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Phase space distributions in quantum mechanics and signal analysis

Lee, Chongmoon, Ph.D.

City University of New York, 1989

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PHASE SPACE DISTRIBUTIONS
IN QUANTUM MECHANICS AND SIGNAL ANALYSIS

by

CHONGMOON LEE

A dissertation submitted to the Graduate Faculty in Physics in partial fulfillment of the requirements for the degree of Doctor of Philosophy, The City University of New York

1989

This manuscript has been read and accepted for the Graduate Faculty in Physics in satisfaction of the dissertation requirement for the degree of Doctor of Philosophy.

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Abstract

PHASE SPACE DISTRIBUTIONS
IN QUANTUM MECHANICS AND SIGNAL ANALYSIS

by

Chongmoon Lee

Advisor: Professor Leon Cohen

We have extended the theory and applications of quasi-distributions in a number of directions. A general method for calculating the conditional expectation value of one operator for a fixed value of another has been developed. We have used this method to clarify the local virial theorem in quantum mechanics where we have shown how a phase space distribution can always be chosen so that the local virial theorem is satisfied for a particular wave function. We have also used this method to calculate the local spread of frequencies about the instantaneous frequency of a signal and obtained explicitly the expression for the instantaneous frequency and its spread for the short time energy spectrum. Having an explicit expression for the standard deviation of instantaneous frequencies allows one to calculate optimal windows for the analysis and estimation of instantaneous frequencies. Using the expression for local spread of frequencies we have been able to clarify and to find a criterion for the concept of a multicomponent signal. We have also calculated the standard deviation of the local momentum for a quantum system.

We have used a reduced density matrix approach to study certain aspects of the correlation energy problem for atomic and molecular systems. We developed an explicit model where the reduced density matrices can be calculated analytically and have applied this model to study the Colle-Salvetti method. We have shown that the Colle-Salvetti functional does not produce a N-representable reduced density matrix, however we have demonstrated why it none the less gives very accurate results for the correlation energy. In particular we have shown that it satisfies the momentum and position correlation hole very well. We have used the model problem to study the relationships between the fitting of the correlation holes and the closeness of an approximate physical quantity to the exact one.

ACKNOWLEDGEMENTS

It is a pleasure to thank Professor Leon Cohen for his guidance during the course of this work and also for the stimulation afforded from being associated with him.

Introduction to the world of physics by two friends, Young-Jik Ahn and Young Kuk, is acknowledged.

All the support given by Hyosoon Lee for during the course of this work is greatly appreciated.

To the memory of my mother,
Ok-Kyung Shon

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Chapter 1

INTRODUCTION

In the past few years there has been an immense development in the theory and application of quasi-distributions. The two main areas where these applications are giving considerable profit are in quantum mechanics and signal analysis. In quantum mechanics the concept of local quantities has become an active field of research because considerable insight into quantum systems is obtained by these considerations and furthermore these methods offer practical computational advantages. In the field of signal analysis the concept of a local spectrum, that is the distribution of frequencies at a given time has become a powerful tool for the analysis of non-stationary signals. As we will see the two fields are almost mathematically identical although the variables they deal with are different. Furthermore there has been a realization that these quasi-distribution and associated operator methods are not only useful as approximation to quantum systems as they approach classical mechanics, but also are equivalent to the standard Schrödinger and Heisenberg formulation of quantum mechanics. In fact one may think of these quasi-distributions as particular representations of the density matrix, a representation which has certain advantages and conveniences.

We have extended the theory and applications of these quasi-distributions in a number of directions:

1. We developed a general method of the conditional expectation value of one operator for a fixed value of another.
2. We have clarified the local virial theorem in quantum mechanics and we have shown how a distribution can always be chosen so that the local virial theorem is satisfied for a particular wave function.
3. We have found a method, using the bilinear distributions, for calculating the local spread of frequencies about the instantaneous frequency for a signal.
4. We have obtained the explicit expression for the instantaneous frequency and its spread for the short time energy spectrum. Having an explicit expression for the standard

deviation of instantaneous frequencies allows one to calculate optimal windows for the analysis and estimation of instantaneous frequencies.

5. Using the concept of local spread of frequencies we have been able to clarify and to find a criterion for the concept of a multicomponent signal.

6. In analogy with the signal analysis case we have calculated the standard deviation of the local momentum for a quantum system.

In addition to the above we have used a reduced density matrix approach to study certain aspects of the correlation energy for atomic and molecular systems. Our results in this regard are:

7. We have developed an explicit model where the reduced density matrices can be calculated explicitly.

8. We have applied this model to the Colle-Salvetti method and have shown that the functional does not produce a N-representable reduced density matrix. However, we have demonstrated why it none the less gives very good answers for the correlation energy. In particular we have shown that it satisfies the correlation hole of position and momentum very well. Using these results we suggest some methods for the systematic improvement of the functional.

9. We have studied the relationships between the correlation hole of Coulson and Nielson and the correlation energy, and between correlation hole and the closeness of an approximate physical quantity to the exact one. Also, we present a convenient method for the calculation of the two particle distribution in momentum space, and generalize the concept of the correlation hole by defining it in the pseudo phase space of position and momentum.

Organization of Thesis

As mentioned, the methods we have developed are applicable to both quantum mechanics and signal analysis. However, as we will see, the appropriate variables in each subject are quite different. Furthermore "time" in signal analysis does not correspond to "time" in quantum mechanics and hence if both subjects are discussed together a great deal of confusion may arise. What we will do when a particular method or result is derived, is to keep that chapter totally self-contained to either quantum mechanics or signal analysis. Subsequent sections will transcribe and describe the result to the other subject. The only exception to this is the next chapter where we review the fundamental ideas and applications of these distributions to signal analysis and quantum mechanics and in addition indicate the mathematical relationship between the two.

Papers Published

1. "Exact Reduced Density Matrices for a Model Problems" (with L. Cohen), *J. Math. Phys. (N.Y.)* **26**, 3105 (1985)
2. "A Study of the Colle-Salvetti Functional for ρ_2 via an Exactly Soluble Problem" (with L. Cohen), *Int. J. Quantum Chem.* **19**, 535 (1986)
3. "Correlation Energy for a Slater Determinant Fitted to the Electron Density" (with L. Cohen, C. Frishberg and L. J. Massa), *Int. J. Quantum Chem.* **19**, 525 (1986)
4. "Correlation Hole and Physical Properties: A Model Calculation" (with L. Cohen), *Int. J. Quantum Chem.* **29**, 407 (1986)
5. "Conditional Expectation Values in Quantum Mechanics" (with L. Cohen), *Found. Phys.* **17**, 561 (1987)
6. "Instantaneous Mean Quantities in Time-Frequency Analysis" (with L. Cohen), *IEEE Proc. Int. Conf. on Acoustics, Speech and Signal Processing* 2188 (1988)
7. "Instantaneous Frequency, Its Standard Deviation and Multicomponent Signals" (with L. Cohen), *Advanced Algorithms and Architectures for Signal Processing III, SPIE* : to appear in 1988 or 1989
8. "Local Virial Theorem" (with L. Cohen): submitted for publication

Chapter 2

REVIEW OF QUASI-DISTRIBUTIONS IN QUANTUM MECHANICS AND SIGNAL ANALYSIS AND THEIR RELATIONSHIP

2.1 Quasi-Distributions in Quantum Mechanics

The concept of a quasi-distribution originated with Wigner[77] who devised a classical type distribution of momentum and position to study the N-body quantum problem. At that time quantum statistical mechanics had not been developed and Wigner argued that if we could find a joint classical-like distribution of position and momentum which contained quantum mechanics then it could be used to calculate quantum results using the classical phase space approach. In this manner he calculated the quantum correction to the second virial coefficient of a gas. The fundamental requirement that Wigner sought in these functions is that they satisfy the quantum marginal distributions of position and momentum. That is if $P(q,p)$ is the joint distribution then

$$\int P(q,p)\,dp = |\psi(q)|^2 \tag{2.1}$$

and

$$\int P(q,p)\,dq = |\phi(p)|^2\,, \tag{2.2}$$

where $\psi(q)$ is the wave function and $\phi(p)$ is the momentum wave function. Wigner gave such an a distribution which has now become known as the Wigner distribution,

$$P_W(q,p) = W(q,p) = \frac{1}{2\pi}\int e^{-i\tau p}\psi^*(u - \tfrac{1}{2}\tau\hbar)\,\psi(u + \tfrac{1}{2}\tau\hbar)\,d\tau\,. \tag{2.3}$$

Although the Wigner distribution satisfies the marginal it is not a proper distribution because in general it is not everywhere positive. Hence it is sometimes called a quasi or pseudo distribution.

A year later Kirkwood[47] gave another distribution and argued that it has advantages over the Wigner distribution because the two particle fermion distribution can be written in terms of the one particle distribution in a much simpler way than is the case of the Wigner distribution. Other distributions have been proposed over the years and in addition a variety of derivations have been given for each distribution. In Table I, we list some of the well known distributions.

Table I. Various Distributions and their Kernels

Name	Kernels; $f(\theta,\tau)$	Distribution; $P(q,p)$
Wigner	1	$\frac{1}{2\pi}\int e^{-i\tau p}\psi^*(q-\frac{1}{2}\tau)\psi(q+\frac{1}{2}\tau)\,d\tau$
Margenau-Hill	$\cos\frac{1}{2}\theta\tau$	Real $\frac{1}{\sqrt{2\pi}}\psi(q)\,e^{-iqp}\phi^*(p)$
Sinc Function	$\frac{\sin a\theta\tau}{a\theta\tau}$	$\frac{1}{4\pi a}\int\int_q^{q+a\tau}\frac{1}{\tau}e^{-ip\tau}$ $\times\quad\psi^*(u-\frac{1}{2}\tau)\,\psi\,(u+\frac{1}{2}\tau)\,du\,d\tau$
Rihaczek	$e^{\frac{1}{2}\theta\tau}$	$\frac{1}{\sqrt{2\pi}}\psi(q)\,e^{-iqp}\phi^*(p)$
Page	$e^{\frac{1}{2}i\theta\lvert\tau\rvert}$	$\frac{\partial}{\partial q}\left\lvert\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{q}s(q')\,e^{-ipq'}\,dq'\right\rvert^2$
STFT	$\int h^*(u-\frac{1}{2}\tau)\,e^{-i\theta\tau}$ $h\,(u+\frac{1}{2}\tau)\,du$	$\left\lvert\frac{1}{\sqrt{2\pi}}\int e^{-ip\tau}s\,(\tau)h\,(\tau-q)\,d\tau\right\rvert^2$
Choi-Williams	$e^{-\theta^2\tau^2/\sigma}$	$\frac{1}{4\pi^{3/2}}\int\int\sqrt{\sigma/\tau^2}\,e^{-\frac{\sigma\,(u-q)^2}{4\tau}-ip\tau}$ $\times\quad\psi^*(u-\frac{1}{2}\tau)\,\psi(u+\frac{1}{2}\tau)\,du\,d\tau$
Hussimi-Cartwright-Bopp	$e^{-\alpha\theta^2-\beta\tau^2}$	Special Case of STFT

General Approach

A general approach to study these distributions was given by Cohen[22] where he gave an explicit method to generate an infinite number of them. This general class of distributions is given by

$$P(q,p,t)=\frac{1}{4\pi^2}\int\int\int e^{-i\theta q-i\tau p+i\theta u}f(\theta,\tau)\psi^*(u-\tfrac{1}{2}\tau\hbar,t)\,\psi(u+\tfrac{1}{2}\tau\hbar,t)\,du\,d\tau\,d\theta\ , \qquad (2.4)$$

where $f(\theta,\tau)$ is any arbitrary function. By choosing different f's particular cases are obtained. In Table I, the kernels for the different distributions are listed. In Eq. (2.4) we have explicitly put in the time variable, however we will henceforth suppress it unless explicitly needed. Requirement of the distribution are reflected in constraints on the kernel. For example if the kernel satisfies $f(\theta,\tau) = f^*(-\theta,-\tau)$ then the distribution is real. It is particularly convenient to define a subclass of kernel by

$$f_p(\theta,\tau) = f(\theta\cdot\tau)\,, \tag{2.5}$$

and we shall call such kernels product kernels.

Expectation Values

One of the main motivations of developing phase space methods is to be able to calculate expectation values by way of phase space integration. The correspondence between operators and phase functions was developed by Moyal[63] for the Wigner distribution, and Metha and Sudarshan,[62] and Margenau and Hill[56] for the symmetric distribution. The approach was given by Cohen[22] and subsequently used by Agarwal and Wolf[2].

Quantum mechanical averages can be calculated by phase space integration since one can always set

$$\int \psi^*(q)\,G(\mathbf{Q},\mathbf{P})\,\psi(q)\,dq = \iiint g(q,p)\,P(q,p)\,dq\,dp \tag{2.6}$$

where $G(\mathbf{Q},\mathbf{P})$ is the quantum mechanical operator and $g(q,p)$ is the classical function associated with it. For the condition of Eq.(2.7), we must take[22]

$$G(\mathbf{Q},\mathbf{P}) = \iint \gamma(\theta,\tau)\,f(\theta,\tau)\,e^{i\theta\mathbf{Q}+i\tau\mathbf{P}}d\theta\,d\tau \tag{2.7}$$

where

$$\gamma(\theta,\tau) = \frac{1}{4\pi^2}\iint g(q,p)\,e^{i\theta q+i\tau p}dq\,dp\,. \tag{2.8}$$

or equivalently

$$G(\mathbf{Q},\mathbf{P}) = \frac{1}{4\pi^2}\int\int g(q,p)\,f(\theta,\tau)\,e^{i\theta(\mathbf{Q}-q)+i\tau(\mathbf{P}-p)}d\theta\,d\tau\,dq\,dp\,. \tag{2.9}$$

Inversely, given a quantum mechanical operator the "classical" function is obtained from

$$g(q,p) = \frac{e^{\frac{i}{2}\frac{\partial^2}{\partial q \partial p}}}{f\left(-i\frac{\partial}{\partial q}, -i\frac{\partial}{\partial p}\right)}\, G_Q(q,p) \tag{2.10}$$

where G_Q is the quantum mechanical operator rearranged so that all the $\mathbf{Q}$ factors precede the $\mathbf{P}$ factors before the substitution of $\mathbf{Q}$ and $\mathbf{P}$ by q and p, respectively.

Relationship among Quasi-Distributions[23]

The characteristic function of the distribution is sometimes more advantageous to work with than the distribution itself[22]. The characteristic function is defined as the expectation value of $e^{i\theta p + i\tau q}$, that is

$$M(\theta,\tau) = \left\langle e^{i\theta q + i\tau p} \right\rangle = \iint e^{i\theta q + i\tau p} P(q,p)\, dq\, dp\ . \tag{2.11}$$

From Eq. (2.4) we see that it is given by

$$M(\theta,\tau) = f(\theta,\tau) \int \psi^*(u - \tfrac{1}{2}\tau) e^{i\theta u} \psi(u + \tfrac{1}{2}\tau) du\ , \tag{2.12}$$

Suppose we have two distribution P_1 and P_2 with corresponding kernels f_1 and f_2. Their characteristic functions are

$$M_1(\theta,\tau) = f_1(\theta,\tau) \int e^{i\theta u} \psi^*(u - \tfrac{1}{2}\tau)\, \psi(u + \tfrac{1}{2}\tau)\, du\ , \tag{2.13}$$

$$M_2(\theta,\tau) = f_2(\theta,\tau) \int e^{i\theta u} \psi^*(u - \tfrac{1}{2}\tau)\, \psi(u + \tfrac{1}{2}\tau)\, du\ , \tag{2.14}$$

and dividing one by the other we have

$$M_1(\theta,\tau) = \frac{f_1(\theta,\tau)}{f_2(\theta,\tau)} M_2(\theta,\tau)\ . \tag{2.15}$$

Taking the Fourier transform to obtain the distribution we have[23]

$$P_1\,(q,p) = \frac{1}{4\pi^2} \int \frac{f_1(\theta,\tau)}{f_2(\theta,\tau)}\, e^{i\theta(q'-q) + i\tau(p'-p)}\, P_2(q',p')\, d\theta\, d\tau\, dq'\, dp'\ . \tag{2.16}$$

It is sometimes convenient to write this as

$$P_1(q,p) = \iint g(q' - q, p' - p) P_2(q',p') dq' dp' \tag{2.17}$$

with

$$g(q,p) = \frac{1}{4\pi^2} \iint e^{i\theta q + i\tau p} \frac{f_1(\theta,\tau)}{f_2(\theta,\tau)}\, d\theta\, d\tau\,. \tag{2.18}$$

This form was derived by Claasen and Mecklenbrauker[20] for the case where P_2 is the Wigner distribution. Another very useful way of expressing the results is in operator form[23],

$$P_1(q,p) \;=\; \frac{f_1(i\frac{\partial}{\partial q}, i\frac{\partial}{\partial p})}{f_2(i\frac{\partial}{\partial q}, i\frac{\partial}{\partial p})} P_2(q,p)\;. \tag{2.19}$$

Relation to Density Matrices

As previously mentioned quasi distributions can be considered as particular representation of density matrix. In particular for the one body case the distribution as given by Eq. (2.4) can clearly be written in terms of the density matrix,

$$P(q,p) = \frac{1}{4\pi^2} \iiint e^{-i\theta q - i\tau p + i\theta u}\, f(\theta,\tau)\, \rho(u + \tfrac{1}{2}\tau, u - \tfrac{1}{2}\tau)\, du\, d\theta\, d\tau\,, \tag{2.20}$$

and conversely the density matrix can be uniquely obtained from the distribution. For the general N-body case the reduced distributions can be related to reduced density matrices and it can be shown that they are equivalent[26].

Quasi-Distribution for Arbitrary Operators

Most of the work done with these quasi-distributions has been for the case of position and momentum. Barut[11] considered the case for two arbitrary operator using the symmetrization rule. Recently a generalized method for arbitrary two operators has been given by Scully and Cohen[69]. We will use this method to define conditional expectation values for operators.

The approach is to define the characteristic function of two operators $\mathbf{A}$ and $\mathbf{B}$

$$M^{ab} = \left\langle e^{i\theta \mathbf{A} + i\tau \mathbf{B}} \right\rangle\,, \tag{2.21}$$

and obtain the distribution by Fourier inversion

$$P^{ab}(a,b) = \frac{1}{4\pi^2} \iint M^{ab}(\theta,\tau)\, e^{-i\theta a - i\tau b}\, d\theta\, d\tau\,. \tag{2.22}$$

A general characteristic function may be defined by

$$M_g^{ab}(\theta,\tau) = f(\theta,\tau)\, M^{ab}\,, \tag{2.23}$$

and the distribution is

$$P_g^{ab}(a,b) = \frac{1}{4\pi^2} \iint M_g^{ab}(\theta,\tau)\, e^{-i\theta a - i\tau b}\, d\theta\, d\tau\,. \tag{2.24}$$

Smoothed Distributions

Another development in regard to these distributions is the concept of smoothing[18,45,46] them to enhance the desirable characteristics, and to suppress the undesirable ones. Smoothing may also convert the distribution into a positive one. Though this may change some of the fundamental desirable properties, it is hoped that these changes are minimal. Recently there has been considerable progress made by Andrieux *et al*[5]. where they consider the question of the least amount of smoothing which will make the distribution positive. Nuttall[64] has made a major advance in this direction by considering local optimal smoothing, by using different smoothing functions in different components of the time-frequency plane. We point out that a smoothed distribution can also be put in the form of Eq. (1.1) by choosing the appropriate kernel. Smoothing one distribution with a particular function is equivalent to smoothing any other distribution with a different smoothing function. To show this we consider any two distributions, P_1 and P_2, with corresponding kernels f_1 and f_2. The distributions are related by Eqs. (2.16)–(2.18).

Suppose we smooth distribution P_1 with a function $S_1(q',p';q,p)$ which may or may not be a function of $q'-q$ and $p'-p$. The smoothed distribution is

$$P_1^S(q,p) = \iint P_1(q',p')\; S_1(q',p';q,p)\; dq'\; dp'. \tag{2.26}$$

Due to the linearity of the smoothing operation we can always find another function $S_2(q',p';q,p)$ that when applied to P_2 will produce the same smoothed distribution. To obtain the relationship substitute Eq. (2.26) into Eq. (2.17) to obtain

$$P_1^S(q,p) = \iiiint g_{12}(q''-q',p''-p')\; P_2(q'',p'')\; S_1(q',p';q,p)\; dq'\; dp'\; dq''\; dp''\;, \tag{2.27}$$

This can be made equal to P_2^S if we take

$$S_2(q'',p'';q,p) = \iint g_{12}(q''-q',p''-p')\; S_1(q',p';q,p)\; dq'\; dp'\;. \tag{2.28}$$

What this shows is that smoothing is a distribution-independent process. Any particular smoothed distribution is characterized only be the kernel as defined in Eq. (1.1).

2.2 Quasi-Distribution in Signal Analysis

In standard Fourier analysis, the energy density spectrum indicates what fraction of the total energy was put into each frequency for the complete duration of the signal. That is, if we have a signal $s(t)$ and its Fourier transform defined by

$$S(\omega) \;=\; \frac{1}{\sqrt{2\pi}} \int s(t)\; e^{-j\omega t} dt \; . \tag{2.29}$$

then $|S(\omega)|^2$ is the distribution of frequencies of the signal. Similarly, $|s(t)|^2$ is the instantaneous energy of the signal. However suppose the frequency contents of the signal is changing rapidly in time. The energy density spectrum would not tell us that this is happening because it is independent of time. It considers the frequency content of the whole duration of the signal. What is needed is a method which will give the distribution of frequencies at a particular time or equivalently a joint distribution of time and frequency. The formulation of such a method is one of the most challenging aspects of analysis and may be considered the generalization of standard Fourier analysis. A generalization would indicate how much energy is in each frequency at any one time. In the ideal case, such a theory would have a joint time-frequency distribution which would describe the intensity of a signal at a particular time and frequency. At present, there is no comprehensive and consistent theory for such a description although many methods give very reasonable results. The spectrogram, or short-time Fourier transform, which will be described in detail in Chapter 6, is the most widely used method. The fundamental ideas is to consider the region of time that one is interested in, that is to window the signal around a particular time and take the Fourier transform which will then indicate the frequency content of the signal around that time. If this is repeated for all time one obtains a joint distributions of frequency and time. This method was initiated in the Forties by a hardware implementation, and in the Seventies was implemented on digital computer. However the spectrogram has a number of shortcomings, the principle one being the trade of frequency and time resolution. In addition it does not reproduce the energy density spectrum and the instantaneous power, that is it does not satisfy the marginals. We point out that the spectrogram is a member of the general class of distributions given by Eq. (1.1).

Independent of the development of the spectrogram Gabor[39] and Ville[73] initiated another development in close analogy to quantum mechanics and over the past few years this development has become a powerful new tool for the analysis of signal. In 1948, by applying the quantum analogy, Ville devised a method which is totally analogous to Moyal's method[63], and derived the Wigner distribution which we rewrite in terms of signal analysis language,

$$P_W(t,\omega) = W(t,\omega) = \frac{1}{2\pi}\int e^{-j\tau\omega} s^*(u - \tfrac{1}{2}\tau)\, s(u + \tfrac{1}{2}\tau)\, d\tau\,. \tag{2.30}$$

In the later years other time-frequency distributions have been derived such as the Page[65] and Rihaczek[68] distribution and has been studied in detail. These distributions are bilinear in the signal and have the property that they may preserve the energy density spectrum and instantaneous power

$$\int P(t,\omega)\; d\omega \;= |s(t)|^2\;, \tag{2.31}$$

and

$$\int P(t,\omega)\; dt \;=\; |S(\omega)|^2\,. \tag{2.32}$$

Claasen and Mecklenbrauker[20] and Boashash[13] and others realized the analogy between the quantum case and signal analysis and used Cohen's general equation to study the set of distributions. Boashash was the first one who used these distributions in practical applications, in particular, has used for obtaining the instantaneous frequency of a signal. Escudie and Grea[35] transcribed Cohen's 1966 paper into signal analysis language. That is, as in the quantum case all bilinear distributions (including the spectrogram) may be generated from

$$P(t,\omega) = \frac{1}{4\pi^2}\iiint e^{-j\theta t - j\tau\omega + j\theta u} f(\theta,\tau) s^*(u - \tfrac{1}{2}\tau)\, s(u + \tfrac{1}{2}\tau)\, du\, d\tau\, d\theta\,. \tag{2.33}$$

As in the quantum case, particular distributions are obtained by choosing different kernels, $f(\theta,\tau)$. A shortcoming of some of these distributions is that sometimes they indicate the presence of energy where no energy is expected. In particular, the Wigner distribution often produces spurious values and it has been felt by many investigators that this behavior is typical of all bilinear distributions. However the recent work of Choi and Williams[19] has made it clear that there are many distributions which to a large extent eliminate or suppress the undesirable characteristics of the Wigner distribution. Another difficulty with these distributions is that while they often predict sensible expectation values, frequently they do not. For example, while the Wigner distribution gives a sensible answer for the frequency at a given time, the value it gives for the variance makes no sense at all and can not be used or be interpreted properly. None the less, these distributions have been used with considerable profit.

From a mathematical point of view we can see that there is a direct analogy between the quantum mechanical case and signal analysis case if we make the following association.

Table II. The Relationship between Quantum Mechanics and Signal Analysis

Quantum Mechanics	Signal Analysis
Position; q	Time; t
Momentum; p	Frequency; ω
Wave Function; $\psi(q)$	Signal; $s(t)$
Momentum Wave Function; $\phi(p)$	Spectrum; $S(\omega)$
Probability of Position; $\lvert\psi(q)\rvert^2$	Energy Density; $\lvert s(t)\rvert^2$
Probability of Momentum; $\lvert\phi(p)\rvert^2$	Energy Density Spectrum; $\lvert S(\omega)\rvert^2$

Chapter 3

CONDITIONAL EXPECTATION VALUES IN QUANTUM MECHANICS

Conditional expectation values play a fundamental role in probability and statistical theory. For example, in classical statistical mechanics the kinetic energy and current at a fixed point in space are fundamental quantities that enter into kinetic equations. The conditional expectation value for a random variable b, with a second variable, a, fixed, is †

$$\langle b\rangle_a = \int bP(a,b)\,db\,, \tag{3.1}$$

where $P(a,b)$ is the joint probability distribution of a and b. Although in quantum mechanics joint probabilities for non-commuting variables are not well defined, so called quasi-probability distributions have been used with considerable profit. These quasi-distributions behave to a large extent as ordinary probability distributions and in particular expectation values can be calculated in the classical manner. In the case of position and momentum there have been an number of quasi-distributions which have been studied[43,7] and an infinite number of them can readily be generated[22,23]. For the case of arbitrary operators the writing of a joint distribution was considered by Barut[11] who studied a particular distribution and developed a number of its properties. Recently, a general method for studying joint quasi-distributions for two arbitrary operators has been developed by Scully and Cohen[29,69]. We consider here the general question of conditional expectation values in using that approach.

We now briefly summarize some of the applications and previous work which have used conditional expectation values for quantum mechanical situations. These considerations have dealt mostly with expectation values of operators for a fixed position. In the work of Ziff *et al.*[80] and Putterman[67], local quantities for the quantum case were considered

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† Strictly speaking we should divide the right hand side of Eq. (3.1) by the probability distribution of a. However for the sake of simplicity and because that definition has been previously used by a number of authors in the case for local kinetic energy we continue to use Eq. (3.1) for the definition of $\langle \mathbf{B}\rangle_a$. This has the consequence that to calculate the unconditional expectation value of b we do not have to multiply by the probability of a. In what follows all integral go from minus infinity to infinity unless otherwise noted. We shall designate operators by bold face letters and the random variables associated with them by lower case. We assume a continuous spectrum for the operators as the discrete case can be readily written by analogy.

in formulating kinetic equations for quantum systems. Bader[6] and co-workers considered local kinetic energy and the kinetic energy in a region. In this manner they were able to study spatial partitioning of molecular properties by determining regions for which local virial theorem holds. The general question of local kinetic energy was considered from the point of view of quasi-probability distributions where an infinite number of expressions were given[24]. Local quantities and applications to density functional theory were used by Springborg and Dahl[71]. The concept of local total energy was used by Frost *et al.*[38] for the practical calculation of molecular eigenfunctions. The concept of reduced local energy was introduced by Thomas *et al.*[72] and explicit expressions in terms of reduced density matrices were given by Massa and Cohen[60] who also defined reduced local energy matrices. Leaf[52] used a particular definition to define local quantities which corresponds to Eq. (3.40) below. In the general formulation which we shall give we show how the above considerations are special cases.

The fundamental requirement of a quantum conditional expectation value is that it integrates to the correct quantum value when the conditional variable is integrated out. That is

$$\int \langle \mathbf{B} \rangle_a \, da = \int \psi^*(q) \mathbf{B} \psi(q) \, dq \,. \tag{3.2}$$

To derive expressions for $\langle \mathbf{B} \rangle_a$ it is convenient to use the characteristic function of the variables a and b

$$M^{ab}(\theta, \tau) = \iint P(a,b) e^{i\theta a + i\tau b} \, da \, db \tag{3.3}$$

$$= \langle e^{i\theta a + i\tau b} \rangle \,, \tag{3.4}$$

and by inversion we also have

$$P(a,b) = \frac{1}{4\pi^2} \int M_{ab}(\theta, \tau) e^{-i\theta a - i\tau b} \, d\theta \, d\tau \,. \tag{3.5}$$

Substituting Eq. (3.5) into Eq. (3.1) we have

$$\langle \mathbf{B} \rangle_a = \frac{1}{4\pi^2} \int b M_{ab}(\theta, \tau) e^{-i\theta a - i\tau b} \, db \, d\theta \, d\tau \tag{3.6}$$

$$= \frac{1}{2\pi i} \int \left. \frac{\partial M_{ab}(\theta, \tau)}{\partial \tau} \right|_{\tau = 0} e^{-i\theta a} \, d\theta \,. \tag{3.7}$$

3.1 Two Approaches to Conditional Expectation Values

There are two general approaches which can be used to calculate conditional quantum expectation values. The first approach is to write a joint distribution of the two variables and then uses Eq. (3.1). The second approach starts with the distribution of position and momentum and finds the conditional expectation values by expressing the physical quantities in terms of variables q and p. We now explicitly work out on these two methods.

A) Method 1: Operator Method

Although the characteristic function is an expectation value and hence the quantum mechanical procedure for calculating it should be straightforward, there is an ambiguity since there are many expressions which reduce to the classical definition when the operators are considered ordinary functions. In general we seek an operator, $\mathbf{M}(\theta,\tau)$, whose expectation value corresponds to the classical characteristic function when its expectation value is calculated in the usual quantum mechanical manner as

$$M_{ab}(\theta,\tau)=\int\psi^*(q)\mathbf{M}_{ab}(\theta,\tau)\psi(q)\,dq\,. \tag{3.8}$$

The ambiguity arises because of the non-commutivity of the operators. For example, we can take the following different expressions, each of which reduce to the classical case when the operators commute

$$e^{i\theta a+i\tau b}\rightarrow e^{i\theta\mathbf{A}+i\tau\mathbf{B}}\equiv\mathbf{M}_W^{ab}(\theta,\tau) \tag{3.9a}$$

and

$$e^{i\theta a+i\tau b}\rightarrow\tfrac{1}{2}\left[e^{i\theta\mathbf{A}},e^{i\tau\mathbf{B}}\right]_+\equiv\mathbf{M}_S^{ab}(\theta,\tau) \tag{3.9b}$$

where $\mathbf{A}$ and $\mathbf{B}$ are the quantum operators corresponding to the classical functions $a(q,p)$ and $b(q,p)$. Many other expressions are clearly possible. This is of course the same ambiguity which arises for the case of position and momentum and which gives rise to the different correspondence rules[22,23]. In addition we can take any particular characteristic function and form a new one by multiplying it with any function or functional $f(\theta,\tau)$

$$M_1(\theta,\tau)=f(\theta,\tau)M(\theta,\tau)\,, \tag{3.10}$$

where $f(\theta,\tau)$ must satisfy

$$f(\theta,0)=f(0,\tau)=1\,. \tag{3.11}$$

Substituting Eq. (3.8) into (3.7) we have that

$$\langle \mathbf{B} \rangle_a = \frac{1}{2\pi i} \int \left\{ \left. \frac{\partial M_{ab}(\theta,\tau)}{\partial \tau} \right|_{\tau=0} + M(\theta,0) \left. \frac{\partial f(\theta,\tau)}{\partial \tau} \right|_{\tau=0} \right\} e^{-i\theta a} \, da \, . \tag{3.12}$$

By choosing different functions $f(\theta,\tau)$, an infinite number of expressions for the conditional expectation can be generated, each of which satisfies Eq. (3.2).

We now proceed to obtain explicit expressions for $\langle \mathbf{B} \rangle_a$ for the correspondences given by Eqs. (3.9a) and (3.9b).

a) Calculation of $\langle \mathbf{B} \rangle_a$ *for* $\mathbf{M}_W$

The derivative of $\mathbf{M}_W$ is obtained by the use of the Feynman[36] formula

$$\left. \frac{\partial \mathbf{M}_W}{\partial \tau} \right|_{\tau=0} = i \int_0^1 e^{(1-s)i\theta \mathbf{A}} \, \mathbf{B} \, e^{i\theta s \mathbf{A}} \, ds \, . \tag{3.13}$$

Calculating the expectation value we have

$$\langle \mathbf{B} \rangle_a = \frac{1}{2\pi} \iiint_0^1 \psi^*(q) \, e^{(1-s)i\theta \mathbf{A}} \, \mathbf{B} \, e^{i\theta s \mathbf{A}} \, e^{-i\theta a} \, \psi(q) \, ds \, d\theta \, dq \, . \tag{3.14}$$

This expression can be simplified in a number of ways although for calculation purposes it is often the simplest. If we take the eigenfunctions and eigenvalues of $\mathbf{A}$ to be defined by

$$\mathbf{A} u_\alpha(q) = \alpha \, u_\alpha(q) \, , \tag{3.15}$$

and expand the position wave function in terms of the eigenfunctions of $\mathbf{A}$

$$\psi(q) = \int \phi(\alpha) \, u_\alpha(q) \, d\alpha \, , \tag{3.16}$$

where ϕ is the wave function in the $\mathbf{A}$ representation, we obtain

$$\langle \mathbf{B} \rangle_a = \frac{1}{2\pi} \iiiint_{-\frac{1}{2}}^{\frac{1}{2}} \phi^*(\alpha') \phi(\alpha) \langle \alpha' | \mathbf{B} | \alpha \rangle \, e^{-i\theta\{a-(\alpha+\alpha')/2-s(\alpha-\alpha')\}} \, ds \, d\alpha \, d\alpha' \, d\theta \, , \tag{3.17}$$

where

$$\langle \alpha' | \mathbf{B} | \alpha \rangle = \int u_{\alpha'}^*(q) \mathbf{B} u_\alpha(q) \, dq \, . \tag{3.18}$$

Performing the s integration

$$\langle \mathbf{B} \rangle_a = \frac{1}{2\pi} \iiint \phi^*(\alpha')\phi(\alpha)\langle \alpha' | \mathbf{B} | \alpha \rangle \, e^{-i\theta\{a-(\alpha+\alpha')/2\}} \operatorname{sinc}\tfrac{1}{2}\theta(\alpha - \alpha') \, d\alpha \, d\alpha' \, d\theta \,, \tag{3.19}$$

where

$$\operatorname{sinc} x = \frac{\sin x}{x} \,. \tag{3.20}$$

Depending on the operator, the expansion in terms of repeated commutators is sometimes convenient. Using[36,79]

$$e^{-i\theta s \mathbf{A}} \mathbf{B} \, e^{i\theta s \mathbf{A}} = \mathbf{B} - i\theta s[\mathbf{A}, \mathbf{B}] + \tfrac{1}{2}(i\theta s)^2 \left[\mathbf{A}, [\mathbf{A}, \mathbf{B}]\right] + \cdots \tag{3.21}$$

and substituting in Eq. (3.14) we have, after performing the s integration

$$\langle \mathbf{B} \rangle_a = \langle \delta(\mathbf{A} - a)\mathbf{B} \rangle + \frac{1}{2!}\frac{\partial}{\partial a}\langle \delta(\mathbf{A} - a) \, [\mathbf{A}, \mathbf{B}] \rangle + \frac{1}{3!}\frac{\partial^2}{\partial a^2}\langle \delta(\mathbf{A} - a) \, \left[\mathbf{A}, [\mathbf{A}, \mathbf{B}]\right] \rangle + \cdots \tag{3.22}$$

b) Calculation of $\langle \mathbf{B} \rangle_a$ *for* $\mathbf{M}_S$

From Eq. (3.9b) we have that

$$\left. \frac{\partial \mathbf{M}_s}{\partial \tau} \right|_{\tau = 0} = \frac{i}{2} \left[e^{i\theta \mathbf{A}}, \mathbf{B} \right]_+ \,, \tag{3.23}$$

and hence

$$\langle \mathbf{B} \rangle_a = \frac{1}{4\pi} \int \psi^*(q)[e^{-i\theta \mathbf{A}}, \mathbf{B}] \, e^{-i\theta a} \psi(q) \, d\theta \, dq \tag{3.24}$$

$$= \tfrac{1}{2}\phi(a) \int \phi^*(\alpha)\langle \alpha | \mathbf{B} | a \rangle \, d\alpha + \tfrac{1}{2}\phi^*(a) \int \phi(\alpha)\langle a | \mathbf{B} | \alpha \rangle \, d\alpha \,. \tag{3.25}$$

B) Method 2: Joint Position-Momentum Distribution Method

An alternative approach to calculating $\langle \mathbf{B} \rangle_a$ is by way of the joint distribution of position and momentum which in classical statistical mechanics would of course be the standard way. Let us first consider the classical situation and suppose that instead of using a joint distribution of a and b we have the distribution of position and momentum.

From the probability distribution for q and p, the probability distribution for a and b is calculated by ‡

$$P(a,b) = \iint \delta(a - a(q,p))\, \delta(b - b(q,p))\, P(q,p)\, dq\, dp\,, \tag{3.26}$$

where the observables $a(q,p)$ and $b(q,p)$ are expressed in terms of p and q in the integration. Substituting Eq. (3.26) in Eq. (3.1) we have

$$\langle \mathbf{B} \rangle_a = \iiint \delta(a - a(q,p))\, \delta(b - b(q,p))\, b\, P(q,p)\, dq\, dp\, db \tag{3.27}$$

$$= \iint \delta(a - a(q,p))\, b(q,p)\, P(q,p)\, dq\, dp\,. \tag{3.28}$$

For future reference we specialize to the case where a is the position, x, in which case

$$\langle \mathbf{B} \rangle_x = \int b(x,p) P(x,p)\, dp\,. \tag{3.29}$$

To convert this into a quantum mechanical expression we would use a joint quasi–distribution for q and p and for the quantities $a(q,p)$ and $b(q,p)$ we would use the c number expressions which correspond to the operators **A** and **B**. In some cases $a(q,p)$ and $b(q,p)$ may be the classical quantities but in general they are to be obtained from the quantum operator[22,23]. This is the method which has been used for the case of local kinetic energy. By choosing different quasi- distributions an infinite number of expressions can be derived. In the later section, we discuss the implications of these two different approaches and address the question as to which is more convenient in particular circumstances.

3.2 Relationships between Operator Method and Joint Distribution Method

The conditional expectation values defined for the quantum case do not obey constraints and inequalities that the classical conditional expectation values do. For example, the conditional expectation value of a manifestly positive quantity can be negative in the quantum case. None the less, as has been the case with local kinetic energy, conditional expectation values may be profitably used in quantum mechanics. The basic reason

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‡ The P's on the right hand side and left hand side of Eq. (3.26) are not the same. It will be clear for the context whether we are referring to the probability of a, b or q, p. Similarly we drop the superscript ab from $M(\theta, \tau)$ when it is clear from the context which variables we are referring to.

for the non-classical behavior of these expectation values is that they depend on the wave function in a bilinear way. Bilinear quasi-distributions are never positive definite and that is the reason for the considerably different properties that these conditional expectation values have in contrast to their classical counterparts. Positive distributions which give the right quantum mechanical marginal distributions do exist and can be used to define conditional expectation values. This has been done for the case of local kinetic energy[56,24,29]. Another unique feature regarding joint distributions and conditional expectation values in quantum mechanics deals with the range of the random variables. In quantum mechanics the measurable quantities are the eigenvalues of the operator. However, if we consider two operators and derive the joint quasi-probability distributions, then the range for the random variables will in general be larger than the space spanned by the eigenvalues of the operators. A dramatic example of this is the case of spin[29]. If the joint distribution for the spin of two particles is derived using Eq. (3.9b) we obtain four distinct probabilities as one would expect. However if Eq. (3.9a) is used then the range for the two random variables for spin is continuous! We note that for the case of the symmetrization rule the resulting range for a and b will always coincide with the eigenvalues. In regard to conditional expectation values these features manifest themselves in that the quantities we are holding fixed may not be eigenvalues. Considerably more clarification of these effects and their implication is needed.

We now contrast the two general approaches for calculating conditional expectation values. One being directly from the quasi joint distribution of position and momentum, that is by way of Eq. (3.28) and the other from direct calculation of moment generating functions for the two operators using Eqs. (3.9a) and (3.9b). The advantage of the first method is that the distribution remains fixed. However a serious disadvantage is that if one calculates the conditional expectation value of a function of $b(q,p)$, e.g. **B** square then $b^2(q,p)$ cannot be inserted in Eq.(3.28). An elaborate procedure[43,7,23,29,69] is involved to find the expression to be used in the integrand if we want the correct quantum expression to result upon a further integration of the conditional quantity. In contrast the method that uses the characteristic function for the operators **A**, and **B** has the advantage that the expectation value of a function of the variable is obtained by simply putting the function of the operator in the appropriate expressions.

3.3 Examples and Special Cases

a) *Local Quantities*

A particularly interesting case arises when a is the position, x. We shall use the phrase local quantity to connote that situation. From Eq. (3.14)

$$\langle \mathbf{B} \rangle_x = \frac{1}{2\pi} \iint_0^1 \psi^*(q)\, e^{(1-s)i\theta q} \mathbf{B}(\mathbf{Q},\mathbf{P})\, e^{i\theta s q - i\theta x} \psi(q)\, ds\, dq\, d\tau . \tag{3.30}$$

We now expand the operator $\mathbf{B}(\mathbf{Q},\mathbf{P})$ in the form[22]

$$\mathbf{B}(\mathbf{Q},\mathbf{P}) = \iint \gamma_B(\theta,\tau)\, f(\theta,\tau)\, e^{i\theta \mathbf{Q} + i\tau \mathbf{P}}\, d\theta\, d\tau \,, \tag{3.31}$$

where

$$\gamma_B(\theta,\tau) = \frac{1}{4\pi^2} \iint b(q,p)\, e^{-i\theta q - i\tau p}\, dq\, dp \,, \tag{3.32}$$

and $b(q,p)$ is the c number variable corresponding to the quantum operator. It is given by

$$b(q,p) = \frac{\exp\left(\dfrac{i\hbar}{2}\dfrac{\partial^2}{\partial q \partial p}\right)}{f\left(-i\dfrac{\partial}{\partial q}, -i\dfrac{\partial}{\partial p}\right)} B_Q(q,p) \,, \tag{3.33}$$

where $B_Q(q,p)$ is $\mathbf{B}(\mathbf{Q},\mathbf{P})$ after rearranging it such that the Q factors proceed the P factors. The expansion of operators in the above form is particularly convenient and unifies so-called correspondence rules between classical quantities and quantum mechanical operators[22]. By choosing different values for the function $f(\theta,\tau)$ different correspondence rules are obtained. Substituting Eq. (3.31) into Eq. (3.30) we have, after some straightforward transformations,

$$\begin{aligned} \langle \mathbf{B} \rangle_x = \frac{1}{2\pi} \iint_{-\frac{1}{2}}^{\frac{1}{2}} & \psi^*(u - \tfrac{1}{2}\tau\hbar)\psi(u + \tfrac{1}{2}\tau\hbar)\, \gamma(\theta',\tau') f(\theta',\tau') \\ & e^{i\theta\tau\hbar s + i(\theta+\theta')u' - i\theta x}\, ds\, d\theta\, d\theta'\, d\tau\, du \,. \end{aligned} \tag{3.34}$$

Now we can write this in terms of the characteristic function for an arbitrary quasi-distribution of position and momentum[22,23]

$$M_{qp}(\theta,\tau) = f(\theta,\tau) \int \psi^*(u - \tfrac{1}{2}\tau\hbar)\, e^{i\theta u} \psi(u + \tfrac{1}{2}\tau\hbar)\, du \,, \tag{3.35}$$

and therefore

$$\langle \mathbf{B} \rangle_x = \frac{1}{2\pi} \iint_{-\frac{1}{2}}^{\frac{1}{2}} M^{qp}(\theta + \theta', \tau)\, e^{i\theta\tau\hbar s - i\theta x} \gamma_B(\theta', \tau)\, d\theta\, d\theta'\, d\tau \tag{3.36}$$

$$= \int P(q,p)\, b(q',p)\, K(q - q', q - x, p - p')\, dq\, dq'\, dp\, dp' \,, \tag{3.37}$$

where

$$K = \frac{1}{(2\pi)^3} \iint_{-\frac{1}{2}}^{\frac{1}{2}} e^{i\theta'(q-q') + i\tau(p-p') + i\theta(q-x) + i\theta\tau s\hbar} \frac{f(\theta,\tau)}{f(\theta+\theta',\tau)}\, ds\, d\tau\, d\theta\, d\theta' \,. \tag{3.38}$$

We note that if K is expanded in powers of $\hbar$ the first term yields delta functions of $q - q'$, $q - x$, and $p - p'$ which, upon the substitution in Eq. (3.37) yields Eq. (3.29).

Similarly for the symmetrical characteristic function we have that

$$\langle \mathbf{B} \rangle_x = \frac{1}{4\pi} \int \psi^*(q)\, e^{i\theta(q-x)}\, \mathbf{B}(\mathbf{Q},\mathbf{P})\, \psi(q)\, dq + \mathrm{C.C.} \tag{3.39}$$

$$= \tfrac{1}{2} \psi^*(x) \mathbf{B}(\mathbf{x}, \mathbf{p}_x)\, \psi(x) + \mathrm{C.C.} \tag{3.40}$$

b) Local Kinetic Energy

If we take $\mathbf{B}$ to be the kinetic energy operator, we have that

$$\langle \mathrm{K.E.} \rangle_x = \frac{1}{2\pi} \iint_0^1 \psi^*(q) \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} \right) \psi(q)\, e^{i\theta s q}\, ds\, dq\, d\theta \,, \tag{3.41}$$

which evaluates to

$$\langle \mathrm{K.E.} \rangle_x = \frac{\hbar^2}{2m} \left\{ \frac{\partial \psi^*(x)}{\partial x} \frac{\partial \psi(x)}{\partial x} - \frac{1}{3} \frac{\partial^2 |\psi(x)|^2}{\partial x^2} \right\} . \tag{3.42}$$

We point out that this expression can be obtained from Eq. (3.29) if the distribution used is the one obtained by the use of the Born and Jordan correspondence rule[22,23].

For the symmetrical case we have that

$$\langle \mathrm{K.E.} \rangle_x = -\frac{\hbar^2}{4m} \left\{ \psi^*(x) \frac{\partial^2}{\partial x^2} \psi(x) + \mathrm{C.C.} \right\} . \tag{3.43}$$

which can be derived from Eq. (3.29) with the Margenau-Hill[22,23,56] distribution.

c) Local Total Energy

In Frost *et al.*[38] work the local energy (Hamiltonian) is defined as (in our notation)

$$\langle \mathbf{H} \rangle_x = \tfrac{1}{2}\{\psi^* \mathbf{H} \psi + c.c.\} . \tag{3.44}$$

Also he defines

$$\langle \mathbf{H}^2 \rangle_x = \tfrac{1}{2}\{\psi^* \mathbf{H}^2 \psi + c.c.\} . \tag{3.45}$$

This corresponds to the use of Eq. (3.40). If the wave function is an energy eigenstate then the local variance defined by

$$\langle \sigma^2 \rangle_x = \langle (\mathbf{H} - \langle \mathbf{H} \rangle_x)^2 \rangle_x \tag{3.46}$$

will be is zero and also

$$\langle \mathbf{H} \rangle_x = E|\psi(x)|^2 \tag{3.47}$$

where E is the eigenvalue of the Hamiltonian.

By expanding a wave function in terms of an arbitrary set of functions and minimizing the local variance with respect to the expansion coefficient Frost *et al.*[38] devised a practical way to obtain approximate wave functions. In general other rules for defining local energy will not produce zero local variance although of course the integration of the local variance over all space will be zero for an eigenstate. None the less it is still possible to derive schemes in the sense of Frost using other definitions then Eq. (3.44) for local energy. Since there is a wide choice, it would be of interest to see whether there are any numerical advantages to the different expressions.

d) Current

To calculate the local momentum we use $\mathbf{B} = (\hbar/i)(\partial/\partial x)$ in Eq. (3.30) which straightforwardly results in

$$\langle \mathbf{P} \rangle_x = \frac{\hbar}{2i}\left\{\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right\} . \tag{3.48}$$

When the wavefunction is written as

$$\psi(x) = R(x) e^{iS(x)/\hbar} , \tag{3.49}$$

where $R(x)$ and $S(x)$ are real functions of x, then Eq. (3.48) can be expressed in a concise form,

$$\begin{aligned}\langle \mathbf{P} \rangle_x &= \frac{\hbar}{2i}\{R(\frac{\partial R}{\partial x}+iR\frac{\partial S}{\partial x}) - R(\frac{\partial R}{\partial x}-iR\frac{\partial S}{\partial x})\} \\ &= R^2\frac{\partial S}{\partial x}\,.\end{aligned} \tag{3.50}$$

This is the usual expression for the quantum mechanical current. If we use Eq. (3.40) the identical result is obtained. This will be elaborated in Chapter 8.

e) Operators at Different Times

In Eq. (3.14) we can take **A** and **B** to be the same quantity but at different times. For **B** we take $\mathbf{A}(t)$ and for **A** we take $\mathbf{A}(0)$. Therefore the conditional expectation value for $a(t)$ for a given value of $a(0) = a_0$ is, using Eq. (3.14)

$$\langle \mathbf{A}(t)\rangle_{a_0} = \frac{1}{2\pi}\iiint_0^1 \psi^*(q,0)\, e^{(1-s)i\theta\mathbf{A}(0)}\mathbf{A}(t)e^{i\theta s\mathbf{A}(0)}\, e^{-i\theta a_0}\psi(q,0)\, ds\, d\theta\, dq\,. \tag{3.51}$$

Similarly for the symmetrical rule, Eq. (3.24) we have

$$\langle \mathbf{A}(t)\rangle_{a_0} = \frac{1}{4\pi}\iint \psi^*(q,0)\, e^{i\theta(\mathbf{A}(0)-a)}\mathbf{A}(t)\psi(q,0)\, dq\, d\theta + c.c.\,. \tag{3.52}$$

As an example consider the position of a free particle and harmonic oscillator. Whether one uses Eq. (3.51) or Eq. (3.52) the result are identical as shown below.

Suppose we seek the joint quasi probability for the position of a particle at the different times $q(t_0), q(t_1), \ldots, q(t_N)$. To calculate it we find the characteristic function

$$M(\theta_0,\ldots,\theta_N) = \left\langle e^{i\sum_{k=0}^{N}\theta_k \mathbf{q}(t_k)}\right\rangle \tag{3.53}$$

$$= \int \psi^*(q_0,0)e^{i\sum_{k=0}^{N}\theta_k \mathbf{q}(t_k)}\psi(q_0,0)\, dq_0\,, \tag{3.54}$$

and the quasi probability is then

$$P(q_0,\ldots,q_N) = \frac{i}{(2\pi)^{N+1}}\int M(\theta_0,\ldots,\theta_N)\, e^{-i\sum_{k=0}^{N}\theta_k \mathbf{q}(t_k)}\, d\theta_0,\ldots,\, d\theta_N\,. \tag{3.55}$$

For the case of a free particle and a harmonic oscillator the position operator at a time t depends linearly on the initial position and momentum operators

$$\mathbf{q}(t_k) = \alpha_k \mathbf{q}(t_0) + \beta_k \mathbf{p}(t_0)\,, \tag{3.56}$$

where

$$\begin{aligned} \alpha_k &= 1, & \beta_k &= \frac{t_k - t_0}{m} & &\text{for free particle} \\ \alpha_k &= \cos\omega\,(t_k - t_0), & \beta_k &= \frac{\sin\omega\,(t_k - t_0)}{m\omega} & &\text{for harmonic oscillator} \end{aligned} \tag{3.57}$$

In that case the characteristic function operator can be disentangled,

$$e^{i\sum_{k=0}^{N}\theta_k \mathbf{q}(t_k)} = e^{i\hbar/2(\theta_0+\sum_{k=1}^{N}\theta_k\alpha_k)\sum_{k=1}^{N}\theta_k\beta_k}\, e^{i(\theta_0+\sum_{k=1}^{N}\theta_k\alpha_k)\mathbf{q}_0}\, e^{i\sum_{k=1}^{N}\theta_k\beta_k\mathbf{p}_0}, \tag{3.58}$$

and hence

$$M(\theta_0,\dots,\theta_N) = \int \psi^*\left(q - \frac{\hbar}{2}\sum_{k=1}^{N}\theta_k\beta_k\right) e^{i(\theta_0+\sum_{k=1}^{N}\theta_k\alpha_k)q}\,\psi\left(q + \frac{\hbar}{2}\sum_{k=1}^{N}\theta_k\beta_k\right) dq\,. \tag{3.59}$$

The joint distribution is then

$$\begin{aligned} P(q_0,\dots,q_N) = \frac{1}{2\pi\beta_N}\int \psi^*\left(q_0 - \frac{\hbar}{2}\tau\right)\psi\left(q_0 + \frac{\hbar}{2}\tau\right) e^{-i\tau(q_N-\alpha_N q_0)/\beta_N} \\ \times \prod_{k=1}^{N-1}\delta\left\{(q_k - \alpha_k q_0) - \frac{\beta_k}{\beta_N}(q_N - \alpha_N q_0)\right\} d\tau\,. \end{aligned} \tag{3.60}$$

For the case of $N = 1$, we have

$$P(q_0,q_1) = \frac{1}{2\pi\beta_1}\int \psi^*\left(q_0 - \frac{\hbar}{2}\tau\right) e^{-i\tau(q_0-\alpha_1 q_0)/\beta_1}\,\psi\left(q_0 + \frac{\hbar}{2}\tau\right) d\tau\,. \tag{3.61}$$

If one calculates the expectation value of $\langle\, q(t)\,\rangle_{q_0}$, using this expression, we obtain

$$\langle q(t)\rangle_{q_0} = q_0 + \frac{\langle p\rangle_{q_0}}{m}t \qquad \text{(free particle)} \tag{3.62}$$

and

$$\langle q(t)\rangle_{q_0} = q_0\cos\omega t + \frac{\langle p\rangle_{q_0}}{m}\frac{\sin\omega t}{\omega} \qquad \text{(harmonic oscillator)} \tag{3.63}$$

where $\langle p\rangle_{q_0}$ is the local momentum and where we have dropped the probability distribution from the first term. For the case of a free particle and harmonic oscillator, the N time joint distributions can be explicitly calculated and the conditional expectation values calculated directly from the distribution.

f) Conditional Expectation Values in Phase Space

An interesting consideration which arises in quantum mechanics but is trivial in classical mechanics is the expectation value of an operator in phase space. In classical mechanics the expectation value of $b(q,p)$ for a fixed value of q and p is of course the value of the function itself at q,p. However in quantum mechanics the situation is considerably different. Using the same methods as before we have that

$$\langle \mathbf{B} \rangle_{qp} = \frac{1}{4\pi^2 i} \iint \left. \frac{\partial \mathbf{M}(\xi,\theta,\tau)}{\partial \xi} \right|_{\xi=0} e^{-i\theta q - i\tau p} \, d\theta \, d\tau \,, \tag{3.64}$$

where now $\mathbf{M}(\xi,\theta,\tau)$ is the characteristic function of the three variables, $\mathbf{B}$, q and p. Again, different expressions for $\mathbf{M}(\xi,\theta,\tau)$ are possible and we list some of them

$$\mathbf{M}(\xi,\theta,\tau) = e^{i\xi\mathbf{B}+i\theta\mathbf{q}+i\tau\mathbf{p}} \tag{3.65}$$

$$\mathbf{M}(\xi,\theta,\tau) = \tfrac{1}{2}[e^{i\xi\mathbf{B}}, e^{i\theta\mathbf{q}+i\tau\mathbf{p}}]_+ \tag{3.66}$$

$$\mathbf{M}(\xi,\theta,\tau) = e^{i\xi\mathbf{B}}\, e^{i\theta\mathbf{q}}\, e^{i\tau\mathbf{p}} \,. \tag{3.67}$$

We shall not work out the details here, however we note that in general none of these choices will result in the value for $\langle \mathbf{B} \rangle_{qp}$ to be $b(q,p)$ as would be the classical case.

Chapter 4

LOCAL VIRIAL THEOREM

We now consider the question local kinetic energy in detail and formulate the local virial theorem in quantum mechanics. We briefly mention the previous work done in this area.

Bader[6] and co-workers developed the concept of the virial theorem in a region and used it to study the spatial partitioning of molecules. They considered regions of space where the total flux vanished and showed that with their definition of local kinetic energy the virial theorem was satisfied in the region. Mazziotti, Parr and Simons[61] derived the conditions for the local virial theorem to hold in a region. It was subsequently shown that there are an infinite number of possible definitions of local kinetic energy each one associated with different quasi-probability distributions and that for a very wide class of definitions the concept of virial partitioning holds[24]. In the work of Ghosh, Berkowitz and Parr[40] in formulating ground state density functional theory as a local thermodynamic theory, the local kinetic energy plays a central role. Various definitions of local kinetic energy have been used in developing kinetic equations by Ziff, Kac and Uhlenbeck[80] and Putterman[67]. Dahl and Springborg[71] have considered the question of whether the virial theorem can be satisfied at each point, however they considered only a few possible expressions for local kinetic energy. They showed that one particular definition does yield a local virial theorem for the ground state of the hydrogen atom (see section 4.1).

We will show that one can always choose a quasi-distribution so that the local virial theorem holds and give an explicit method for finding it. In particular we show that there are an infinite number of distributions which generate a particular expression for the local kinetic energy and for which the local virial theorem is satisfied.

By the local virial theorem we shall mean

$$2\,T(q) = q \cdot \frac{\partial V(q)}{\partial q} \tag{4.1}$$

where $T(q)$ is the local kinetic energy and $V(q)$ is the potential. When the potential is a homogeneous function one can also write, As for the global virial theorem

$$T(q) = \frac{n}{2} V(q), \tag{4.2}$$

or

$$T(q) = \frac{n}{n+2} E(q), \tag{4.3}$$

$$V(q) = \frac{2}{n+2} E(q), \tag{4.4}$$

where $E(q)$ is the local total energy. This follows because the sum of two local quantities is the local quantity of the sum[30]. (We note that this is not so for the product of two local quantities.) It is convenient to define

$$K(q) = T(q)\,|\psi(q)|^2. \tag{4.5}$$

Although we will show that the local virial theorem can always be satisfied, one particular expression for the local kinetic energy can not be universally used. Even for the same potential different expressions for local kinetic energy have to be used for different eigenstates as is clear from the examples to follow. We point out that even if the local virial theorem is not satisfied the regional virial theorem may still be satisfied. This is so since the integration over a region puts considerably less stringent conditions on the choice of distributions or expressions for local kinetic energy.[24]

As previously mentioned one of the advantages of the phase space formulation and the use of local quantities is that it provides a classical like treatment of quantum mechanics and hence has certain conceptual advantages. However, it must be emphasized that these quasi distributions are particular representations of the density matrix and all yield the same quantum mechanical result. One should not be surprised that for different problems different distributions or expressions for local kinetic energy may be more convenient than others. As is the case with the traditional method of choosing an appropriate representation when working with the wave function or the density matrix, the choice of distribution function should be made on the basis of mathematical convenience and the insight the representation may give for that particular problem.

4.1 Local Kinetic Energy and Joint Distributions

Before proceeding to the local virial theorem we summarize the concept of local kinetic energy, the various expressions possible and their relationship to joint quasi-probability distributions of position and momentum. There are an infinite number of possible definitions for $K(q)$, the main requirement being that it yields to the proper quantum mechanical result when integrated over all space

$$\int K(q)\,dq = -\frac{\hbar^2}{2m}\int \psi^* \nabla^2 \psi\, dq = \left\langle \frac{p^2}{2m} \right\rangle . \tag{4.6}$$

Using the quantum quasi-probability distributions the local kinetic energy can be obtained from the distribution as in the classical case[24]

$$K(q) = \int P(q,p) \ \ (p^2/2m)\, dp , \tag{4.7}$$

where $P(q,p)$ is the quasi-probability distribution of position and momentum. As there are an infinite number of distributions there are an infinite number of expressions for $K(q)$. In addition, as we will discuss, there are an infinite number of distributions which generate the same particular expression for local kinetic energy.

As previously mentioned, all bilinear quasi-distribution can be generated from Eq. (2.4) which we write in three dimensions

$$P(q,p) = \left(\frac{1}{4\pi^2}\right)^3 \iiint e^{-i\theta\cdot q - i\tau\cdot p + i\theta\cdot u} f(\theta,\tau)\psi^*(u - \tfrac{1}{2}\tau\hbar)\psi(u + \tfrac{1}{2}\tau\hbar)\, du\, d\theta\, d\tau\,, \tag{4.8}$$

where $f(\theta,\tau)$ is any arbitrary function.

To obtain the possible expressions for local kinetic energy one substitutes Eq. (4.8) into Eq. (4.7) to obtain[24]

$$K(q) = -(\hbar^2/8m)(\nabla^2|\psi| - |\nabla\psi|^2) - \left(\frac{1}{2\pi}\right)^3 \int e^{i\theta\cdot(u-q)} \Big[\frac{|\psi(u)|^2}{2m} h_2(\theta) + i h_1(\theta)\cdot J(u)\Big] du\, d\theta\ , \tag{4.10 - 1}$$

where J is the quantum mechanical current

$$J = (\hbar/2mi)(\psi^*\nabla\psi - \psi\nabla\psi^*), \tag{4.11}$$

and h_1 and h_2 are defined by

$$h_1(\theta) = \nabla_\tau f(\theta,\tau)|_{\tau=0} \tag{4.12}$$

$$h_2(\theta) = \nabla_\tau^2 f(\theta, \tau)|_{\tau=0}. \qquad (4.13)$$

We note that the first term in Eq. (4.10) is distribution independent and the dependence of the second term on the distribution is only by way of the first and second partial derivatives of the kernel, $f(\theta, \tau)$.

For the subclass where $f(\theta, \tau)$ is a function of $\theta \cdot \tau$, the product kernels,

$$f_P(\theta, \tau) = f(\theta \cdot \tau) \qquad (4.14)$$

Eq. (4.10) reduces to

$$K(q) = -(\hbar^2/8m)\left[1 - 4f_P''(0)/\hbar^2\right]\nabla^2|\psi|^2 + (\hbar^2/2m)|\nabla\psi|^2 + f_P'(0)\nabla\cdot J \qquad (4.15)$$

where the primes denote differentiation with respect to the argument of f.

Some expressions for local kinetic energy which have been used in the literature are

$$K_A = -(\hbar^2/2m)\psi^*\nabla^2\psi, \qquad (4.16)$$

$$K_B = (\hbar^2/2m)|\nabla\psi|^2, \qquad (4.17)$$

$$K_C = -(\hbar^2/4m)(\psi^*\nabla^2\psi + \psi\nabla^2\psi^*), \qquad (4.18)$$

$$K_D = (\hbar^2/2m)|\nabla\psi|^2 - (\hbar^2/8m)\nabla^2|\psi^2|, \qquad (4.19)$$

and each follows by taking the class of distributions where the first and second derivatives of $f(x)$ are given by

$$f_A'(0) = -\tfrac{1}{2}i\hbar \quad ; \quad f_A''(0) = -\tfrac{1}{4}\hbar^2, \qquad (4.20)$$

$$f_B'(0) = 0 \quad ; \quad f_B''(0) = \tfrac{1}{4}\hbar^2, \qquad (4.21)$$

$$f_C'(0) = 0 \quad ; \quad f_C''(0) = -\tfrac{1}{4}\hbar^2, \qquad (4.22)$$

$$f_D'(0) = 0 \quad ; \quad f_D''(0) = 0, \qquad (4.23)$$

respectively.

4.2 Non–Uniqueness of the Expression for Local Kinetic Energy

We emphasize that for any particular expression for local kinetic energy there are an infinite number of distributions which will yield it. That is so since there are an infinite number of different kernels which have identical h_1 and h_2. Consider for example the expression given by K_D which is usually derived from the Wigner distribution. For the Wigner distribution

$$f_W(\theta,\tau) = 1 \tag{4.24}$$

and hence it is clear from (4.23) that one can obtain K_D from it. However there are an infinite number of other distributions which yield K_D. To obtain them one chooses kernels so that its first and second derivative are equal to zero at zero. For example the distributions obtained by using any one of the following kernels

$$f(x) = \cos \alpha x + \tfrac{1}{2}\alpha^2 x^2 \tag{4.25}$$

$$f(x) = 1 + \sin \alpha x - \alpha x \tag{4.26}$$

$$f(x) = e^{-\frac{1}{2}\alpha^2 x^2 + \alpha x} - \alpha x \tag{4.27}$$

where α is an arbitrary constant and $x = \theta\tau$, will all yield the same expression for local kinetic energy as the Wigner distribution, namely, K_D, because they satisfy Eq. (4.23). Hence from a particular favorite choice for local kinetic energy one distribution cannot be favored since there are an infinite number which give the same expression.

A procedure to generate an infinite number of kernels which have the identical expression for local kinetic energy is as follows. Chose any $f(\theta,\tau)$ which satisfies Eq. (4.9) and for given $h_1(\theta)$ and $h_2(\theta)$ form the new distribution

$$f_{\text{new}}(\theta,\tau) = f(\theta,\tau) + \tau\left[\, h_1(\theta) - \nabla_\tau f(\theta,\tau)|_{\tau=0}\, \right] + \tfrac{1}{2}\tau^2\left[\, h_2(\theta) - \nabla_\tau^2 f(\theta,\tau)|_{\tau=0}\, \right] . \tag{4.28}$$

This assures that f_{new} will satisfy Eqs. (4.12) and (4.13). In this way we generate an infinite number of kernels and hence an infinite number of distributions which will give the same expression for the local kinetic energy. For the case of product kernels where the local kinetic energy is determined by $f'(0)$ and $f''(0)$ chose an arbitrary $f_P(\theta\tau)$ for a given $f'(0)$ and $f''(0)$ form

$$f_{\text{new}}(\theta\tau) = f_P(\theta\tau) + \theta\tau\left[f'(0) - f_P'(0)\right] + \tfrac{1}{2}\theta^2\tau^2\left[f''(0) - f_P''(0)\right] . \tag{4.29}$$

We now ask under what conditions can one find a product kernel to give the same expression for local kinetic energy as given by a particular h_1 and h_2. We obtain the conditions by substituting $f_P(\theta\tau)$ for $f(\theta,\tau)$ into (2.14) and (2.15) which results in

$$\theta f_P'(0) = h_1(\theta) \tag{4.30}$$

$$\theta^2 f_P''(0) = h_2(\theta) \ . \tag{4.31}$$

Hence we must have that

$$h_1(\theta) \sim \theta \tag{4.32}$$

$$h_2(\theta) \sim \theta^2 \tag{4.33}$$

That is, for expressions for local kinetic energy determined by h_1 and h_2 as given by Eqs. (4.32) and (44.33) we can find a product kernel which gives the same expression. Examples of such situations are the ground states of the Hydrogen atom and harmonic oscillator.

4.3 Local Virial Theorem

We now address the question whether one can always find a distribution such that the local viral theorem is satisfied. We restrict ourselves to real wavefunctions and hence take $J = 0$. Consider first the subclass where the local kinetic energy is given by Eq. (4.15). Substituting Eq. (4.15) into Eq. (4.1) yields

$$f''(0) = \frac{\hbar^2}{4} + \frac{m\,q \cdot \dfrac{\partial V(q)}{\partial q}|\psi|^2 - \hbar^2|\nabla\psi|^2}{\nabla^2|\psi|^2} \ . \tag{4.34}$$

Now, in general, the right had side of Eq. (3.1) will be a function of position and hence will not be a constant although in particular situations it could be so. Thus, in general one can not satisfy the local virial theorem if one is restricted to the class of distributions where the kernel is a product kernel.

However we now show that one can always find an $f(\theta, \tau)$ which will satisfy the virial theorem. Substituting Eq. (4.10) into (4.1)

$$-2(\hbar^2/8m)(\nabla^2|\psi| - |\nabla\psi|^2) - \left(\frac{1}{2\pi}\right)^3 \int e^{i\theta\cdot(u-q)}\left[\frac{|\psi(u)|^2}{2m} h_2(\theta)\right] du\, d\theta \; = q \cdot \frac{\partial V(q)}{\partial q} \ . \tag{4.35}$$

By taking the fourier transform we can solve $h_2(\theta)$

$$h_2(\theta) = -2m\, \frac{\int \left[q \cdot \dfrac{\partial V(q)}{\partial q}|\psi|^2 + (\hbar^2/8m)(\nabla^2|\psi| - |\nabla\psi|^2)\right] e^{i\theta\cdot q}\, dq}{\int |\psi(q)|^2 e^{i\theta\cdot q}\, dq} \ . \tag{4.36}$$

Hence for a wave function and potential we obtain h_2 by Eq. (4.36) and use it to obtain the corresponding expression for local kinetic energy. That particular choice for local kinetic energy will assure that the local virial theorem is satisfied. In addition, once we have

$h_2(\theta)$ an infinite number of distributions can be generated having the same h_2 by using Eq. (4.28).

4.4 Examples

a) Hydrogen Atom

Consider the ground state of the hydrogen atom. We take

$$\psi(r) = \frac{1}{\sqrt{4\pi}} \frac{2}{a_0^{3/2}} e^{-r/a_0} \tag{4.37}$$

and straightforward substitution in Eq.(4.34) yields that

$$f_P''(0) = 0 \ . \tag{4.38}$$

This corresponds to Eq. (4.23) which gives K_D for the expression for local kinetic energy. Hence the use of K_D as given by Eq. (4.19) results in the local virial theorem being satisfied for the ground state of the hydrogen atom. This was previously shown by Dahl and Springborg[31] where they concluded that the Wigner distribution is preferred because it yields K_D. However as we have pointed out K_D also follows from an infinite number of other distributions.

Calculation of $h_2(\theta)$ gives

$$h_2(\theta) = 0 \tag{4.39}$$

For the first excited state we take

$$\psi(r) = \frac{1}{\sqrt{4\pi}} \frac{1}{(2a_0)^{3/2}} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0} \tag{4.40}$$

and by direct substitution we get

$$f_P''(0) = \frac{\hbar^2}{4} \frac{6a_0 r - 2a_0 r^2 - r^3}{16a_0^3 - 26a_0^2 r + 10a_0 r^2 - 2r^3} \tag{4.41}$$

and

$$h_2(\theta) = \frac{3\hbar^2}{2a_0^2} \frac{1 + a_0^2\theta^2}{(1 - a_0^2\theta^2)(1 - 2a_0^2\theta^2)} \ . \tag{4.42}$$

Hence for the first excited state a product kernel can not be found which gives an expression for local kinetic energy which satisfies the local virial theorem.

b) Harmonic Oscillator

Substituting the ground state of the harmonic oscillator

$$\psi(r) = \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}r^2} \tag{4.43}$$

into Eq. (4.34) yields

$$f_P''(0) = \frac{\hbar^2}{4} \tag{4.44}$$

which corresponds to the case given by Eq. (2.23) and therefor K_B may be used for the local kinetic energy if one wants to satisfy the local virial theorem. A wider class is obtained if we use $h_2(\theta)$

$$h_2(\theta) = \frac{\hbar^2}{4}\theta^2 \ . \tag{4.45}$$

For the first excited state

$$\psi(r) = \left(\frac{4m^3\omega^3}{\pi\hbar^3}\right)^{\frac{1}{4}} r\, e^{-\frac{m\omega}{2\hbar}r^2} \tag{4.46}$$

we have

$$f_P''(0) = \frac{\hbar^2}{4}\left(1 + \frac{4m\omega r^2 - 2\hbar^2}{2m^2\omega^2 r^4 - 5\hbar m\omega r^2 + \hbar^2}\right) \tag{4.47}$$

and

$$h_2(\theta) = \frac{\hbar^2}{4}\left(1 + \frac{8m\omega}{2m\omega - \hbar\theta^2}\right)\theta^2 \ . \tag{4.48}$$

We note that for examples given by Eq. (4.39) and (4.45) $h_2(\theta)$ is of the form of Eq. (4.33) and that is why a product kernel as given by (4.38) and (4.44) exists for those two cases.

Chapter 5

INSTANTANEOUS FREQUENCY AND ITS STANDARD DEVIATION

We consider instantaneous frequency and its variance using the bilinear joint time-frequency distributions. It is well known that these quasi distributions give the instantaneous frequency as the time derivative of the phase. We show that they also lead to a reasonable definition for the standard deviation of instantaneous frequency, namely

$$\sigma_\omega^2(t) = \left(\frac{A'(t)}{A(t)} \right)^2 \tag{5.1}$$

where $A(t)$ is the amplitude of the signal. We will demonstrate the relationship with the bandwidth of the spectrum. In the next chapter we derive the corresponding quantities for the short-time Fourier spectrum and show the relation to and consistency with the above definition.

In Chapter 7, the concept of local spread of frequencies is used to define and clarify the meaning of multicomponent signals. We will argue that the breaking up of a signal into components is a local phenomenon and that the criteria for a meaningful decomposition is that the standard deviations of instantaneous frequency of each part about their own individual instantaneous frequencies be well separated and small in comparison to the standard deviations of the signal.

Although the concept of the frequency at a given time has meaning for certain types of signals, the mathematical and physical description of this concept has not been fully developed. In particular, the way in which frequency is used in reference to the energy density spectrum compared to instantaneous frequency is not altogether identical and the relationship is not obvious. Furthermore, although instantaneous frequency is a local phenomenon, it is usually defined as the derivative of the phase of the analytic signal. However, calculation of the analytic signal at a particular time requires knowledge of the whole time period of the actual signal. For some signals it certainly is the case that the derivative of the phase meets our expectations of what instantaneous frequency should be. Boashash[14,15] and coworkers pioneered the idea of using the Wigner distribution to extract the instantaneous frequency even though the predictions for other physical quantities may make no sense. The application for obtaining the random instantaneous frequency has recently been formulated by White and Boashash[74,75,76].

It is usually the case that the resulting equations are more revealing when the signal is expressed in terms of amplitude and phase of the signal,

$$s(t) = A(t)\ e^{j\varphi(t)}\ . \tag{5.2}$$

We will examine whether the concept of the local spread can be meaningfully defined by way of these distributions, and indeed we will show that there are an infinite number of distributions for which this is so.

Although we have already considered the general definition of conditional expectation values we repeat the general ideas, in signal analysis language here for the sake of clarity and continuity.

For a function, $g(t,\omega)$, of time and frequency the global expectation value is

$$\langle\ g(t,\omega)\ \rangle = \iint g(t,\omega)\ P(t,\omega)\ d\omega\ dt\ , \tag{5.3}$$

where $P(t,\omega)$ is the density or distribution .

The density of frequency for a given time, and the density of time for a given frequency, are respectively given by

$$P(\omega|t) = \frac{P(t,\omega)}{P_1(t)} \qquad ; \qquad P(t|\omega) = \frac{P(t,\omega)}{P_2(\omega)}\ , \tag{5.4}$$

where $P_1(t)$and $P_2(\omega)$ are the marginal distributions

$$P_1(t) = \int P(t,\omega)\ d\omega \qquad ; \qquad P_2(\omega) = \int P(t,\omega)\ dt\ . \tag{5.5}$$

Hence the expectation value of a function g at a given time or frequency is

$$\langle\ g(t,\omega)\ \rangle_t = \frac{1}{P_1(t)} \int g(t,\omega)\ P(t,\omega)\ d\omega \quad ; \quad \langle\ g(t,\omega)\ \rangle_\omega = \frac{1}{P_2(\omega)} \int g(t,\omega)\ P(t,\omega)\ dt\ . \tag{5.6}$$

To avoid repetition of similar formulas we will restrict ourselves to consideration of expectation values at a given time. It will be obvious how to write the corresponding equation for a given frequency.

The spread of a function at a given time is defined in the usual way

$$\begin{aligned}\sigma_g^2(t) &= \frac{1}{P_1(t)}\int \{\ g(t,\omega) - \langle\ g(t,\omega)\ \rangle_t\}^2\ P(t,\omega)\ d\omega \\ &= \frac{1}{P_1(t)}\int \left\{g^2(t,\omega) - 2g(t,\omega)\langle g(t\omega)\rangle_t + \langle g(t,\omega)\rangle_t^2\right\} P(t,\omega)\,d\omega \\ &= \frac{1}{P_1(t)}\int g^2(t,\omega)P(t,\omega)\,d\omega - \frac{2\langle g(t,\omega)\rangle_t}{P_1(t)}\int g(t,\omega)P(t,\omega)\,d\omega + \langle g(t,\omega)\rangle_t^2 \\ &= \langle g^2(t,\omega)\rangle_t - 2\langle g(t,\omega)\rangle_t^2 + \langle g(t,\omega)\rangle_t^2 \\ &= \langle\ g^2(t,\omega)\ \rangle_t - \langle\ g(t,\omega)\ \rangle_t^2\,.\end{aligned} \tag{5.7}$$

We point out that while the global expectation value may be obtained by integrating the local expectation value

$$\int \langle\ g(t,\omega)\ \rangle_t\ P_1(t)\ dt = \langle\ g(t,\omega)\ \rangle\ , \tag{5.8}$$

that is not generally the case with the spread. In general

$$\int \sigma_g^2(t)\ P_1(t)\ dt\ \neq\ \iint \{\ g(t,\omega) - \langle\ g(t,\omega)\ \rangle\}^2\ P(t,\omega)\ d\omega\ dt\ . \tag{5.9}$$

This is the case even if g is only a function of ω. The significance of the left hand side of Eq. (5.9) is that it gives the average local spread.

5.2 Spread of Instantaneous Frequency

From the point of view of a joint distribution one may ask for the average frequency at a certain time

$$\langle\ \omega\ \rangle_t = \frac{1}{P_1(t)}\int \omega\ P(t,\omega)\ d\omega\ , \tag{5.10}$$

and in addition one may ask for the spread of that value at that time,

$$\sigma_\omega^2(t) = \int (\ \omega - \langle\ \omega\ \rangle_t\ )^2\ P(t,\omega)\ d\omega = \langle\ \omega^2\ \rangle_t - \langle\ \omega\ \rangle_t^2\ , \tag{5.11}$$

where

$$\langle\ \omega^2\ \rangle_t = \frac{1}{P_1(t)}\int \omega^2\ P(t,\omega)\ d\omega\ . \tag{5.12}$$

Whether we want to identify $\langle\ \omega\ \rangle_t$ with the concept of instantaneous frequency we leave aside for the moment. However it is clear that from a distribution point of view, that quantity is the average frequency at a particular time.

Now we confine ourselves to the product kernels,

$$f_p(\theta,\tau) = f(\theta\tau)\,, \tag{5.14}$$

because they belong to one of the important classes of kernels, and they gives a clear insight to the problem. In Chapter 6, we will give the results for a general kernel. From the context it will usually be clear whether we are considering the product kernels or the general ones.

Inserting Eq. (2.36) into Eq. (5.10), and using primes to denote differentiation with respect to the argument, we have

$$\begin{aligned}
\langle \omega \rangle_t \, P_1(t) &= \frac{1}{4\pi^2} \iiiint e^{-j\theta t - i\omega\tau + j\theta u} \omega f(\theta\tau) s^*(u - \tfrac{1}{2}\tau) s(u + \tfrac{1}{2}\tau)\, du\, d\theta\, d\tau\, d\omega \\
&= -\frac{1}{4\pi^2 j} \iint du\, d\theta\, e^{-j\theta(t-u)} \int d\tau \left\{ \frac{\partial}{\partial\tau} \int d\omega\, e^{-j\tau\omega} \right\} f(\theta\tau) s^*(u - \tfrac{1}{2}\tau) s(u + \tfrac{1}{2}\tau) \\
&= -\frac{1}{4\pi^2 j} \iint du\, d\theta\, e^{-j\theta(t-u)} \int d\tau \left\{ \frac{\partial}{\partial\tau} 2\pi\delta(\tau) \right\} f(\theta\tau) s^*(u - \tfrac{1}{2}\tau) s(u + \tfrac{1}{2}\tau) \\
&= \frac{1}{2\pi j} \iint du\, d\theta\, e^{-j\theta(t-u)} \int d\tau\, \delta(\tau) \left\{ \frac{\partial}{\partial\tau} f(\theta\tau) s^*(u - \tfrac{1}{2}\tau) s(u + \tfrac{1}{2}\tau) \right\} \\
&= \frac{1}{2\pi j} \iint du\, d\theta\, e^{-j\theta(t-u)} \; \frac{\partial}{\partial\tau} \left\{ f(\theta\tau) s^*(u - \tfrac{1}{2}\tau) s(u + \tfrac{1}{2}\tau) \right\} \Big|_{\tau=0} \\
&= \frac{1}{2\pi} f(0) \iint du\, d\theta\, e^{-j\theta(t-u)} \frac{1}{2j} \left\{ s^*(u) \frac{\partial}{\partial u} s(u) - s(u) \frac{\partial}{\partial u} s^*(u) \right\} \\
&\quad + \frac{1}{2\pi j} f'(0) \iint du\, d\theta\, e^{-j\theta(t-u)}\, \theta\, |s(u)|^2 \\
&= \frac{1}{2\pi} f(0) \int du\, \frac{1}{2j} \left\{ s^*(u) \frac{\partial}{\partial u} s(u) - s(u) \frac{\partial}{\partial u} s^*(u) \right\} \int d\theta\, e^{-j\theta(t-u)} \\
&\quad - \frac{1}{2\pi} f'(0) \int du\, |s(u)|^2 \frac{\partial}{\partial u} \int d\theta\, e^{-j\theta(t-u)} \\
&= f(0)\, \frac{1}{2j} \left\{ s^*(t) \frac{\partial}{\partial t} s(t) - s(t) \frac{\partial}{\partial t} s^*(t) \right\} + f'(0) \frac{\partial}{\partial t} |s(t)|^2 \,.
\end{aligned} \tag{5.15}$$

Using Eq. (5.2), we have

$$\langle\, \omega \,\rangle_t \; P_1(t) = f(0) \; A^2(t) \; \varphi'(t) + 2 f'(0) \; A(t) \; A'(t)\,. \tag{5.16}$$

A similar calculation with Eqs. (2.36) and (5.12) yields

$$\begin{aligned}
\langle\, \omega^2 \,\rangle_t \; P_1(t) &= \tfrac{1}{2} \left[f(0) + 4 f''(0) \right] A(t)'^2 - \tfrac{1}{2} \left[f(0) - 4 f''(0) \right] A(t) \; A''(t) \\
&\quad + f(0) \; A^2(t) \; \varphi'^2(t) + 2 f'(0) \left[2\, A(t) \; A'(t) \; \varphi'(t) + A^2(t) \; \varphi''(t) \right] \,.
\end{aligned} \tag{5.18}$$

As has been pointed out many times, and as can be seen from Eq. (5.17), if we want the first conditional moment to be the derivative of the phase then we must take

$$f(0)=1\ , \qquad ; \qquad f'(0)=0\ , \tag{5.19}$$

in which case we have that

$$\langle\ \omega\ \rangle_t=\varphi'(t)\ . \tag{5.20}$$

We note that this result is independent of whether we use the analytic signal or not. It is true for all signals. Therefore we can not associate the conditional expectation value with instantaneous frequency unless the analytic signal is used. Also, even for the case of an analytic signal the concept of instantaneous frequency is not always applicable. A proper theory would of course give for the expected value the derivative of the phase of the analytic signal even when the real signal is used in the distribution. What this indicates is that the proper variable to use for instantaneous frequency may not be ω as it appears in the distribution but some other function. None the less we will continue to use the phrase "instantaneous frequency" for the first conditional moment of frequency. Before proceeding we note that the conditions of Eq. (5.19) are necessary for the distribution to give the instantaneous power and energy density spectrum.

We point out that Eq. (2.36) is a general bilinear distribution and other distributions which do not satisfy the marginals but which are important and useful may be put into that form. A prime example is the spectrogram which we consider in Chapter 6.

Standard Deviation

We now consider the spread of instantaneous frequency at a given time. The local spread was considered by Claasen and Mecklenbrauker[20] for the Wigner distribution. Also, the question of the second conditional moment arises under the concept of local kinetic energy in quantum mechanics as we have discussed in Chapter 4. Janssen[45,46] in his comprehensive work on spread, squared the distribution to avoid negative spreads. Our approach is to see if there are distributions which predict a manifestly positive standard deviation.

If the kernel satisfies Eq. (5.19), then we have

$$\langle\ \omega^2\ \rangle_t=\tfrac{1}{2}\left[1+4f''(0)\right]\left(\frac{A'(t)}{A(t)}\right)^2-\tfrac{1}{2}\left[1-4f''(0)\right]\frac{A''(t)}{A(t)}\ +\ \varphi'^2(t)\ , \tag{5.21}$$

and

$$\langle\, \sigma_\omega^2 \,\rangle_t = \tfrac{1}{2}\,[1+4f''(0)]\left(\frac{A'(t)}{A(t)}\right)^2 - \tfrac{1}{2}\,[1-4f''(0)]\,\frac{A''(t)}{A(t)}\ . \tag{5.22}$$

For an arbitrary choice of $f''(0)$, the spread will not be positive. For the Wigner distribution, where $f=1$ the spread is obtained by taking $f''(0)=0$ which results in

$$\langle\, \sigma_\omega^2 \,\rangle_t = \tfrac{1}{2}\left(\frac{A'(t)}{A(t)}\right)^2 - \tfrac{1}{2}\,\frac{A''(t)}{A(t)}\ , \tag{5.23}$$

a result obtained by Claasen and Mecklenbrauker[20]. As they have pointed out this is in general negative and cannot be properly interpreted.

There is a class of distributions for which the spread is manifestly positive. If we take

$$f''(0) = \frac{1}{4}\ , \tag{5.24}$$

then the spread becomes

$$\sigma_\omega^2(t) = \left(\ \frac{A'(t)}{A(t)}\ \right)^2\ , \tag{5.25}$$

which is always positive. Also the conditional second moment is manifestly positive

$$\langle\, \omega^2 \,\rangle_t = \left(\ \frac{A'(t)}{A(t)}\ \right)^2 + \varphi'^2(t)\ . \tag{5.26}$$

Even though the spread is positive it does not follow that it has any meaning because we obtained it from distributions which may go negative. The results obtained from improper distributions should always be suspected. However we will argue that the above definition of spread is useful in a variety of contexts and show how it enters into the consideration of the relationship between the concept of frequency as expressed by the energy density spectrum and instantaneous frequency. This is done in the next section. Before proceeding there are two other notions which are useful and revealing.

Modulation

Consider the product of two signals,

$$s(t) = s_1(t)\,s_2(t) = A_1(t)\,e^{j\varphi_1(t)}\,A_2(t)\,e^{j\varphi_2(t)} \ = A(t)\,e^{j\varphi(t)}\ , \tag{5.27}$$

with

$$A(t) = A_1(t)\,A_2(t) \quad ; \quad \varphi(t) = \varphi_1(t) + \varphi_2(t)\ . \tag{5.28}$$

We attempt to express the spread of the modulated signal in terms of the individual spreads. We keep things general for the moment and substitute Eq. (5.28) into Eq. (5.22). The result is

$$\sigma_\omega^2(t) = \sigma_\omega^2(t)_1 + \sigma_\omega^2(t)_2 + 8f''(0)\,\frac{A_1'(t)}{A_1(t)}\frac{A_2'(t)}{A_2(t)} \ . \tag{5.29}$$

We now ask, for what kernels may in the right hand side be expressed in terms of the spreads of the individual signals only. Since the third term in Eq. (5.29) only depends on the first derivative of the amplitude, the term must either be eliminated by taking $f''(0) = 0$ in which case we have

$$\sigma_\omega^2(t) = \sigma_\omega^2(t)_1 + \sigma_\omega^2(t)_2 \ , \tag{5.30}$$

or we must use a kernel which leads to a spread which only depends on the first derivative. The only such case is $f''(0) = \frac{1}{4}$. The spread of the modulated signal is then

$$\sigma_\omega(t) = \sigma_\omega(t)_1 + \sigma_\omega(t)_2 \ . \tag{5.31}$$

Hence if we want the spread of a modulated signal to be expressible only in terms of the spread of each signal there are only two classes of kernels. We emphasize that the spreads in Eq. (5.30) are generally not positive, however in Eq. (5.31) the spreads are always positive.

Average Local Spread

Eq. (5.25) defines the standard deviation at each instant in time. To get an idea how the frequencies of a signal have spread for the duration of the signal we can define the average local spread by

$$\langle\ \sigma_\omega^2(t)\ \rangle = \int \left(\frac{A'(t)}{A(t)} \right)^2 |s(t)|^2\, dt = \int A'^2(t)\ dt \ . \tag{5.31}$$

One can also define the average spread in an interval of time

$$\langle\ \sigma_\omega^2(t)\ \rangle_{t_1,t_2} = \int_{t_1}^{t_2} \left(\frac{A'(t)}{A(t)} \right)^2 |s(t)|^2\, dt = \int_{t_1}^{t_2} A'^2(t)\ dt \ . \tag{5.32}$$

This allows us to compare the spreading in different intervals.

5.3 Relation between Spectral Bandwidth and Spread of Instantaneous Frequency

The relationship between frequencies that appear in the spectrum and the instantaneous frequencies which exist during the course of the signal, has been one of the fundamental issues. The question has been investigated by a number of people, particularly Ville[73], Fink[37] and Mandel[55]. We shall re-derive their results in a simple manner and relate them to the notions of local spread as we have discussed. We first consider the question of average frequency for which there are three possible definitions. First is the average frequency as defined by way of the spectrum

$$\langle \omega \rangle_S = \int \omega \, |S(\omega)|^2 \, d\omega \, , \qquad \text{(spectral average)} \tag{5.33}$$

Next we can define the time average of the instantaneous frequency

$$\langle \omega \rangle_T = \int \varphi'(t) \, |s(t)|^2 \, dt \, , \qquad \text{(time average)} \tag{5.34}$$

and last by way of a joint distribution

$$\langle \omega \rangle_D = \iint \omega \, P(t,\omega) \, d\omega \, dt \, . \qquad \text{(distribution average)} \tag{5.35}$$

There is no inherent reason why these three differently defined averages should be equal and indeed it was Ville[73] who approached the problem from the point of view of making them equal.

That $\langle \omega \rangle_T = \langle \omega \rangle_D$ is readily seen to be the case as long as the distribution satisfies the marginals. To show that $\langle \omega \rangle_S = \langle \omega \rangle_T$ we have

$$\langle \omega \rangle_S = \int \omega \, |S(\omega)|^2 \, d\omega = \int s^*(t) \left(\frac{1}{j} \frac{d}{dt} \right) s(t) \, dt \tag{5.36}$$

$$= \int A(t) \{ \, -jA'(t) + A(t)\,\varphi'(t) \, \} \, dt = \int \varphi'(t)\, A^2(t) \, dt = \langle \omega \rangle_T \, . \tag{5.37}$$

The first term vanishes if $A(t)$ vanishes at the end points. Hence we have that

$$\langle \omega \rangle_S \; = \; \langle \omega \rangle_T \; = \; \langle \omega \rangle_D \tag{5.38}$$

We now turn to the question of how the spreads are related. We first consider this from a physical point of view. We note that even if the spectrum is a line spectrum, that is a sum of delta functions, the instantaneous frequency will in general be a continuous function of time. Second, even if the spectrum is band limited there can be instantaneous frequencies which are outside the band. As a corollary of this, even for analytic signals where the spectrum is zero for negative frequencies, the instantaneous frequency may become negative. One may be tempted to therefore conclude that global spread of instantaneous frequencies should be broader than the spread of the energy density spectrum. The opposite is true as was first shown by Fink[37]. What this must mean is that the distribution of instantaneous frequencies is generally narrower than the energy density spectrum.

As before we define three kinds of spreads. First the standard bandwidth

$$\sigma_S^2 = \int (\omega - \langle \omega \rangle)^2 \, |S(\omega)|^2 \, d\omega, \tag{5.39}$$

then the global deviation of instantaneous frequency around the global average frequency

$$\sigma_T^2 = \int (\varphi'(t) - \langle \omega \rangle)^2 \, |s(t)|^2 \, dt \, , \tag{5.40}$$

and last the average local spread

$$\sigma_D^2 = \int (\omega - \varphi'(t))^2 \, P(t,\omega) \, dt \, d\omega = \int \left(\frac{A'(t)}{A(t)} \right)^2 |s(t)|^2 \, dt \, . \tag{5.41}$$

Now consider

$$\begin{aligned}
\sigma_S^2 &= \int (\omega - \langle \omega \rangle)^2 \, |S(\omega)|^2 \, d\omega && (5.42)\\
&= \int s^*(t) \Big(\frac{1}{j}\frac{d}{dt} - \langle \omega \rangle \Big)^2 s(t) \, dt && (5.43)\\
&= \int \left| \Big(\frac{1}{j}\frac{d}{dt} - \langle \omega \rangle \Big) s(t) \right|^2 dt && (5.44)\\
&= \int \left| \frac{1}{j}\frac{A'(t)}{A(t)} + \varphi'(t) - \langle \omega \rangle \right|^2 A^2(t) \, dt && (5.45)\\
&= \int \left[\Big(\frac{A'(t)}{A(t)} \Big)^2 + \Big(\varphi'(t) - \langle \omega \rangle \Big)^2 \right] A^2(t) \, dt && (5.46)\\
&= \int \Big(\frac{A'(t)}{A(t)} \Big)^2 A^2(t) \, dt + \int \Big(\varphi'(t) - \langle \omega \rangle \Big)^2 A^2(t) \, dt \, . && (5.47)
\end{aligned}$$

Hence we have that

$$\sigma_S^2 = \sigma_T^2 + \sigma_D^2 \tag{5.47}$$

a relation obtained by Fink[37] and later by Mandel[55]. Thus the spectral bandwidth is always larger than the spread of instantaneous frequencies.

Examples of Distribution of Instantaneous Frequency and Its Range

As previously mentioned, for a band limited spectrum the instantaneous frequencies may go outside the band which must mean that they are generally more concentrated around the average frequency. The distribution of instantaneous frequency can be calculated as follows. Let us call ω_i the variable denoting instantaneous frequency. Then the distribution of frequency $P(\omega_i)$ is related to the instantaneous power, $|s(t)|^2$ by

$$P(\omega_i)\ d\omega_i = |s(t)|^2\ dt\ , \tag{5.49}$$

or

$$P(\omega_i) = \frac{|s(t)|^2}{\varphi''(t)}\ . \tag{5.50}$$

The right hand side of equation (5.50) must be expressed in terms of ω_i which is done by solving for time in terms of ω_i from

$$\omega_i = \varphi'(t)\ . \tag{5.51}$$

From the distribution we can also calculate

$$\sigma_T^2 = \int (\omega_i - \langle\ \omega_i\ \rangle)^2\ P(\omega_i)\ d\omega_i\ . \tag{5.52}$$

As an example we calculate the distribution of instantaneous frequency for the chirp like signal

$$s(t) = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\alpha t^2 + \frac{1}{2}j\beta t^2 + j\omega_0 t}\ . \tag{5.53}$$

The instantaneous frequency is

$$\omega_i = \omega_0 + \beta t\ , \tag{5.54}$$

and its derivative is simply β. Hence

$$P(\omega_i) = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} \frac{1}{\beta}\, e^{-\alpha\left(\frac{\omega_i - \omega_0}{\beta}\right)^2}\ . \tag{5.55}$$

We now compare it to the distribution of frequencies as given by the energy density spectrum. The spectrum and energy density spectrum are readily worked out.

$$S(\omega) = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{\alpha - j\beta}}\, e^{-\frac{(\omega - \omega_0)^2}{2(\alpha - j\beta)}}\ , \tag{5.56}$$

and

$$|S(\omega)|^2 = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} \frac{1}{\sqrt{\alpha^2+\beta^2}}\, e^{-\dfrac{\alpha(\omega-\omega_0)^2}{\sqrt{\alpha^2+\beta^2}}} \; . \tag{5.57}$$

Thus we see that both distributions are peaked at ω_0 which of course is expected from Eq. (5.38).

Another example illustrating these points is to consider the sum of two signals,

$$s(t) = s_1(t) + s_2(t) = A_1(t)\, e^{j\varphi_1(t)} + A_2(t)\, e^{j\varphi_2(t)} = A(t)\, e^{j\varphi(t)} \; . \tag{5.58}$$

Solving for the amplitude and phase of the resulting signal we have (suppressing t for brevity)

$$A^2 = A_1^2 + A_2^2 + 2A_1A_2\cos(\varphi_2 - \varphi_1) \; , \tag{5.59}$$

and

$$\tan\varphi = \frac{A_1\sin\varphi_1 + A_2\sin\varphi_2}{A_1\cos\varphi_1 + A_2\cos\varphi_2} \; . \tag{5.60}$$

An alternative convenient form is

$$s(t) = A(t)\, e^{\frac{1}{2}(\varphi_2+\varphi_1)+j\tilde{\varphi}} = e^{\frac{1}{2}(\varphi_2+\varphi_1)} \left[A_1(t)\, e^{j\frac{1}{2}(\varphi_1-\varphi_2)} + A_2(t)\, e^{j\frac{1}{2}(\varphi_2-\varphi_1)} \right] \; , \tag{5.61}$$

in which case we have that

$$\tan\tilde{\varphi} = \frac{A_2 - A_1}{A_2 + A_1}\tan\tfrac{1}{2}(\varphi_2 - \varphi_1) \; , \tag{5.62}$$

and the two phases are related by

$$\varphi = \tfrac{1}{2}(\varphi_2 + \varphi_1) + \arctan\tilde{\varphi} \; . \tag{5.63}$$

Now the instantaneous frequency may be obtained from differentiating Eq. (5.60).

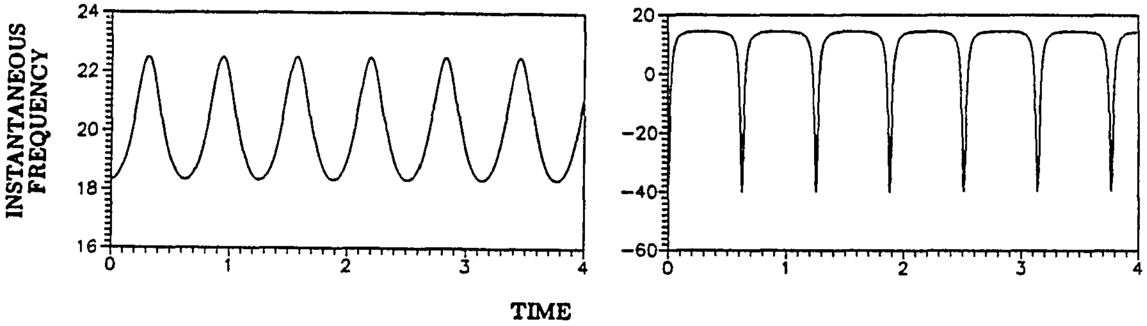
$$\varphi' = \frac{A_1^2\varphi_1' + A_2^2\varphi_2' + A_1A_2(\varphi_1' + \varphi_2')\cos(\varphi_2 - \varphi_1) + (A_2'A_1 - A_1'A_2)\sin(\varphi_2 - \varphi_1)}{A^2} \; , \tag{5.64}$$

or equivalently by differentiating Eq. (4.31)

$$\varphi' = \tfrac{1}{2}(\varphi_2' + \varphi_1') + \frac{\frac{1}{2}(\varphi_2' - \varphi_1')(A_2^2 - A_1^2)}{A^2} + \frac{(A_2'A_1 - A_1'A_2)\sin(\varphi_2 - \varphi_1)}{A^2} \; . \tag{5.65}$$

To illustrate that the instantaneous frequency can be outside the band consider the case where

$$\varphi_1 = \omega_1 t \quad ; \quad \varphi_2 = \omega_2 t \; , \tag{5.66}$$



Figures 1 and 2. Examples illustrating the behavior of the instantaneous frequency for the signal $s(t) = A_1 e^{10jt} + A_2 e^{20jt}$. In Figures 1 and 2 the amplitudes are $A_1 = 0.2$, $A_2 = 1$ and $A_1 = 1.2$, $A_2 = 1$, respectively.

and constant amplitudes. The instantaneous frequency is then given by

$$\varphi' = \frac{A_1^2\omega_1 + A_2^2\omega_2 + A_1A_2(\omega_1+\omega_2)\cos(\omega_2-\omega_1)t}{A^2} = \tfrac{1}{2}(\omega_2+\omega_1) + \tfrac{1}{2}(\omega_2-\omega_1)\,\frac{A_2^2 - A_1^2}{A(t)^2}\,. \tag{5.67}$$

We emphasize that A_1 and A_2 are constants but $A(t)$ is a function of time. We point out that even when A_2 is close to A_1 the last term is not necessarily small. For times for which $\cos(\omega_2-\omega_1)t$ is close to -1 the last term becomes very large, but the intensity of the signal is very small near those times. The spectrum of this signal consists of only two frequencies ω_1 and ω_2,

$$S(\omega) = A_1\delta(\omega-\omega_1) + A_2\delta(\omega-\omega_2)\ . \tag{5.68}$$

However the instantaneous frequency is continuous for a broader range than $\omega_2 - \omega_1$. Depending on the relative magnitudes of A_1 and A_2, the instantaneous frequency can be to the left of ω_1 or to the right of ω_2. This is illustrated in Figures 1 and 2. We note that in Figure 2 the instantaneous frequencies become negative even though the signal is analytic.

Chapter 6

SHORT TIME ENERGY SPECTRUM OR SPECTROGRAM

The spectrogram or short-time Fourier energy spectrum has been the most widely used tool for the study of signals with time varying spectrum contents because the understanding and classification of human speech and sound has become a major development of science. The first implementation of the spectrogram was hardware, but in the Seventies, with the development of the fast Fourier transform, the spectrogram has become the main tool in the signal analysis of non-stationary signals. The basic idea of the spectrogram is simple. Consider a signal which has at time varying spectrum. Suppose we are interested in what is happening around time t, then we can merely cut off the signal with a box window around time t and take the Fourier transform of the piece of the signal. Instead of abruptly cutting of the signal, we can window it with some other windows.

Therefore windowing the signal at time t means mathematically

$$S_t(\omega) = \frac{1}{\sqrt{2\pi}} \int e^{-j\omega\tau} s(\tau) h(\tau - t) d\tau \ , \tag{6.1}$$

and $h(t)$ is the window function. The spectrogram or short-time energy density is defined by

$$P_{SP}(t,\omega) = |S_t(\omega)|^2 \ . \tag{6.2}$$

This method of short-time Fourier transformation ($STFT$) has continuously been used in all fields of science. For example, if one analyzes a short burst of light at a given time, he is really taking the short-time Fourier spectrum. In the field of laser physics this is sometimes called the physical spectrum of light and has recently been elaborated by Eberly and Wódkiewicz[32]. Their approach is similar to that developed by Mark[59] who was probably the first one to call it the physical spectrum. We also point out that it was realized by Ackroyd[1] that there is a close relationship between the spectrogram and Rihaczek distribution. Mark[59] and later Claasen and Mecklenbrauker[20] derived the relationship between the spectrogram and the Wigner distribution. Recently Cohen showed that there is a large class of quasi distributions for which the above relations can be generalized.

6.1 Standard Deviation Using STFT

We now derive the first and second conditional moment and the spread of the spectrogram. For $h(t)$, we write in terms of its amplitude and phase

$$h(t) = A_h(t)\, e^{j\varphi_h(t)} \ . \tag{6.3}$$

First we note that by direct integration of Eq. (6.1) we have

$$P_1(t) = \int |S_t(\omega)|^2 \ d\omega = \int A^2(\tau) \ A_h^2(\tau - t) \ d\tau \ , \tag{6.4}$$

For convenience we define the windowed signal by

$$\eta_t(\tau) = s(\tau)h(\tau - t) \ , \tag{6.5}$$

and note that t is to be a considered a parameter. Now $\eta_t(\tau)$ and $S_t(\omega)$ form a Fourier transform pair between the variables τ and ω. Then

$$\langle \ \omega \ \rangle_t P_1(t) = \int \omega \ |S_t(\omega)|^2 \ d\omega \ , \tag{6.6}$$

which may be readily written † in terms of $\eta_t(\tau)$

$$\langle \ \omega \ \rangle_t \ P_1(t) = \int \eta_t^*(\tau) \ \frac{1}{j}\frac{d}{d\tau} \ \eta_t(\tau) \ d\tau \ . \tag{6.7}$$

Direct evaluation gives

$$\langle \ \omega \ \rangle_t P_1(t) = \int A^2(\tau) \ A_h^2(\tau - t) \ \{ \ \varphi'(\tau) + \varphi_h'(\tau - t) \ \} \ d\tau \ . \tag{6.8}$$

This result is well known and is the main reason for the use of the spectrogram.

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† We recall that for any real function $G(t)$ of time its expected value can be calculated from either the signal $s(t)$ or its Fourier transform, $S(\omega)$

$$\langle \ G(t) \ \rangle = \int G(t) \ |s(t)|^2 \ dt = \int S^*(\omega) \ G\left(j\frac{d}{d\omega}\right) \ S(\omega) d\omega \ ,$$

and similarly for any real function of frequency

$$\langle \ H(\omega) \ \rangle = \int H(\omega) \mid S(\omega)|^2 \ d\omega = \int s^*(t) \ H\left(-j\frac{d}{dt}\right) \ s(t) \ dt \ .$$

Spread

We shall give a number of different derivations for the standard deviation because each method has its own mathematical interest. In a particular method, we will show that the simple application of well known quantum mathematical maneuvers saves a considerable amount of algebra. Also we will give the brute force method.

Similar to Eqs. (6.7)-(6.8), we have

$$\langle \omega^2 \rangle_t P_1(t) = \int \eta_t^*(\tau) \left(\frac{1}{j} \frac{d}{d\tau} \right)^2 \eta_t(\tau)\, d\tau = \int \left| \frac{1}{j} \frac{d}{d\tau} \eta_t(\tau) \right|^2 d\tau \tag{6.9}$$

$$= \int \left(\frac{d}{d\tau}\, A(\tau)\, A_h(\tau - t) \right)^2 d\tau + \int A^2(\tau) A_h^2(\tau - t) \{\, \varphi'(\tau) + \varphi_h'(\tau - t)\, \}^2\, d\tau\, . \tag{6.10}$$

The local spread is given by

$$\sigma_\omega^2(t) = \langle\, \omega^2 \,\rangle_t - \langle\, \omega \,\rangle_t^2 \tag{6.11}$$

$$\begin{aligned} &= \frac{1}{P_1(t)} \int \{\, A'(\tau) A_h(\tau - t) + A(\tau) A_h'(\tau - t)\, \}^2\, d\tau \\ &\quad + \frac{1}{P_1(t)} \int A^2(\tau) A_h^2(\tau - t) \{\, \varphi'(\tau) + \varphi_h'(\tau - t)\, \}^2\, d\tau \\ &\quad - \frac{1}{P_1^2(t)} \iint A^2(\tau_1) A^2(\tau_2) A_h^2(\tau_1 - t) A_h^2(\tau_2 - t) \{\, \varphi'(\tau_1) + \varphi_h'(\tau_1 - t)\, \} \\ &\qquad \times \{\, \varphi'(\tau_2) + \varphi_h'(\tau_2 - t)\, \}\, d\tau_1\, d\tau_2\, . \end{aligned} \tag{6.12}$$

Combining the last two terms of Eq. (6.12) we have

$$\begin{aligned} \sigma_\omega^2(t) &= \frac{1}{P_1(t)} \int \{\, A'(\tau) A_h(\tau - t) + A(\tau) A_h'(\tau - t)\, \}^2 d\tau \\ &\quad + \frac{1}{P_1^2(t)} \iint A^2(\tau_1) A^2(\tau_2) A_h^2(\tau_1 - t) A_h^2(\tau_2 - t) \big[\{\, \varphi'(\tau_1) + \varphi_h'(\tau_1 - t)\, \}^2 \\ &\qquad - \{\varphi'(\tau_1) + \varphi_h'(\tau_1 - t)\}\{\varphi'(\tau_2) + \varphi_h'(\tau_2 - t)\} \big] d\tau_1 d\tau_2\, . \end{aligned} \tag{6.13}$$

Interchanging τ_1 with τ_2 in the last integration and adding and dividing by two we have

$$\begin{aligned} \sigma_\omega^2(t) &= \frac{1}{P_1(t)} \int \{A'(\tau) A_h(\tau - t) + A(\tau) A_h'(\tau - t)\}^2\, d\tau \\ &\quad + \frac{1}{2P_1^2(t)} \iint A^2(\tau_1) A^2(\tau_2) A_h^2(\tau_1 - t) A_h^2(\tau_2 - t) \\ &\qquad \times \left[\, \varphi'(\tau_1) - \varphi'(\tau_2) + \varphi_h'(\tau_1 - t) - \varphi_h'(\tau_2 - t) \right]^2 d\tau_1\, d\tau_2\, , \end{aligned} \tag{6.14}$$

which shows that the variance for the spectrogram is manifestly positive as it should be since the spectrogram is a proper positive distribution.

An alternate expression is obtained by starting with

$$\sigma_\omega^2(t)P_1(t) = \int (\, \omega - \langle\, \omega \,\rangle_t)^2 \; |S_t(\omega)|^2 \; d\omega \,, \tag{6.15}$$

and by using the fact that for any two functions f and g

$$\int |f(x)|^2\, dx \int |g(y)|^2\, dy \;-\; \left| \int f^*(x) g(x) dx \right|^2 = \frac{1}{2} \int \int |f(x)g(y) - f(y)g(x)|^2\, dx\, dy \,, \tag{6.16}$$

one obtains that

$$\sigma_\omega^2(t) = \frac{1}{2P_1^2(t)} \iint \left| \eta_t(\tau_1) \frac{1}{j} \frac{d}{d\tau_2}\; \eta_t(\tau_2) - \eta_t(\tau_2) \frac{1}{j} \frac{d}{d\tau_1}\; \eta_t(\tau_1) \right|^2 d\tau_1 d\tau_2 \,. \tag{6.17}$$

This result can be used to obtain Eq. (6.14) straightforwardly. In addition, one may write

$$\sigma_\omega^2(t)P_1(t) = \int \eta_t^*(\tau) \left(\frac{1}{j}\frac{d}{d\tau} - \langle\, \omega \,\rangle_t \right)^2 \eta_t(\tau)\, d\tau = \int \left| \left(\frac{1}{j}\frac{d}{d\tau} - \langle\, \omega \,\rangle_t \right) \eta_t(\tau) \right|^2 d\tau \,. \tag{6.18}$$

Real Window

If the window is real then we have

$$\langle\, \omega \,\rangle_t P_1(t) = \int A^2(\tau) A_h^2(\tau - t) \; \varphi'(\tau) d\tau \,, \tag{6.19}$$

$$\langle\, \omega^2 \,\rangle_t P_1(t) = \int \{A'(\tau)\, A_h(\tau-t) + A(\tau)\, A_h'(\tau-t)\}^2 d\tau + \int A^2(\tau)\, A_h^2(\tau-t)\, \varphi'^2(\tau) d\tau \,, \tag{6.20}$$

and

$$\begin{aligned} \sigma_\omega^2(t) = & \frac{1}{P_1(t)} \int [\; A'(\tau) A_h(\tau - t) + A(\tau) A_h'(\tau - t) \;]^2 \; d\tau \\ & + \frac{1}{2P_1^2(t)} \iint A^2(\tau_1)\, A^2(\tau_2)\, A_h^2(\tau_1 - t)\, A_h^2(\tau_2 - t)\, [\, \varphi'(\tau_1) - \varphi'(\tau_2)]^2 \; d\tau_1 \, d\tau_2 \,. \end{aligned} \tag{6.21}$$

Alternate Derivation

We point out that there is an alternate method for obtaining the above results by noting that the spectrogram is a member of the general bilinear class with the kernel (the τ appearing in the following expressions bears no relation to the τ in the above equations)

$$f_{SP}(\theta,\tau) = \int h^*(u - \tfrac{1}{2}\tau)h(u + \tfrac{1}{2}\tau)\, e^{-j\theta u}\, du. \tag{6.22}$$

This kernel is not a product kernel and hence we can not use Eqs. (5.17) and (5.18) in Chapter 5.

For a general kernel the mean conditional frequency and the mean square frequency at a given time are

$$\langle\, \omega\, \rangle_t\ P_1(t) = \frac{1}{2\pi} \iint A^2(t)\,[\,g_0(\theta)\,\varphi'(u) - j g_1(\theta)\,]\ e^{j\theta(u-t)}\ d\theta\ du\ , \tag{6.23}$$

and

$$\langle\, \omega^2\, \rangle_t\ P_1(t) = \frac{1}{2\pi} \iint \Big[g_0(\theta)\, \{A^2(u)\,\varphi'^2(u) + \tfrac{1}{2}A'^2(u) - \tfrac{1}{2}A(t)A''(u)\} \\ - 2j\, g_1(\theta)\, A^2(u)\, \varphi'(u) - g_2(\theta)\, A^2(u) \Big]\ e^{j\theta(u-t)}\ d\theta\ du \tag{6.24}$$

where for convenience we have defined

$$g_0(\theta) = f(\theta,0) \quad ; \quad g_1(\theta) = \frac{\partial f(\theta,\tau)}{\partial \tau}\Big|_{\tau=0} \quad ; \quad g_2(\theta) = \frac{\partial^2 f(\theta,\tau)}{\partial \tau^2}\Big|_{\tau=0}\ . \tag{6.25}$$

Then using Eq. (6.22), we can obtain the various quantities,

$$g_0(\theta) = \int A_h^2(u)\, e^{-j\theta u}\, du\,, \tag{6.26}$$

$$g_1(\theta) = j \int A_h^2(u)\, \varphi_h'(u)\, e^{-j\theta u}\, du\,, \tag{6.27}$$

and

$$g_2(\theta) = \frac{1}{2} \int\ [\ A_h''(u)A_h(u) - A_h'^2(u) - 2A_h^2(u)\varphi_h'^2(u)\ ]\, e^{-j\theta u}\ du\,. \tag{6.28}$$

By substituting these values into Eqs. (6.24) and (6.25) one readily obtains Eqs. (6.19)–(6.21).

A further approach is to use the fact there is a close relationship between the short-time Fourier transform and the bilinear distributions. In particular, for any distribution whose kernel satisfies

$$f(-\theta,\tau)\ f(\theta,\tau) = 1. \tag{6.29}$$

the spectrogram and distribution are related by

$$P_{SP}(t,\omega) = \iint P_s(t',\omega')P_h(t'-t,\omega-\omega')dt'\,d\omega' \,. \tag{6.30}$$

This is a generalization of the relation derived by Ackroyd[1] and Altes[4] for the Rihaczek distribution, and by Mark[59] and Claasen and Mecklenbrauker[20] for the Wigner distribution. By taking conditional moments of both sides the relations given above can be alternatively derived.

Limiting Values and Comparison with Distribution Spread

We now compare this result for the short-time Fourier spectrum to Eq. (3.17) which is the inherent spread of the signal. Suppose that we narrow the window and in particular suppose $A_h^2(t)$ approaches a delta function

$$A_h^2(t) \sim \delta(t) \,. \tag{6.31}$$

In that limit we have that

$$P_1(t) = \int A^2(\tau)A_h^2(\tau-t)d\tau \sim \int A^2(\tau)\delta(\tau-t)d\tau = A^2(t) \,, \tag{6.32}$$

and from Eq. (6.19) we also then have that

$$\langle\, \omega \,\rangle_t \sim \varphi'(t) \,. \tag{6.33}$$

Now consider the spread as given by Eq. (6.21). The last term goes as

$$\begin{aligned} &\frac{1}{2P_1(t)}\iint A^2(\tau_1)A^2(\tau_2)A_h^2(\tau_1-t)A_h^2(\tau_2-t)\,[\,\varphi'(\tau_1)-\varphi'(\tau_2)]^2\,d\tau_1 d\tau_2 \\ &\quad\sim \frac{1}{2P_1(t)}\int A^2(\tau_1)A^2(\tau_2)\delta(\tau_1-t)\delta(\tau_2-t)\,[\,\varphi'(\tau_1)-\varphi'(\tau_2)]^2\,d\tau_1 d\tau_2 = 0 \,. \end{aligned} \tag{6.34}$$

The first term of the first part of Eq.(6.21)

$$\frac{1}{P_1(t)}\int A'^2(\tau)\;A_h^2(\tau-t)\,d\tau \sim \frac{1}{P_1(t)}\int \;A'^2(\tau)\delta(\tau-t)\,d\tau \;= \left(\frac{A'(t)}{A(t)}\right)^2 \tag{6.35}$$

and hence we have that the spread of the spectrogram goes as

$$\begin{aligned} \sigma_\omega^2(t) \sim \left(\frac{A'(t)}{A(t)}\right)^2 &+ \frac{2}{P_1(t)}\int A(\tau)\,A'(\tau)\,A_h(\tau-t)\,A_h'(\tau-t)\,d\tau \\ &+ \frac{1}{P_1(t)}\int A^2(\tau)\,A_h'^2(\tau-t)\,d\tau \,. \end{aligned} \tag{6.36}$$

We see that in the limit the standard deviation approaches a window independent term which is identical to that given by the bilinear distributions, Eq. (3.17), plus window dependent terms. The window dependent terms are generally infinite as we approach a delta function as is expected from the uncertainty principle. This can be seen in the following way. For a particular time, t, we can consider the Fourier transform pairs between the variables τ and ω for the signal $\eta_t(\tau) = s(\tau)h(\tau - t)$. In the limit as the window approaches a delta function the windowed signal becomes infinitely narrow as a function of τ and hence by the uncertainty principle the spreading in frequency must become large.

Non-normalizable Signals

If the signal can not be normalized, that is the signal energy is infinite, then $P_1(t)$ will not exist. However expectation values can still be calculated. The equation and calculations are the same as before except that one does not divide by $P_1(t)$.

6.2 Examples

Consider a chirp with a Gaussian envelope

$$s(t) = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\alpha t^2 + \frac{1}{2}j\beta t^2 + j\omega_0 t} \ , \tag{6.37}$$

and where we take the window to be

$$h(t) = \left(\frac{a}{\pi}\right)^{\frac{1}{4}} e^{-\frac{1}{2}at^2 + \frac{1}{2}jbt^2} \ . \tag{6.38}$$

Using the Eqs. (6.4), (6.8), (6.10) and (6.12) one readily calculates

$$P_1(t) = \sqrt{\frac{a\alpha}{\pi(\alpha + a)}} \, e^{-\frac{a\alpha}{(\alpha + a)}t^2} \ , \tag{6.39}$$

$$\langle \, \omega \, \rangle_t = \frac{a\beta - b\alpha}{\alpha + a} \, t + \omega_0 \ , \tag{6.40}$$

$$\langle \, \omega^2 \, \rangle_t = \langle \, \omega \, \rangle_t^2 + \tfrac{1}{2} \, (\alpha + a) + \tfrac{1}{2} \, \frac{(\beta + b)^2}{\alpha + a} \ , \tag{6.41}$$

$$\langle \, \sigma_\omega^2 \, \rangle_t = \tfrac{1}{2} \, (\alpha + a) + \tfrac{1}{2} \, \frac{(\beta + b)^2}{\alpha + a} \ . \tag{6.42}$$

It is interesting that the spread about the *estimated* instantaneous frequency is a constant. As the window becomes narrow, that is as $a \to \infty$ the estimate for the instantaneous frequency approaches $\beta t + \omega_0$ and the spread approaches infinity. The second term of Eq. (6.42) which comes from the second term in Eq. (6.21) goes to zero as $a \to \infty$. The first part of Eq. (6.42), which corresponds to the first term of Eq. (6.21), can be broken up into three terms as previously discussed,

$$\frac{1}{P_1(t)} \int A'^2(\tau) A_h^2(\tau - t) d\tau = \frac{\alpha^2\, a^2}{(a+\alpha)^2}\, t^2 + \tfrac{1}{2} \frac{\alpha^2}{\alpha + a} \,, \tag{6.43}$$

$$\frac{2}{P_1(t)} \int A'(\tau) A_h(\tau - t) A(\tau) A_h'(\tau - t) d\tau = -\frac{2\alpha^2\, a^2}{(a+\alpha)^2}\, t^2 + \tfrac{1}{2} \frac{\alpha a}{\alpha + a} \,, \tag{6.44}$$

$$\frac{1}{P_1(t)} \int A^2(\tau) A_h'^2(\tau - t) dt = \frac{\alpha^2\, a^2}{(a+\alpha)^2}\, t^2 + \tfrac{1}{2} \frac{a^2}{\alpha + a} \,. \tag{6.45}$$

In conformity with our previous discussion the first part of Eq. (6.43) remains finite as $a \to \infty$ and indeed approaches the inherent spreading of the signal

$$\frac{\alpha^2\, a^2}{(a+\alpha)^2}\, t^2 + \tfrac{1}{2} \frac{\alpha^2}{\alpha + a} \;\to\; \alpha^2\, t^2 = \left(\frac{A'(t)}{A(t)} \right)^2 \,. \tag{6.46}$$

The last two terms, Eq. (6.44) and Eq. (6.45) become infinite. From the view point presented here there is an inherent spread of the instantaneous frequency given by Eq. (6.46) but the spectrogram adjusts the window so that the spreading is compensated to give a constant spread about the estimate of instantaneous frequency, Eq. (6.40). If a different window were used then of course the spread would not be independent of time. None the less the first term, in the sense described above would always give the inherent spread, namely that given by Eq. (3.17).

Finally, we note that the short-time Fourier transform for this case can be done exactly. There are a number of ways to express the final answer. Particulary revealing one is

$$P_{SP}(t,\omega) = |S_t(\omega)|^2 \;=\; \frac{P_1(t)}{\sqrt{2\pi\sigma_\omega^2(t)}}\; e^{-\dfrac{(\,\omega - \langle\, \omega \,\rangle_t)^2}{2\pi\sigma_\omega^2(t)}} \,, \tag{6.47}$$

and

$$S_t(\omega) = |S_t(\omega)|\; e^{-\frac{1}{2} i\phi} \,, \tag{6.48}$$

where

$$\begin{aligned} \phi &= \arctan\left(\frac{\beta + b}{\alpha + a} \right) \\ &+ \frac{(\beta + b)\omega^2 - 2(\alpha a + \beta b + a^2 + b^2)\omega t - \left[(\alpha^2 + \beta^2) b + (a^2 + b^2)\beta \right]\, t^2}{(\beta + b)^2 + (\alpha + a)^2} \,. \end{aligned} \tag{6.49}$$

We may know ask for what value of a the standard deviation will be minimum. If we differentiate Eq. (6.42) with respect to a,

$$\frac{\partial}{\partial a}\sigma_{\omega}^{2}(t) = \tfrac{1}{2} - \tfrac{1}{2}\left(\frac{\beta+b}{\alpha+a}\right)^{2} , \tag{6.50}$$

which gives that

$$\alpha + a = \beta + b . \tag{6.51}$$

Substituting Eq. (6.51) into Eq. (6.42), we have

$$\sigma_{\omega}^{2}(t)\ _{\text{minimum}} = \alpha + a . \tag{6.52}$$

then we see that the value for a at the minimum spread is the derivative of the instantaneous frequency.

If the chirp has no amplitude modulation, that if

$$s(t) = e^{\frac{1}{2}j\beta t^{2} + j\omega_{0}t} , \tag{6.53}$$

then

$$\langle\ \omega\ \rangle_{t} = \beta t + \omega_{0} , \tag{6.54}$$

$$\langle\ \omega^{2}\ \rangle_{t} = \langle\ \omega\ \rangle_{t}^{2} + \tfrac{1}{2}a + \tfrac{1}{2}\ \frac{(\beta+b)^{2}}{a} , \tag{6.55}$$

$$\langle\ \sigma_{\omega}^{2}\ \rangle_{t} = \tfrac{1}{2}\ a + \tfrac{1}{2}\ \frac{(\beta+b)^{2}}{a} . \tag{6.56}$$

The question of optimal window was considered as early as 1947 by Barber and Ursell[9] and Storey[82]. and it is generally stated that the optimal window is of the order of the derivative of the instantaneous frequency. Using the standard deviation as a measure allows one to calculate explicitly the optimal condition for windowing for any window and set of parameters.

B. Quadratic FM Signal with a Gaussian Window

As a further example we take a signal which has a quadratic frequency dependence

$$s(t) = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\alpha t^{2} - j\frac{1}{3}\gamma t^{3}} , \tag{6.57}$$

and we take a real gaussian window

$$h(t) = \left(\frac{a}{\pi}\right)^{\frac{1}{4}} e^{-\frac{1}{2}at^{2}} . \tag{6.58}$$

Straightforward calculation yields that

$$\langle \omega \rangle_t = \frac{\gamma}{2(\alpha+a)^2}(2a^2t^2+1) \, , \tag{6.59}$$

$$\langle \omega^2 \rangle_t = \tfrac{1}{2}(\alpha+a) + \frac{\gamma^2}{4(\alpha+a)^4}(4a^4t^4+12a^2\alpha^2t^2+12a^3t^2+3\alpha^2+6\alpha+3a^2) \, , \tag{6.60}$$

$$\sigma_\omega^2 = \tfrac{1}{2}(\alpha+a) + \tfrac{1}{2}\frac{\gamma^2}{(\alpha+a)^2} + \frac{2\gamma^2a^2}{(\alpha+a)^3}t^2 \, . \tag{6.61}$$

If we have no amplitude modulation, that is if

$$s(t) = e^{j\frac{1}{3}\gamma t^3} \tag{6.62}$$

then

$$\langle \omega \rangle_t = \gamma t^2 + \frac{\gamma}{2a} \, , \tag{6.63}$$

$$\langle \omega^2 \rangle_t = \tfrac{1}{2}a + \frac{3}{4a^2} + \frac{3\gamma^2}{a}t^2 + \gamma^2t^4 \, , \tag{6.64}$$

$$\sigma_\omega^2 = \tfrac{1}{2}a + \frac{\gamma^2}{2a^2} + \frac{2\gamma^2}{a}t^2 \, . \tag{6.65}$$

C. Sinusoidal FM Signal with a Gaussian Window

As a final example we consider important case of a sinusoidal frequency dependence of the instantaneous frequency. The signal is given by

$$s(t) = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} e^{j(\omega_0 t + \beta \sin \omega_m t)} \tag{6.66}$$

and we take a gaussian window

$$h(t) = \left(\frac{a}{\pi}\right)^{\frac{1}{4}} e^{-\frac{1}{2}at^2} . \tag{6.67}$$

The relevant quantities are then,

$$\phi'(t) = \omega_0 + \beta\omega_m \cos \omega_m t \, , \tag{6.68}$$

$$\langle \omega \rangle_t = \omega_0 + \beta\omega_m \, e^{-\frac{\omega_m^2}{4(\alpha+a)}} \cos \frac{a\omega_m}{\alpha+a} t \, , \tag{6.69}$$

$$\begin{aligned}\left\langle \omega^2 \right\rangle_t =& \tfrac{1}{2}(\alpha+a) + \omega_0^2 + 2\beta\omega_m\omega_0\, e^{-\dfrac{\omega_m^2}{4(\alpha+a)}} \cos\frac{a\omega_m}{\alpha+a}\,t \\ &+ \tfrac{1}{2}\beta^2\omega_m^2 \left(e^{-\dfrac{\omega_m^2}{\alpha+a}} \cos\frac{2a\omega_m}{\alpha+a}\,t + 1 \right) ,\end{aligned} \tag{6.70}$$

$$\sigma_\omega^2 = \tfrac{1}{2}(\alpha+a) + \beta^2\omega_m^2 \left(\tfrac{1}{2}\, e^{-\dfrac{\omega_m^2}{\alpha+a}} \cos\frac{2a\omega_m}{\alpha+a}\,t - e^{-\dfrac{\omega_m^2}{2(\alpha+a)}} \cos^2\frac{a\omega_m}{\alpha+a}\,t \right) . \tag{6.71}$$

It has been known for a long time that almost any window will give unsatisfactory results for the sinusoidal time dependence and we see that the fundamental reason for that is that the standard deviation has a very complicated and oscillatory form and hence any fixed window will give poor results.

Chapter 7

MULTICOMPONENT SIGNALS

The analysis of multicomponent signals have been the main stumbling block in the use of these distributions for the analysis of realistic signals. Our main aim here is to consider the fundamental question of what is a multicomponent signal and to show that the analysis of the previous chapter can help in clarifying the definition of the multicomponent signal. We will give some examples and briefly review the difficulty which they present in their analysis. The sum of two pure tones is a multicomponent signal consisting of two unique parts. When a radar signal is sent out and is reflected form different surfaces, the signal at the receiver may be a multicomponent signal. In the quantum mechanical context, which we will discuss in detail in a different section, the incoming, transmitted and reflected wave functions generally form a multicomponent signal. It is clear that a multicomponent signal is not just a signal which can be expressed as the sum of multiple parts. For example if we subtract a function from a sine wave, and then add the function, clearly then we would not have a multicomponent signal. Generally speaking a signal is a multicomponent signal when each individual part has its identity and uniqueness. Also we will show that if a class of distributions yields a certain expectation value, then the cross terms of the different distributions within that class contribute the identical value towards expectation values. Hence, even though the cross terms may be reduced, they none the less contribute an identical amount towards an expectation value. Before proceeding it may be worthwhile to explicitly illustrate the difficulty which multicomponent signals.

The simplest example is the sum of two sine waves

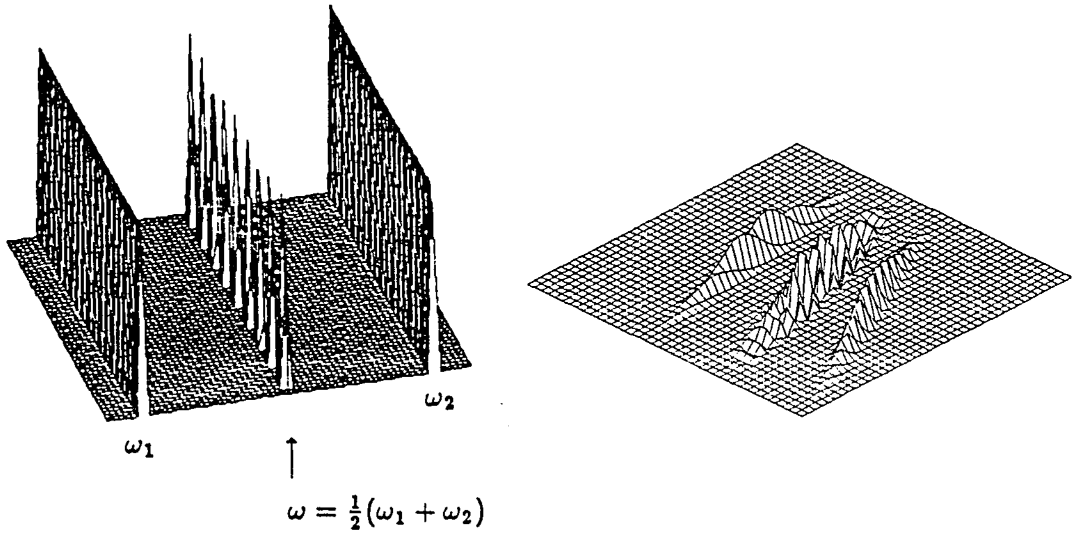
$$s(t) = A_1 e^{j\omega_1 t} + A_2 e^{j\omega_2 t}\,. \tag{7.1}$$

then the Wigner distribution is

$$W(t,\omega) = A_1^2\delta(\omega-\omega_1) + A_2^2\delta(\omega-\omega_2) + 2A_1A_2\delta\{\omega - \tfrac{1}{2}(\omega_1+\omega_2)\}\cos(\omega_2-\omega_1)\,t\,. \tag{7.2}$$

This is illustrated in Figure 3. We see that, besides the two expected self terms there seemingly is energy in places where no energy is expected that is at $\omega = \frac{1}{2}(\omega_1+\omega_2)$. When the frequencies are near each other, the separation is difficult. Another example is the sum of two chirps

$$s(t) = A_1\left(\frac{\alpha_1}{\pi}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\alpha_1 t^2 + \frac{1}{2}j\beta_1 t^2 + j\omega_1 t} + A_2\left(\frac{\alpha_2}{\pi}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\alpha_2 t^2 + \frac{1}{2}j\beta_2 t^2 + j\omega_2 t}\,, \tag{7.3}$$



Figures 3 and 4. The Wigner distributions. Figure 3 is the Wigner distribution for the sum of two sine waves $s(t) = e^{jt} + e^{9jt}$. Note that it is peaked to infinity at the frequencies ω_1, ω_2 and at the spurious value of $\omega = \frac{1}{2}(\omega_1 + \omega_2)$. The delta functions at ω_1 and ω_2 are symbolically represented and are cur off at the value of 700. In figure 4, the Wigner distribution has artifacts and spurious values in between the two concentrations along the instantaneous frequencies of the chirps.

and the Wigner distribution is illustrated in Figure 4.

As the Winger distribution has been the most widely used and studied distribution and always displays these artifacts or spurious values it has been generally felt that other distributions would be even worse in this respect.

If we consider the sum of two signals

$$s(t) = s_1(t) + s_2(t) \ , \tag{7.4}$$

then the distribution is

$$P(t,\omega) = P_{11}(t,\omega) + P_{22}(t,\omega) + P_{12}(t,\omega) + P_{21}(t,\omega) \ , \tag{7.5}$$

where

$$P_{kl}(t,\omega) \ = \ \frac{1}{4\pi^2} \iiint \ e^{-j\theta t - j\tau\omega + j\theta u} \ f(\theta,\tau) s_k^*(u - \tfrac{1}{2}\tau) \ s_l(u + \tfrac{1}{2}\tau) \ du \ d\tau \ d\theta \ . \tag{7.6}$$

The last two terms in Eq. (7.5), the "cross terms", are the terms which *sometimes* place energy in the time-frequency plane where it would not be expected. However, the cross terms are essential although there have been many attempts to "eliminate" them. As Choi and Williams[19] have pointed out, one can not have the desirable properties of a distribution without the cross terms, but they realized is that one can minimize the undesirable effects of the cross terms and still keep the essential contributions that they make. This may seem contradictory but we illustrate this from the point of view of expectation values. For the sum of two signals or equivalently a signal broken up into two parts, whether they are components or not in the sense of the previous section, the expectation value of a function is the sum of the expectation value with the distribution of each part plus the expectation values with the cross term distribution,

$$\langle\, g \,\rangle_{1+2}^{A} \;=\; \langle\, g \,\rangle_{1}^{A} + \langle\, g \,\rangle_{2}^{A} + \langle\, g \,\rangle_{1,2}^{A} \;, \tag{7.7}$$

where A denotes that we are using distribution A with kernel f_A. If we have another distribution, B, with kernel f_B then also

$$\langle\, g \,\rangle_{1+2}^{B} \;=\; \langle\, g \,\rangle_{1}^{B} + \langle\, g \,\rangle_{2}^{B} + \langle\, g \,\rangle_{1,2}^{B} \;. \tag{7.8}$$

Now suppose that both kernels have the property that they predict the correct value for the expectation value then

$$\langle\, g \,\rangle_{1+2}^{A} \;=\; \langle\, g \,\rangle_{1+2}^{B} \;. \tag{7.9}$$

For example if we chose kernels whose first derivative with respect to τ at $\tau = 0$ is zero, then all distributions having such a kernel will predict the same value for the instantaneous frequency. Similarly the identical value will be predicted for the auto terms,

$$\langle\, g \,\rangle_{1}^{A} \;=\; \langle\, g \,\rangle_{1}^{B} \qquad ; \qquad \langle\, g \,\rangle_{2}^{A} \;=\; \langle\, g \,\rangle_{2}^{B} \;. \tag{7.10}$$

Hence the contributions of the cross terms are also the same

$$\langle\, g \,\rangle_{1,2}^{A} \;=\; \langle\, g \,\rangle_{1,2}^{B} \;. \tag{7.11}$$

What this shows is that the contributions of the cross terms toward the expectation value is identical and hence can not be diminished. For example, both the Wigner and the Choi-Williams distribution predict correct averages for frequency and the contributions of the cross terms of each are identical toward that average. However, as we shall see, the cross terms of the Choi-Williams distribution are minuscule in comparison to the Wigner distribution. That is because there is considerable freedom in choosing kernels even though they may be constrained to yield the desirable properties.

Choi-Williams Type Distributions

Choi and Williams[19] gave a general criteria for choosing kernels which minimize the cross terms and greatly enhances the interpretive ability of the bilinear distributions. We briefly summarize their approach. They define a time dependent correlation function

$$R_t(\tau) = \frac{1}{2\pi} \iint e^{j\theta(u-t)} \, f(\theta,\tau) s^*(u - \tfrac{1}{2}\tau) \; s(u + \tfrac{1}{2}\tau) \; d\theta \; du \; , \tag{7.12}$$

in which case the distribution is given by

$$P(t,\omega) = \frac{1}{2\pi} \int R_t(\tau) \, e^{-j\omega\tau} d\tau \; . \tag{7.13}$$

Choi and Williams realized that it can be used to understand how the properties of the kernel relate to the properties of the distributions. They argue that the kernel must be of such a form that the result of the inner integration should be peaked when t is near u. This emphasizes the values of the signal near the point of interest. To suppress the cross terms they argue from the structure of the generalized ambiguity function[66]

$$M(\theta,\tau) = f(\theta,\tau) \int s^*(u - \tfrac{1}{2}\tau) \;\; e^{j\theta u} \;\; s(u + \tfrac{1}{2}\tau) \; du \; , \tag{7.14}$$

that the kernel should be relatively large when θ and τ are small and small otherwise. We shall call such kernels Choi-Williams type kernels or distributions. In particular, they found that the distribution with kernel,

$$f(\theta,\tau) = e^{-\theta^2\tau^2/\sigma} \; , \tag{7.15}$$

gives excellent results for a wide variety of cases.

To get an idea of these effects we consider the simple case of the sum of two pure tones given by Eq. (7.1). We assume that the kernels satisfy the marginal requirements and also take

$$f(\theta,\tau) = f^*(-\theta,-\tau) \; , \tag{7.16}$$

which assures that the distributions are real. In that case, the self terms are independent of the kernel †† and we have that

$$P(t,\omega) = A_1^2 \, \delta(\omega - \omega_1) + A_2^2 \, \delta(\omega - \omega_2) + \left[A_1 A_2 \, e^{-j(\omega_1-\omega_2)t} \; K(\omega) + c.c.\right] \; , \tag{7.17}$$

---

†† In general the auto terms are not independent of the kernel. One of the effects of suppressing the cross terms by choosing Choi-Williams type kernels is that the auto terms may be broadened out somewhat.

where

$$K(\omega) = \frac{1}{2\pi} \int f(\omega_1 - \omega_2, \tau)\, e^{-j\tau(\omega - \bar{\omega}_{12})}\, d\tau \ , \tag{7.18}$$

and

$$\bar{\omega}_{12} = \tfrac{1}{2}(\omega_1 + \omega_2) \ . \tag{7.19}$$

For the case of real product kernels which are even functions

$$P(t,\omega) = A_1^2\, \delta(\omega - \omega_1) + A_2^2\, \delta(\omega - \omega_2) + 2A_1A_2 \cos(\omega_1 - \omega_2)t\ K(y) \ , \tag{7.20}$$

with

$$K(y) = \frac{1}{|\omega_2 - \omega_1|}\ \frac{1}{2\pi} \int f(x)\, e^{-jxy}\, dx \quad ; \quad y = \frac{\omega - \bar{\omega}_{12}}{|\omega_1 - \omega_2|} \ . \tag{7.21}$$

We calculated the $K(\omega)$ for a number of different kernels and summarize the results in Table III. In Figure 5, the cross terms, without the time dependence term, $K(\omega)$ are plotted for various values of the parameter. Our purpose in doing so is to illustrate the rich variety of possibilities opened up by the work of Choi and Williams and to confirm the general conditions on the kernels as formulated by them.

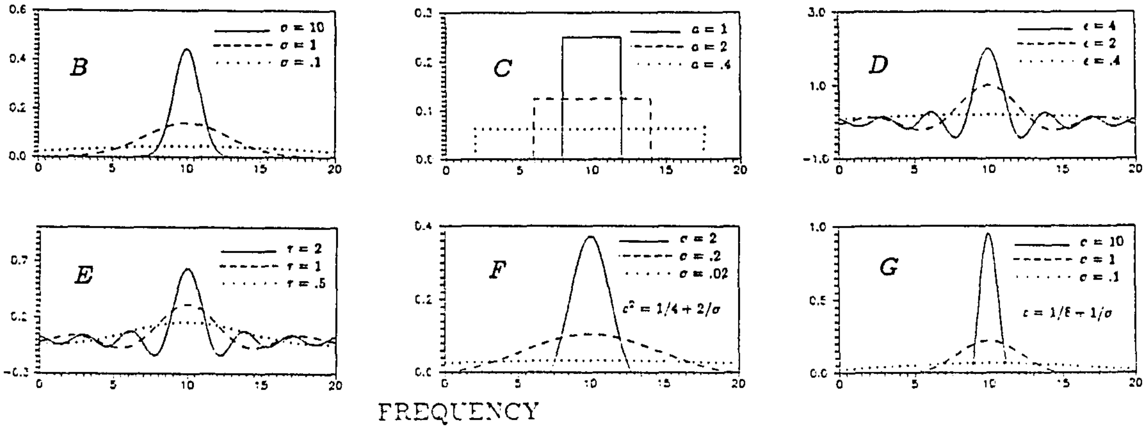


Figure 5. The crossterm (without the oscillatory time dependence), for the signal given by Eq. (7.16) where $\omega_1 = 9$ and $\omega_2 = 11$. Each case represents a different kernel as discussed in the text. A general approach of the behavior of the crossterms has been given by Choi and Williams. These examples illustrate their formulation.

Case A. The choice of $f = 1$ gives an infinite value for the cross term and does not meet the Choi-Williams criteria that it should be peaked for small values of θ and τ. That is why the Wigner distribution behaves poorly in regard to the cross terms.

Case B. This is the exponential kernel studied in detail by Choi and Williams. If we take σ to be large then the kernel becomes flat and the cross terms are peaked. On the other hand when σ is small the kernel is peaked at zero and the cross terms spread out.

Case C. The sinc kernel was derived in Reference 23 and has some interesting properties. The cross terms spread out uniformly between the limits as indicated. Again, if a is taken to be small the kernel is relatively flat and a high value for the cross terms is obtained.

Case D and E. These kernels have sharp cutoffs. By controlling the cutoffs very different affects are achieved. However we point out that in general these two kernels do not satisfy some of the other desirable properties.

Case F and G. These two kernels are variations of case B with an additional parameters. We include these cases to show that similar results to *Case D* can be obtained with the advantage that we have an additional free parameter. In particular by choosing the parameters appropriately we can obtain kernel which have the Choi-Williams properties and satisfy $f''(0) = 1/4$. For *Case F* that is achieved by taking $c^2 = 2/\sigma + 1/4$ and for case G one takes $c = 1/\sigma + 1/8$.

Criteria for Multicomponent Signal

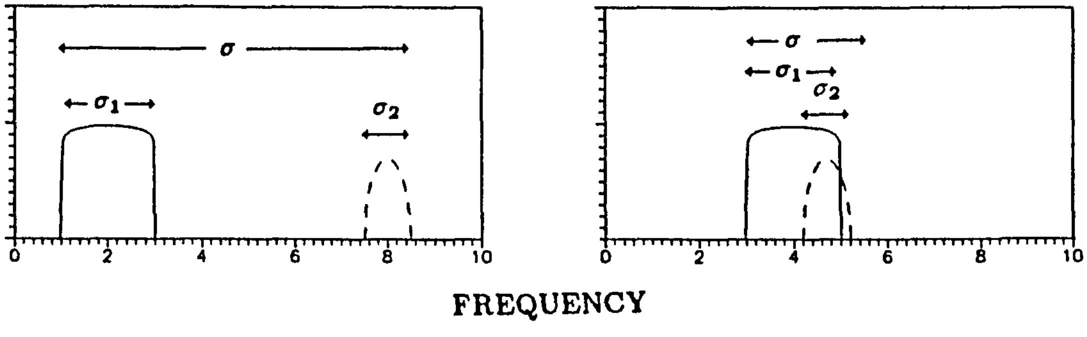
The question of what is a "component" in a multicomponent signal is not fully understood, however it is clear that certain decompositions of a signal often have physical meaning in that each part behaves more or less as a group or unit. Any signal can be broken down in an infinite number of non-unique ways. We emphasize the fact that a signal, written as a sum of two or more signals or parts, does not make it a multicomponent signal. It is the nature of the parts in relation to themselves and the signal which determines whether the decomposition is of physical interest. Is it possible to define a criteria as to when a break up of a signal is of such a nature that we can sensibly speak of a multicomponent signal? First we argue that the breaking up of a signal into meaningful components is a local phenomenon, as the break up may be meaningful for some times but not for others. Secondly we will argue that the criteria for a meaningful break up is whether the conditional distribution is localized into compact parts at that time. A simple

Table III. $K(\omega)$ for a variety of kernels for the case of the sum of two pure tones. $[\,\bar{\omega}_{12} = \frac{1}{2}(\omega_1 + \omega_2)\,]$

Case	Kernel $f(\theta, \tau)$	$K(\omega)$
A	1	$\delta(\omega - \bar{\omega}_{12})$
B	$e^{-\theta^2\tau^2/\sigma}$	$\dfrac{\sqrt{\sigma/4\pi}}{\lvert\omega_1 - \omega_2\rvert} \exp\left\{ -\dfrac{\sigma}{4} \left(\dfrac{\omega - \bar{\omega}_{12}}{\omega_2 - \omega_1} \right)^2 \right\}$
C	$\dfrac{\sin a\theta\tau}{a\theta\tau}$	$\dfrac{1}{2a} \dfrac{1}{\lvert\omega_1 - \omega_2\rvert}$ if $\omega_{12} - a\lvert\omega_1 - \omega_2\rvert \le \omega \le \omega_{12} + a\lvert\omega_1 - \omega_2\rvert$
D	1 if $\lvert\theta\tau\rvert \le \epsilon$; 0 otherwise.	$\dfrac{1}{\omega - \bar{\omega}_{12}} \sin\left(\dfrac{\omega - \bar{\omega}_{12}}{\lvert\omega_1 - \omega_2\rvert} \epsilon \right)$
E	1 if $\lvert\theta\rvert \le \theta_1$ and $\lvert\tau\rvert \le \tau_1$; 0 otherwise.	$\dfrac{1}{\pi} \dfrac{\sin(\omega - \bar{\omega}_{12})\tau_1}{\omega - \bar{\omega}_{12}}$ if $\lvert\omega_1 - \omega_2\rvert \le \theta_1$
F	$\cosh(c\theta\tau)\; e^{-\theta^2\tau^2/\sigma}$	$\dfrac{\sqrt{\sigma/4\pi}}{\lvert\omega_1 - \omega_2\rvert} \cos\left\{ \tfrac{1}{2}c\sigma \left(\dfrac{\omega - \bar{\omega}_{12}}{\omega_2 - \omega_1} \right) \right\} \exp\left\{ -\dfrac{\sigma}{4} \left(\dfrac{\omega - \bar{\omega}_{12}}{\omega_2 - \omega_1} \right)^2 + \tfrac{1}{4}c^2\sigma \right\}$
G	$(1 + c\theta^2\tau^2)e^{-\theta^2\tau^2/\sigma}$	$\dfrac{\sqrt{\sigma/4\pi}}{\lvert\omega_1 - \omega_2\rvert} \left[1 + \tfrac{1}{2}c\sigma - \tfrac{1}{4}c\sigma^2 \left(\dfrac{\omega - \bar{\omega}_{12}}{\lvert\omega_2 - \omega_1\rvert} \right)^2 \right] \exp\left\{ -\dfrac{\sigma}{4} \left(\dfrac{\omega - \bar{\omega}_{12}}{\omega_2 - \omega_1} \right)^2 \right\}$

measure of that is the spread of frequencies of each part as compared to the spread of the whole signal. Furthermore for reasons already discussed we argue that the spread as previously defined by Eq. (5.25) is a good measure for the localization.

To illustrate these points suppose we have, at a particular time, t_1, a break up of the signal into two parts and for that time the distribution of frequency (if we had a sensible one) is as in Figure 6. We have indicated the spread of each by σ_1 and σ_2 and the spread of the signal by $\sigma(t_1)$. Now we emphasize that the spreads are taken with respect to the instantaneous frequency of each component which we assume is somewhere near the middle of the spreads. Clearly for time t_1 we have a signal made up of two parts. Why? because the spreads of each about its own instantaneous frequency is well separated with respect to themselves and the whole signal. Now suppose that at a later time the shape of each part is more or less the same but the instantaneous frequencies have become closer as in Figure 7. Then we would certainly not say that we have two components because the spreads are not well separated in comparison to the spread of the whole signal. Hence the separation of a signal into components is a local phenomenon. Of course a particular separation may last for all time or for a time interval, and the way we would know that is by examining the average local spread. Therefore, generally speaking we can say that a signal is multicomponent at a given time if the local spread of frequencies of each component are well separated and small in relationship to the local spread for the whole signal. Furthermore we can say that a signal is a multicomponent signal in an interval of time (possibly infinity) if the average spreads in the interval as defined by Eq. (5.32) are well separated.



Figures 6 and 7. An idealized example illustrating the relation of spread to the concept of multicomponent signals.

Chapter 8

QUANTUM MECHANICAL CURRENT AND ITS STANDARD DEVIATION

In this chapter we consider quantum mechanical current or local momentum and its standard deviation. We show that the standard deviation can be defined via the quasi-probability distributions. Furthermore we will derive the corresponding quantities using the concept of a "quantum mechanical spectrogram" which is a way of localizing or windowing (or weighing) the wave function around a given point in space. We show that, as the window narrows around the point of interest, the limiting value of the standard deviation goes to infinity in a special way, namely, as an infinite window dependent part plus a window independent part, which is identical to the standard deviation obtained by way of the bilinear distributions. All the results of the previous chapter can be translated mathematically into quantum mechanics language, however the quantum situation presents its own unique language and hence we will make this chapter self-contained even though there is a one to one correspondence between quantum mechanics and signal analysis.

First let us discuss the quantum mechanical current in usual way.

Using Schrödinger equation for the one dimensional case, one derives the equation of continuity

$$\frac{\partial}{\partial t}|\psi(q,t)|^2 = -\frac{\hbar}{2mi}\frac{\partial}{\partial q}\left(\psi^*(q,t)\frac{\partial\psi(q,t)}{\partial q} - \psi(q,t)\frac{\partial\psi^*(q,t)}{\partial q}\right) \tag{8.1}$$

and by analogy with the classical case one defines the current

$$j(q,t) = \frac{\hbar}{2mi}\left(\psi^*(q,t)\frac{\partial\psi(q,t)}{\partial q} - \psi(q,t)\frac{\partial\psi^*(q,t)}{\partial q}\right) . \tag{8.2}$$

If the wave function is written in the form

$$\psi(q,t) = R(q,t)\; e^{iS(q,t)/\hbar} , \tag{8.3}$$

where R and S are real functions of position and time, then the current becomes

$$j(q,t) = \frac{1}{m}\,\frac{\partial S(q,t)}{\partial q} . \tag{8.4}$$

We note that current as defined by Eq. (8.4) is a local quantity since it depends on position. Hence when we speak of current we mean current at a particular point in space. However current is basically a velocity and hence it is certainly against the usual formulation of quantum mechanics to speak of velocity at a point. Perhaps current is the only local quantity which appears in textbooks and is not in keeping with the usual interpretation of quantum mechanics. In addition we point out that no operator is associated with current and hence its observable status is at least unusual. A second point to be made is that in the Bohm theory the derivative of the phase is taken literally as the velocity of the particle. In addition we point out that current possesses the following interesting property. Consider the global average of current defined by

$$\langle j \rangle = \int j(q)|\psi(q)|^2 \, dq \,. \tag{8.5}$$

It is easy to show that this global average is the average velocity calculated by the usual quantum rules. Working with momentum, we have

$$\begin{aligned} \langle \, p \, \rangle &= \int p \, |\phi(p)|^2 \, dp = \int \psi^*(q) \left(\frac{\hbar}{i} \frac{\partial}{\partial q} \right) \psi(q) \, dq \\ &= \int R(q) \{ \, -iR'(q) + R(q) \, S'(q) \, \} \, dq = \int mj(q) \, R^2(q) \, dq \\ &= m \, \langle \, j \, \rangle \, . \end{aligned} \tag{8.6}$$

where the prime denotes differentiation with respect to the argument.

The above arguments certainly indicate that the quantity defined by Eq. (8.4) is acting as a local velocity or current per unit mass. It is therefore natural to ask what is the *local* standard deviation of that velocity or current. That is what is the spread in velocity at a given position?

Before addressing this issue we note that the range of usually defined momentum is very different from the range in current even though their expectation values are the same. This is the same as the case of instantaneous frequency as defined in the previous chapter. For example, if we have the wave function

$$\psi(q) = R_1 \, e^{ik_1 q/\hbar} + R_2 \, e^{ik_2 q/\hbar} = R(q) \, e^{iS(q)/\hbar} \, . \tag{8.7}$$

in which case the only measurable values of momenta are k_1 and k_2.

Solving for the amplitude and phase of $\psi(q)$ we have that

$$R^2(q) = R_1^2 + R_2^2 + 2R_1 R_2 \cos\left[(k_2 - k_1)q/\hbar\right] \, , \tag{8.8}$$

and

$$\tan\left[S(q)/\hbar\right] = \frac{R_1 \sin(k_1 q/\hbar) + R_2 \sin(k_2 q/\hbar)}{R_1 \cos(k_1 q/\hbar) + R_2 \cos(k_2 q/\hbar)} \,. \tag{8.9}$$

Now the current may be obtained by using Eq. (8.4),

$$j(q) = \frac{R_1^2 k_1 + R_2^2 k_2 + R_1 R_2 (k_1 + k_2) \cos\left[(k_2 - k_1) q/\hbar\right]}{A^2(q)} \,. \tag{8.10}$$

First we note that the current may take on a continuous range even though according to the standard interpretation of momentum only two values can be measured. Secondly the range of the current can be almost anything and depends upon the values chosen for the A's. None the less both

quantities give the same global expectation values. However as we shall see they do not give the same value for the higher moments.

Local Momentum via Quasi-Distributions

Suppose we have a joint distribution of position and momentum. Then the local momentum would be the conditional expectation value of momentum for a given position,

$$\langle\, p \,\rangle_q = \frac{1}{P_1(q)} \int p \; P(q,p) \; dp \,, \tag{8.11}$$

where $P_1(q)$ is the distribution of position

$$P_1(q) = \int P(q,p)\, dp \,. \tag{8.12}$$

If the marginals are satisfied then we would have that

$$P_1(q) = |\psi(q)|^2 \,. \tag{8.13}$$

If we use the Wigner distribution for $P(q,p)$, a straightforward calculation yields a very satisfying result,

$$\langle\, p \,\rangle_q = S'(q) \; = m j(q) \,. \tag{8.14}$$

Therefore we see that the local momentum as defined by way of Wigner distribution gives the standard quantum mechanical current. However let us now calculate its standard deviation. For $\langle p^2 \rangle_q$, we obtain, using the Wigner distribution

$$\langle p^2 \rangle_q = \tfrac{1}{2}\left(\frac{R'(q)}{R(q)}\right)^2 - \tfrac{1}{2}\frac{R''(q)}{R(q)} + m^2 j^2(q) , \tag{8.15}$$

and the spread is therefore

$$\sigma_p^2(q) = \tfrac{1}{2}\left(\frac{R'(q)}{R(q)}\right)^2 - \tfrac{1}{2}\frac{R''(q)}{R(q)} . \tag{8.16}$$

However both of these quantities are in general negative and can not be interpreted.

Now consider the expectation value of momentum with other distributions. If the general class of distribution, Eq. (2.4) is put into Eq. (8.11) we have that

$$\langle p \rangle_q \, P_1(q) = f(0)\, R^2(q)\, mj(q) + 2f'(0)\, R(q)\, R'(q) . \tag{8.17}$$

As long as we constrain the kernel by

$$f(0) = 1 , \qquad ; \qquad f'(0) = 0 , \tag{8.18}$$

we will have that the conditional expected value is given by Eq. (8.14) as with the Wigner distribution.

We now calculate $\langle p^2 \rangle_q$. The derivation is identical to the one given in the previous chapter and we just quote the result;

$$\begin{aligned}\langle p^2 \rangle_q \, P_1(q) = {} & \tfrac{1}{2}\left[f(0) + 4f''(0)\right] R'^2(q) - \tfrac{1}{2}\left[f(0) - 4f''(0)\right] R(q)\, R''(q) \\ & + f(0)\, R^2(q)\, m^2 j^2(q) + 2f'(0) m \left[2R(q)\, R'(q)\, j(q) + R^2(q)\, j'(q)\right] .\end{aligned} \tag{8.19}$$

Now if we impose the conditions given by Eq. (8.18) we have that

$$\langle p^2 \rangle_q = \tfrac{1}{2}\left[1 + 4f''(0)\right]\left(\frac{R'(q)}{R(q)}\right)^2 - \tfrac{1}{2}\left[1 - 4f''(0)\right]\frac{R''(q)}{R(q)} + m^2 j^2(q) , \tag{8.20}$$

The standard deviation is obtained in the usual way

$$\sigma_p^2(q) = \int (\, p - \langle p \rangle_q \,)^2 \, P(q,p)\, dp = \langle p^2 \rangle_q - \langle p \rangle_q^2 , \tag{8.21}$$

and hence

$$\sigma_p^2(q) = \tfrac{1}{2}\left[1 + 4f''(0)\right]\left(\frac{R'(q)}{R(q)}\right)^2 - \tfrac{1}{2}\left[1 - 4f''(0)\right]\frac{R''(q)}{R(q)} . \tag{8.22}$$

In general these expressions for $\left\langle p^2 \right\rangle_q$ and the standard deviation $\sigma_p^2(q)$ are not manifestly positive. However let us ask if there are any distributions for which they are manifestly positive for *any* wave function. If we take

$$f''(0) = \frac{1}{4}\,, \tag{8.23}$$

then the spread becomes

$$\sigma_p^2(q) = \left(\frac{R'(q)}{R(q)} \right)^2 \,, \tag{8.24}$$

which is always positive. In addition, the conditional second moment is then also manifestly positive

$$\langle\, p^2 \,\rangle_q = \left(\frac{R'(q)}{R(q)} \right)^2 + m^2 j^2(q)\;. \tag{8.25}$$

Relation between Global Spreads in Momentum and Current and Local Momentum

In the last chapter we discussed theorem due to Fink[37] and Mandel[55] which applied for the signal analysis case. We will derive an equivalent result for the quantum case which connects the spread in momentum and the spread in current. Furthermore we will show that the local spread as defined by Eq. (8.17) enters into these relations in a fundamental way.

We first clarify the terminology which we are going to use. As we have seen both the current and first conditional moment of the joint distribution give the same answer. By the global standard deviation of the current we shall mean the standard deviation calculated using the wave function, that is

$$\sigma_j^2 = \int \big(j(q) - \langle j(q)\rangle\big)^2 |\psi(q)|^2 \, dq\,. \tag{8.26}$$

By the standard deviation (*local*) of the local momentum we shall mean the expression derived by way of the joint distributions, namely by Eq. (8.12) and by its global average we shall mean,

$$\left\langle \left(\frac{R'(q)}{R(q)} \right)^2 \right\rangle = \int \left(\frac{R'(q)}{R(q)} \right)^2 |\psi(q)|^2 dq = \int R^2(q) dq\,. \tag{8.27}$$

By momentum we shall continue to mean what is usually understood in quantum mechanics.

We now calculate the expected value of the square of momentum and relate it to the expected value of the square of current.

$$\langle p^2\rangle = \int p^2\ |\phi(p)|^2\ dp \tag{8.28}$$

$$= \int \psi^*(q)\Big(\frac{\hbar}{i}\frac{\partial}{\partial q}\Big)^2 \psi(q)\ dq \tag{8.29}$$

$$= \int \ \left|\Big(\frac{1}{i}\frac{\partial}{\partial q}\Big)\psi(q)\right|^2 \ \delta q \tag{8.30}$$

$$= \int \left|\frac{1}{i}\frac{R'(q)}{R(q)} + mj(q)\right|^2 R^2(q)\ dq \tag{8.31}$$

$$= \int \left[\ \left(\frac{R'(q)}{R(q)}\right)^2 + m^2 j^2(q)\right] R^2(q)\ dq \tag{8.32}$$

$$= \int \ \left(\frac{R'(q)}{R(q)}\right)^2 R^2(q)\ dq\ +\ \int m^2 j^2(q) R^2(q)\ dq\ . \tag{8.33}$$

Hence we have that

$$\langle\, p^2\,\rangle = m^2\ \langle\, j^2\,\rangle + \left\langle\ \frac{R'(q)}{R(q)}\Big)^2\ \right\rangle . \tag{8.34}$$

Now the spread can be calculated in the usual way. By noting that the relation between $\langle\, p\,\rangle$ and $\langle\, j\,\rangle$ in

Eq. (8.6), we have that

$$\sigma_p^2 = m^2\ \sigma_j^2 + \left\langle\ \frac{R'(q)}{R(q)}\Big)^2\ \right\rangle . \tag{8.35}$$

It is of some interest to obtain Eq. (8.31) directly as we previously have done for the signal analysis case. Consider

$$\sigma_p^2 = \ \int (p - \langle\, p\,\rangle)^2\ |\phi(p)|^2\ dp \tag{8.36}$$

$$= \int \psi^*(q)\Big(\frac{\hbar}{i}\frac{\partial}{\partial q} - \langle\, p\,\rangle\Big)^2 \psi(q)\ dq \tag{8.37}$$

$$= \int \ \left|\Big(\frac{\hbar}{i}\frac{\partial}{\partial q} - \langle\, p\,\rangle\Big)\psi(q)\ \right|^2 \ dq \tag{8.38}$$

$$= \int \left|\frac{1}{i}\frac{R'(q)}{R(q)} + mj(q) - \langle\, p\,\rangle\right|^2 R^2(q)\ dq \tag{8.39}$$

$$= \int \left[\ \left(\frac{R'(q)}{R(q)}\right)^2 + \Big(mj(q) - \langle\, p\,\rangle\Big)^2\right] R^2(q)\ dq \tag{8.40}$$

$$= \int \ \left(\frac{R'(q)}{R(q)}\right)^2 R^2(q)\ dq\ + \int \Big(mj(q) - \langle\, p\,\rangle\Big)^2 R^2(q)\ dq\ . \tag{8.41}$$

which is Eq. (8.35).

Eq. (8.35) is an interesting relation between the spreads of momentum and current. It shows that momentum and current are not the same quantity even though Eq. (8.6) would indicate that perhaps they are. This is the same as for the signal analysis case which pointed out by Mandel[55]. We should point out that in general the global spread of momentum is not the integral of the local spread, that is

$$\int \sigma_p^2(q)\,|\psi(q)|^2\,dq \neq \sigma_p^2\,. \tag{8.42}$$

However we emphasize that it is not unique to quantum mechanical but also true for any situation described by a joint probability.

Quantum Mechanical Spectrogram

We now consider a method for measuring and defining local momentum in quantum mechanics. We will approach this subject in analogy to the spectrogram in signal analysis, although all variables in the two fields have different meaning. As we will see the resulting approach is related to the work of Kuryskin[49,50,51] and coworkers.

The fundamental idea of the spectrogram or short time Fourier transform is to consider the signal near the time of interest and to use it as a means of *estimating* the quantities of interest. We define the quantum mechanical spectrogram in the same fashion, except we consider a region of space about the point of interest, instead of the region of time in the signal analysis case. In particular, suppose we have a wave function and we want to *estimate* the momentum, or anything else, in a region in space, say, at point q_1. An operational approach is to consider only a small region of space around that point, renormalize the wave function, and to calculate its momentum distribution. As we make the region of space smaller we will get a finer and finer estimate of the local quantities. Now, instead of taking a part of the wave function in a finite region and of neglecting the rest, we could taper the wave function. One would hope that the method of tapering or surrounding the point will not influence the answer in the limit. We will see that it is the case in some sense. Now how do we actually localize the wave function near a point? The way to do it is to multiply the wave function with another wave function which peaks at the point of interest. In analogy with signal analysis we shall call such functions window wave functions. That is, we consider a new wave function made up of the following way

$$\eta_{q_1}(q) = N(q_1)\ \psi(q)\ W(q - q_1)\ , \tag{8.43}$$

where $\psi(q)$ is the wave function of interest and $W(q)$ is the window functions and N is a normalizing factor. It will be convenient to write the window function in terms of its amplitude and phase

$$W(q) = R_W(q)\, e^{iS_W(q)/\hbar}\ . \tag{8.44}$$

The normalizing factor is

$$N^{-2}(q_1) = \int |\psi(q)\ W(q - q_1)|^2\ dq = \int R^2(q)\ R_W^2(q - q_1)\ dq\,, \tag{8.45}$$

and is a function of q_1.

To simplify the notation we now will call q_1 which is an arbitrary point q and in the integrations we will integrate over x. That is q will be the point in space we are interested in and x will be the running position variable. For convenience we rewrite some of the above equation in terms of q and x,

$$\eta_q(x) = N(q)\ \psi(x)\ W(x - q)\ , \tag{8.46}$$

and

$$N^2(q) = \frac{1}{\int |\psi(x)\ W(x - q)|^2\, dx} = \frac{1}{\int R^2(x)\ R_W^2(x - q)\, dx}\,. \tag{8.47}$$

The corresponding momentum wave function $\varsigma_q(p)$ to $\eta_q(x)$ is

$$\varsigma_q(p) = \frac{1}{\sqrt{2\pi\hbar}} \int e^{-ipx/\hbar} \eta_q(x) dx = \frac{N(q)}{\sqrt{2\pi\hbar}} \int e^{-ipx/\hbar} \psi(x) W(x - q) dx\ , \tag{8.48}$$

and the distribution of momentum at point q is then

$$P(q,p) = |\varsigma_q(p)|^2\,. \tag{8.49}$$

This can then be interpreted as the joint distribution of position and momentum, however it does not satisfy the marginals.

Two Digressions

1. Kuryshkin-Zaparovanny Development We digress momentarily to mention the above type of functions have been introduced by Kuryshkin, Zaparovanny and Lyabis[51] and they have studied these functions and their consequences in great detail. They have developed quantum mechanics in terms of these probability distributions. Their attempt is to develop a sub-quantum description of quantum mechanics, that is a hidden variable theory of quantum mechanics. In their formulation, $W(q)$ is called the auxiliary function. Our viewpoint here is, in analogy to the signal analysis, to use them as devices to estimate the expectation values in a given region.

2. Relation with Wigner Distribution We digress further to mention the relation of the spectrogram with the Wigner distribution and other distributions. Ackroyd[1] pointed out that the spectrogram can be written using the Margenau-Hill distribution,

$$|\varsigma_q(p)|^2 = \iint e_s(q',p')e_h(q'-q,p-p')\,dq'\,dp'\,, \tag{8.50}$$

where $e_s(q,p)$ and $e_h(q,p)$ are the Margenau-Hill distributions of the signal and window functions respectively. The spectrogram can be thought of as the time-frequency distribution of the signal smoothed with the time-frequency distribution of the window. Mark[59] and Claasen and Mecklenbrauker[20] pointed out a similar relation with the Wigner distribution:

$$|\varsigma_q(p)|^2 = \iint W_s(q',p')W_h(q'-q,p-p')dq'dp'\,. \tag{8.51}$$

Also Cohen[83] has shown that these these two special cases can be generalized for other distributions,

$$|\varsigma_q(p)|^2 = \iint P_s(q',p')P_h(q'-q,p-p') \text{ for all kernels such that } \phi(-\theta,\tau)\phi(\theta,\tau) = 1. \tag{8.52}$$

Recently this type of distributions have been developed and studied by O'Connell and Wigner[81].

Local Momentum

Now let us consider the expected value of momentum and presumably this expected value will be close to the momentum value near the point of interest,

$$\begin{aligned}\langle\, p\,\rangle_q &= \int p\ |\varsigma_q(p)|^2\ dp = \int \eta_q^*(x)\ \frac{1}{i}\frac{\partial}{\partial x}\ \eta_q(x)\ dx \\ &= N^2(q)\ \int R^2(x)\ R_W^2(x-q)\ \{\ mj(x) + S_W'(x-q)\ \}\ dx\,.\end{aligned} \tag{8.53}$$

If the window function is real then we have

$$\langle\, p\,\rangle_q = N^2(q)\, m \int R^2(x)\, R_W^2(x-q)\ j(x)\, dx\,. \tag{8.54}$$

Suppose we narrow the window to get a better estimate of the physical quantities at the point q. In particular, suppose $R_W^2(q)$ approaches a delta function

$$R_W^2(q) \sim \delta(q)\,. \tag{8.55}$$

In that limit we have that

$$N^{-2} = \int R^2(x) R_W^2(x-q) dx \sim \int R^2(x)\delta(x-q)dx = R^2(q)\,, \tag{8.56}$$

and hence

$$N^2(q) \sim \frac{1}{R^2(q)}\,. \tag{8.57}$$

Now we see how the local momentum approaches in the limit of Eq. (8.55). We use Eq. (8.54) which is for the real window so as to avoid the introduction of momentum of the window function. Hence,

$$\langle\, p\,\rangle_q \sim N^2(q)\ \int R^2(x)\delta(x-q)\ \{\ mj(x) + S_W'(x-q)\ \}\ dx = mj(q)\,, \tag{8.58}$$

which is a very satisfactory result.

Spread of Current

We point out that if we make the window go to a delta function the resulting wave function will be very peaked, and by the uncertainty principle the spread in momentum will be infinite even though the average momentum is a well defined quantity as given by Eq. (8.54). However we will see that the spread in momentum approaches infinity in a unique and revealing way.

We now calculate the square of the momentum. There are a number of way of doing that and in the previous chapter we gave four different derivations. We do not repeat them here but outline one of them.

Starting with the wave function given by Eq. (8.34) we have

$$\begin{aligned}\langle\, p^2 \,\rangle_q &= \int \eta_q^*(x)\left(\frac{1}{i}\frac{\partial}{\partial x}\right)^2 \eta_q(x)\; dx = \int \left|\frac{1}{i}\frac{\partial}{\partial x}\eta_q(x)\right|^2 dx \\ &= N^2(q)\int\left(\frac{\partial}{\partial x}\; R(x)\; R_W(x-q)\right)^2 dx \\ &\quad + N^2(q)\int R^2(x)R_W^2(x-q)\{mj(x)+S_W'(x-q)\}^2\; dx\;.\end{aligned} \tag{8.59}$$

The local spread is then

$$\begin{aligned}\sigma_p^2(q) =&\langle\, p^2 \,\rangle_q - \langle\, p \,\rangle_q^2 \\ =&N^2(q)\int\{\; R'(x)R_W(x-q)+R(x)R_W'(x-q)\;\}^2\; dx \\ &+ N^2(q)\int R^2(x)R_W^2(x-q)\{mj(x)+S_W'(x-q)\;\}^2\; dx \\ &- N^4(q)\iint R^2(x_1)R^2(x_2)R_W^2(x_1-q)R_W^2(x_2-q) \\ &\qquad\times\{\; mj(x_1)+S_W'(x_1-q)\;\}\{\; mj(x_2)+S_W'(x_2-q)\;\}\; dx_1\; dx_2\;.\end{aligned} \tag{8.60}$$

Combining the last two terms of Eq. (8.56) we have

$$\begin{aligned}\sigma_p^2(q) =& N^2(q)\int\{\; R'(x)R_W(x-q)+R(x)R_W'(x-q)\;\}^2 dx \\ &+ N^4(q)\iint R^2(x_1)R^2(x_2)R_W^2(x_1-q)R_W^2(x_2-q)\big[\{mj(x_1)+S_W'(x_1-q)\;\}^2 \\ &\qquad - \{mj(x_1)+S_W'(x_1-q)\}\{mj(x_2)+S_W'(x_2-q)\}\big]dx_1dx_2\;.\end{aligned} \tag{8.61}$$

Interchanging x_1 with x_2 in the last integration and adding and dividing by two we have

$$\begin{aligned}\sigma_p^2(q) =&N^2(q)\int\{R'(x)R_W(x-q)+R(x)R_W'(x-q)\}^2\, dx \\ &+\frac{N^4(q)}{2}\iint R^2(x_1)R^2(x_2)R_W^2(x_1-q)R_W^2(x_2-q) \\ &\qquad\times\left[\, mj(x_1)-mj(x_2)+S_W'(x_1-q)-S_W'(x_2-q)\right]^2 dx_1\; dx_2\;.\end{aligned} \tag{8.62}$$

As in the previous chapter a number of alterative expression are possible

$$\sigma_p^2(q) = \frac{1}{2}\iint\left|\eta_q(x_1)\frac{1}{i}\frac{\partial}{\partial x_2}\;\eta_q(x_2)-\eta_q(x_2)\frac{1}{i}\frac{\partial}{\partial x_1}\;\eta_q(x_1)\right|^2 dx_1dx_2\;. \tag{8.63}$$

This result can be used to obtain Et. (8.58) straightforwardly. In addition, one may write

$$\sigma_p^2(q) = \int \eta_q^*(x) \left(\frac{1}{i} \frac{\partial}{\partial x} - \langle\, p \,\rangle_q \right)^2 \eta_q(x)\, dx = \int \left| \left(\frac{1}{i} \frac{\partial}{\partial x} - \langle\, p \,\rangle_q \right) \eta_q(x) \right|^2 dx\,. \qquad (8.64)$$

For real window we have that

$$\begin{aligned} \sigma_p^2(q) &= N^2(q) \int \{R'(x) R_W(x-q) + R(x) R'_W(x-q)\}^2\, dx \\ &+ \frac{N^4(q)}{2} \iint R^2(x_1) R^2(x_2) R_W^2(x_1-q) R_W^2(x_2-q)\, [\, mj(x_1) - mj(x_2)]^2\, dx_1\, dx_2\,. \end{aligned} \qquad (8.65)$$

Limiting Values and Comparison with Distribution Spread

Now let us see what happens when the window approaches a delta function. For the clarity, we consider the real window function. Then the last term in the spread as given by Eq. (8.65) goes as

$$\begin{aligned} &\frac{N^4(q)}{2} \iint R^2(x_1) R^2(x_2) R_W^2(x_1-q) R_W^2(x_2-q)\, [mj(x_1) - mj(x_2)]^2\, dx_1 dx_2 \\ &\sim \frac{N^4(q)}{2} \iint R^2(x_1) R^2(x_2) \delta(x_1-q) \delta(x_2-q)\, [mj(x_1) - mj(x_2)]^2\, dx_1 dx_2 = 0\,. \end{aligned} \qquad (8.66)$$

The first term of the first part of Eq. (8.61) becomes

$$N^2(q) \int R's(x)\; R_W^2(x-q)\, dx \sim N^2(q) \int \;\; R'^2(x) \delta(x-q)\, dx \; = \left(\frac{R'(q)}{R(q)} \right)^2 \qquad (8.67)$$

and hence we have that the spread of the spectrogram goes as

$$\begin{aligned} \sigma_p^2(q) \sim \left(\frac{R'(q)}{R(q)} \right)^2 &+ 2N^2(q) \int R(x)\, R'(x)\, R_W(x-q)\, R'_W(x-q)\, dx \\ &+ N^2(q) \int R^2(x)\, R_W'^2(x-q)\, dx\,. \end{aligned} \qquad (8.68)$$

We see that in the limit the standard deviation approaches a window independent term which is identical to that given by the bilinear distributions, Eq. (8.20), plus window dependent terms. The window dependent terms are generally infinite as we approach a delta function as is expected from the uncertainty principle.

Chapter 9

INTRODUCTION TO THE PART II

The possibility of using reduced density matrices directly for the calculation of atomic properties originates with the observation that the most atomic properties depend only on one and two body properties. Hence, in principle, the full N-body wave function is not necessary and perhaps could be bypassed. In particular, for N-body system with at most two body interaction, the Hamiltonian can be written as,

$$H = \sum_{i=1}^{N} \Omega_i + \sum_{i,j=1}^{N} \Omega_{ij} . \tag{9.1}$$

where Ω_1 and Ω_{12} are the one and two body operators. Then the energy is dependent on only the first and second order reduced density matrix,

$$E = \int \Omega_1 \rho_1(\mathbf{r}_1 ; \mathbf{r}_1') \, d\mathbf{r}_1 + \int \Omega_{12} \rho_2(\mathbf{r}_1, \mathbf{r}_2 ; \mathbf{r}_1', \mathbf{r}_2') \, d\mathbf{r}_1 \, d\mathbf{r}_2 , \tag{9.2}$$

where ρ_1 and ρ_2 are the first and second order density matrices defined by

$$\rho_s(\mathbf{r}_1, \ldots, \mathbf{r}_s ; \mathbf{r}'_1, \ldots, \mathbf{r}'_s) = \binom{N}{s} \int \psi^*(\mathbf{r}'_1, \ldots, \mathbf{r}'_s ; \mathbf{r}_{s+1}, \ldots, \mathbf{r}_N) \times \psi(\mathbf{r}_1, \ldots, \mathbf{r}_s ; \mathbf{r}_{s+1}, \ldots, \mathbf{r}_N) \, d\mathbf{r}_{s+1}, \ldots, d\mathbf{r}_N , \tag{9.3}$$

and where $\psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ is the full N-body wave function.

The second order reduced density matrix is a four variable quantity and is much simpler then the full N body wave function. It would be of immense simplification if the second order reduced density matrix could be obtained directly without the calculation of the full N-body problem.

The first such attempt was made by Mayer,[32] who took a trial density matrix and applied the variational principle to Eq. (9.2) in the usual manner. However the ground state energy obtained by him was lower than the experimental values for the ground state! It was subsequently realized by Tredgold[37], Lowdin[30], Coulson[15], Coleman[14] and others that the seeming violation of the variational principle was due to the fact that the trial second order density matrix was not derivable from any N-body wave function. This led to attempts to find the necessary and sufficient conditions under which the second order density matrix can be derivable from the full N-body wave function. This problem has come to be known as the N-representability problem. A density matrix derivable from a N-body wave function is called a *N-representable* density matrix, a phrase coined by Coleman. If we could solve the N-representability problem then we could choose appropriate trial reduced density matrices and use the variational principle to minimize the energy as given by Eq. (9.2). The minimization of the energy would be with respect to ρ_2 with the appropriate constraints.

While the necessary and sufficient conditions for the first order density matrix are known, the sufficient conditions for the second order density matrix remain untractable. It has been felt that the lack of solution to the N-representability problem for the second order reduced density matrix hinders the possible applications of them to the atomic and molecular problem. The solution of the N-representability problem and the direct calculation of the second order density matrix has always been strongly coupled, however, in the past few years, there have been promising results to indicate that, even without the N-representability conditions, a direct calculation of the second order density matrix is possible, and yields highly accurate results. The approach is not to use the variational principle, but rather to obtain an equation for ρ_2. Colle and Salvetti[13] devised a scheme for the direct calculation of a second order reduced density matrix, and obtained remarkably accurate results, even though their density matrix has been shown not to be N-representable[12]. They obtained the correlation energy of small atoms and molecules to within a few percent. McWeeny[33] has also applied the functional to the uniform electron gas, and obtained excellent results for both the high and low density range. Recently Lee, Yang and Parr[28] have written the expression for the energy given by Colle and Salvetti in terms of the local kinetic energy, and obtained other density functional formulas for the correlation energy. The numerical calculation of Lee[28] *et al.* has also produced very accurate results. Carravetta and Clementi[4] made a wide study of the Colle-Salvetti's method and applied it to the water two body interaction potential with excellent results. In addition, we point out that direct calculation of reduced density matrices in different contexts have been done by a number of investigators, including Clinton[7], Henderson[23] and Scully[36].

Our aim is to study why Colle-Salvetti's functional approximation works so well and how it relates to the N-representability problem. Answers to these questions are essential to the generalization of their method. We have addressed these questions by using the exact second reduced density from a exactly solvable N-body model. Using our model, we are able to compare the exact various expectation values of physical quantities to the values obtained by the Colle-Salvetti's functional approximation. Our work will be discussed in Chapter 11.

Furthermore, in addition to the Colle-Salvetti's functional scheme, the exact solution for the N-body model make us allow to study different ideas relating to the general N-body problem. In particular, we have used our model problem to study the correlation hole of Coulson and Nielson[15], and its extension to momentum space by Banyard and Reed[2]. We have studied the relationships between the correlation hole and the correlation energy, and between correlation hole and the closeness of an approximate physical quantity to the exact one. We have shown that, in general, the better the fit of the correlation hole for an approximate wave function, the closer are the approximate physical quantities to the exact ones. However there are exceptions. Also, we present a convenient method for the calculation of the two particle distribution in momentum space, and generalize the concept of the correlation hole by defining it in the pseudo phase space of position and momentum. This is done within the phase space formulation of quantum mechanics by the use of the Wigner distribution and its generalizations. It is shown that, in the phase space, the distribution of the correlation hole has its marginals as the distributions of Coulson and Nielson's in position space[15], and that of Banyard and Reed's in momentum space[2].

In the next chapter, we develop a model where the reduced density matrix can be calculated exactly, and in the subsequent chapter we address the questions outlined above.

Chapter 10

EXACT REDUCED DENSITY MATRICES FOR A MODEL PROBLEM

10.1 An Exactly Solvable Model of N-Body Problem

The system we consider consists of N bosons of unit mass, each one harmonically attracted to a "nucleus" with spring constant ω^2 and interacting with each other with a harmonic force whose spring constant is γ^2. Various aspects regarding this model problem have been previously developed.[29,16,34] The Hamiltonian is

$$H = \tfrac{1}{2}\sum_{i=1}^{N}(-\nabla_i^2 + \omega^2 r_i^2)) \pm \tfrac{1}{2}\gamma^2 \sum_{i<j}^{N} r_{ij}^2 \,, \tag{10.1}$$

where the minus sign signifies mutual repulsion and the plus sign attraction. Schrödinger's equation

$$H\,\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) = E\,\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) \tag{10.2}$$

can be decoupled by making the following coordinate transformation developed by Hirschfelder *et al.*[25,26]

$$\begin{aligned} \mathbf{Q}_k &= \frac{1}{\sqrt{k(k+1)}}\sum_{i=1}^{k}(\mathbf{r}_{k+1} - \mathbf{r}_i) \qquad \text{for } 1 \leq k \leq N-1\,, \\ \mathbf{Q}_N &= \frac{1}{\sqrt{N}}\sum_{i=1}^{N}\mathbf{r}_i\,, \end{aligned} \tag{10.3}$$

in which case the Hamiltonian becomes

$$H = \tfrac{1}{2}\sum_{k=1}^{N-1}(P_k^2 + \delta_N^2 Q_k^2) + \tfrac{1}{2}\omega^2 Q_N^2 \tag{10.4}$$

with

$$P_k = -i\nabla_{Q_k}\,, \tag{10.5}$$

$$\delta_N^2 = \omega^2 \pm N\gamma^2\,. \tag{10.6}$$

This is the Hamiltonian for N independent harmonic oscillators in the coordinates Q_i, the first $N-1$ having spring constant δ_N^2 and the last one ω^2. The ground state wave function is therefore

$$\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \left(\frac{\delta_N}{\pi}\right)^{\frac{3}{4}(N-1)} \left(\frac{\omega}{\pi}\right)^{\frac{3}{4}} \exp\left\{ -\tfrac{1}{2}\delta_N \sum_{k=1}^{N-1} Q_k^2 - \tfrac{1}{2}\omega Q_N^2 \right\}, \tag{10.7}$$

and corresponding energy is

$$E = \frac{3}{2}(N-1)\,\delta_N + \tfrac{1}{2}\omega\,. \tag{10.8}$$

We now express the wave function in terms of the spatial coordinates. Using Eq. (10.3) one may show that

$$Q_k^2 = r_{k+1}^2 - \frac{1}{k+1}\sum_{i=1}^{k+1}\sum_{j=1}^{k+1} \mathbf{r}_i \cdot \mathbf{r}_j + \frac{1}{k}\sum_{i=1}^{k}\sum_{j=1}^{k} \mathbf{r}_i \cdot \mathbf{r}_j\,, \tag{10.9}$$

$$\sum_{k=1}^{N-1} Q_k^2 = \left(1 - \frac{1}{N}\right)\sum_{k=1}^{N} r_k^2 - \frac{2}{N}\sum_{i\leq j}^{N} \mathbf{r}_i \cdot \mathbf{r}_j\,, \tag{10.10}$$

$$Q_N^2 = \frac{1}{N}\sum_{i=1}^{N} r_i^2 + \frac{2}{N}\sum_{i\leq j}^{N} \mathbf{r}_i \cdot \mathbf{r}_j\,. \tag{10.11}$$

Substituting Eqs. (10.9)-(10.11) into Eq. (10.7) the ground state wave function is expressed in terms of the space coordinates as

$$\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \left(\frac{\delta_N}{\pi}\right)^{\frac{3(N-1)}{4}} \left(\frac{\omega}{\pi}\right)^{\frac{3}{4}}$$
$$\times \exp\left[-\frac{1}{2N}\{(N-1)\,\delta_N + \omega\}\sum_{i=1}^{N} r_i^2 - \frac{1}{N}(\omega - \delta_N)\sum_{i\leq j}^{N} \mathbf{r}_i \cdot \mathbf{r}_j \right]. \tag{10.12}$$

10.2 Exact Reduced Density Matrices

We now derive the exact reduced density matrices for the above wave function. However it will be convenient and advantageous to derive the reduced density matrices for a somewhat wider class of wave functions,

$$\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) = K_N \exp\left(-2A\sum_{i=1}^{N} r_i^2 - 4B\sum_{i\leq j}^{N} \mathbf{r}_i \cdot \mathbf{r}_j \right), \tag{10.13}$$

where A and B are constants and K is a normalizing factor. The wave function given by Eq. (10.12) is a special case. The full N-body density matrix is

$$\rho_N\,(\mathbf{r}_1,\ldots,\mathbf{r}_N\,;\,\mathbf{r}'_1,\ldots,\mathbf{r}'_N) = K_N^2 \exp\{-2A\sum_{I=1}^{N}(r_i^2+r_i'^2) - 4B\sum_{i\leq j}^{N}(\mathbf{r}_i\cdot\mathbf{r}_j+\mathbf{r}'_i\cdot\mathbf{r}'_j)\}\,. \tag{10.14}$$

For convenience we define the following function

$$\begin{aligned} &g_N\,(\mathbf{r}_1,\ldots,\mathbf{r}_N\,;\,\mathbf{r}'_1,\ldots,\mathbf{r}'_N\,;\,A,B,C_N) \\ &\quad = \exp\{-2A\sum_{i=1}^{N}(r_i^2+r_i'^2) - 4B\sum_{i\leq j}^{N}(\mathbf{r}_i\cdot\mathbf{r}_j+\mathbf{r}'_i\cdot\mathbf{r}'_j)^2 - C_N R_N^2\}\,, \end{aligned} \tag{10.15}$$

where C_N is a constant and

$$R_N = \sum_{i=1}^{N}(\mathbf{r}_i+\mathbf{r}'_i)\,. \tag{10.16}$$

The factor $-C_N R_N^2$ has been inserted for reasons which will become clear below. Eventually we will take C_N to be zero.

Now, consider integration with respect to the N-th particle. Using the fact that

$$\int e^{-a\mathbf{r}^2-b\mathbf{r}\cdot\mathbf{J}}\,d\mathbf{r} = \left(\frac{\pi}{a}\right)^{\frac{3}{2}} e^{\frac{b^2J^2}{4a}}\,, \tag{10.17}$$

and

$$R_N^2 = 4r_N^2 + 4\mathbf{r}_N\cdot\mathbf{R}_{N-1} + R_{N-1}^2\,, \tag{10.18}$$

we have

$$\begin{aligned} \int g_N\,d\mathbf{r}_N &= \exp\{-2A\sum_{i=1}^{N-1}(r_i^2+r_i'^2) - 4B\sum_{i\leq j}^{N-1}(\mathbf{r}_i\cdot\mathbf{r}_j+\mathbf{r}'_i\cdot\mathbf{r}'_j) - C_N R_{N-1}^2\} \\ &\qquad\times\int\exp\{-4(A+C_N)\,r_N^2 - 4(B+C_N)\,\mathbf{r}_N\cdot\mathbf{R}_{N-1}\}\,d\mathbf{r}_N \\ &= \left\{\frac{\pi}{4(A+C_N)}\right\}^{\frac{3}{2}} \exp\left\{\frac{(B+C_N)^2 R_N^2}{A+C_N}\right\} g_{N-1}(\mathbf{r}_1,\ldots,\mathbf{r}_{N-1}\,;\,\mathbf{r}'_1,\ldots,\mathbf{r}'_{N-1}\,;\,A,B,C_N) \\ &= \left\{\frac{\pi}{4(A+C_N)}\right\}^{\frac{3}{2}} g_{N-1}(\mathbf{r}_1,\ldots,\mathbf{r}_{N-1}\,;\,\mathbf{r}'_1,\ldots,\mathbf{r}'_{N-1}\,;\,A,B,C_{N-1})\,, \end{aligned} \tag{10.19}$$

where we have taken

$$C_{N-1} = C_N - \frac{(B+C_N)^2}{(A+C_N)}\,. \tag{10.20}$$

Hence, integrating the $N - (s+1)$ coordinates out of Eq. (10.15) yields

$$\int g_N \, d\mathbf{r}_{s+1}, \ldots, d\mathbf{r}_N = \left\{ \frac{\pi^{N-s}}{4^{N-s} \prod_{j=s+1}^{N} (A + C_j)} \right\}^{\frac{3}{2}} g_s(\mathbf{r}_1, \ldots, \mathbf{r}_s \, ; \mathbf{r}'_1, \ldots, \mathbf{r}'_s \, ; A, B, C_s) \tag{10.21}$$

where in general

$$C_i = C_{i+1} - \frac{(B + C_{i+1})^2}{A + C_i} \, . \tag{10.22}$$

To complete the solution we must find C_i explicitly and evaluate the product that appears in the denominator of Eq. (10.21). Eq. (10.22) is a non-linear difference equation which can be transformed into a linear difference equation by making the transformation

$$C_i = -A + \frac{(B - A) Z_i}{Z_{i+1}} \, . \tag{10.23}$$

Substituting this into Eq.(10.22) results in

$$Z_{i+2} + 2 Z_{i+1} + Z_i = 0 \, , \tag{10.24}$$

which is linear and can be solved by standard methods. Taking

$$Z_i = m^i \, , \tag{10.25}$$

where m is to be determined, results in the requirement that

$$m^{i+2} + 2 m^{i+1} + m^i = 0 \, , \tag{10.26}$$

or

$$(m + 1)^2 = 0 \, . \tag{10.27}$$

As both roots are equal to -1 the general solution is

$$Z_i = (-1)^i (\eta_1 + i \, \eta_2) \, , \tag{10.28}$$

where η_1 and η_2 are arbitrary constants. Substituting this solution in to Eq. (10.23) results in

$$C_i = -A + \frac{(A - B)(1 + i \, \eta)}{1 + (i + 1)\eta} \, , \tag{10.29}$$

where

$$\eta = \frac{\eta_2}{\eta_1} \, . \tag{10.30}$$

We see therefore that there is only one arbitrary constant to be solved for. We express it in terms of C_N:

$$C_N = -A + \frac{(A-B)(1+\eta N)}{1+\eta\,(N+1)} \,. \tag{10.31}$$

For our case $C_N = 0$ which results in

$$\eta = -\frac{B}{(A+NB)} \,. \tag{10.32}$$

We now evaluate the product that appears in the numerator in Eq. (10.21):

$$\begin{aligned} \prod_{s=i+1}^{N} (A+C_i) &= \prod_{s=i+1}^{N} \left\{ A - B - \frac{(A-B)\eta}{1+(i+1)\eta} \right\} \\ &= (A-B)^{N-s} \prod_{s=i+1}^{N} \frac{1+i\eta}{1+(i+1)\eta} \\ &= (A-B)^{N-s} \frac{\prod_{s=i+1}^{N}(1+i\eta)}{\prod_{s=i+1}^{N}\{1+(i+1)\eta\}} \\ &= (A-B)^{N-s} \frac{1+(s+1)\eta}{1+(N+1)\eta} \\ &= (A-B)^{N-s} \frac{A+(N-s-1)\,B}{A-B} \,. \end{aligned} \tag{10.33}$$

By taking $s = 0$ for the first factor in Eq. (10.21) and Using Eq. (10.33) we obtain the normalizing factor,

$$K_N^2 = \left\{ \frac{4(A-B)}{\pi} \right\}^{\frac{3N}{2}} \left\{ \frac{A+(N-1)\,B}{A-B} \right\}^{\frac{3}{2}} \,. \tag{10.34}$$

Specialization to Exactly Solvable Model

We now specialize to the wave function given by Eq. (10.12). Comparing Eq. (10.13) with Eq. (10.12) we take

$$A = \frac{1}{4} N\{(N-1)\,\delta_N + \omega\} \,, \tag{10.35}$$

$$B = \frac{1}{4} N(\omega - \delta_N) \,, \tag{10.36}$$

from which

$$A - B = \tfrac{1}{4}\delta_N \,, \tag{10.37}$$

$$A + B(N-1) = \tfrac{1}{4}\omega \,, \tag{10.38}$$

$$A + B(N-s-1) = \tfrac{1}{4} N\{(N-s)\,\omega + s\,\delta_N\} \,. \tag{10.39}$$

Also, the factor in Eq. (10.21) is,

$$\left(\frac{\delta_N}{\pi}\right)^{\frac{3s}{2}} \left\{\frac{N\omega}{(N-s)\omega + s\,\delta_N}\right\}^{\frac{3}{2}} . \tag{10.41}$$

The reduced density matrix of order s is defined by

$$\rho_s(\mathbf{r}_1,\ldots,\mathbf{r}_s\,;\mathbf{r}'_1,\ldots,\mathbf{r}'_s) = \binom{N}{s} \int \psi^*(\mathbf{r}'_1,\ldots,\mathbf{r}'_s\,;\mathbf{r}_{s+1},\ldots,\mathbf{r}_N) \times \psi(\mathbf{r}_1,\ldots,\mathbf{r}_s\,;\mathbf{r}_{s+1},\ldots,\mathbf{r}_N)\,d\mathbf{r}_{s+1},\ldots,d\mathbf{r}_N\,, \tag{10.42}$$

where $\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ is the full N-body wave function.

Using Eqs. (10.38)-(10.42) we have the reduced density matrices,

$$\rho_s = \binom{N}{s} \left\{\frac{\delta_N}{\pi}\right\}^{\frac{3s}{2}} \left\{\frac{N\omega}{(N-s)\omega + s\,\delta_N}\right\}^{\frac{3}{2}} \times g_s\left(\mathbf{r}_1,\ldots,\mathbf{r}_s\,;\mathbf{r}'_1,\ldots,\mathbf{r}'_s\,;\frac{1}{4N}\{(N-1)\,\delta_N+\omega\},\frac{1}{4N}(\omega-\delta_N),C_N\right), \tag{10.43}$$

where for convenience we rewrite some of the previous expressions in terms of the physical parameters:

$$g_s = \exp\left[-\frac{1}{2N}\{\omega+(N-1)\,\delta_N\}\sum_{i=1}^{s}(r_i^2+r_i'^2) - \frac{1}{N}\sum_{i\leq j}^{s}(\mathbf{r}_i\cdot\mathbf{r}_j+\mathbf{r}'_i\cdot\mathbf{r}'_j) - C_s R_s^2\right], \tag{10.44}$$

where

$$\mathbf{R}_s = \sum_{i=1}^{s}(\mathbf{r}_i+\mathbf{r}'_i)\,, \tag{10.45}$$

$$C_s = -\frac{1}{4N}\frac{(N-s)(\omega-\delta_N)^2}{(N-s)\,\omega+s\,\delta_N}\,. \tag{10.46}$$

We write out the cases $s=1$ and $s=2$

$$\rho_1(\mathbf{r}_1,\mathbf{r}'_1) = N\left\{\frac{\delta_N\,N\omega/\pi}{(N-1)\,\omega+\delta_N}\right\}^{\frac{3}{2}} \exp\{-a_1(r_1^2+r_1'^2)+a_2\mathbf{r}_1\cdot\mathbf{r}'_1\}\,, \tag{10.47}$$

$$\begin{aligned}\rho_2(r_1,r_2\,;r'_1,r'_2) = & \frac{N(N-1)}{2}\left\{\frac{\delta_N^2\,N\omega/\pi^2}{(N-2)\,\omega+2\,\delta_N}\right\}^{\frac{3}{2}} \\ & \times\exp\{-b_1(r_1^2+r_1'^2+r_2^2+r_2'^2) - b_2\,(\mathbf{r}_1\cdot\mathbf{r}_2+\mathbf{r}'_1\cdot\mathbf{r}'_2) \\ & + b_3\,(\mathbf{r}_1\cdot\mathbf{r}'_2+\mathbf{r}'_1\cdot\mathbf{r}_2+\mathbf{r}_1\cdot\mathbf{r}'_1+\mathbf{r}_2\cdot\mathbf{r}'_2)\}\,,\end{aligned} \tag{10.48}$$

where

$$a_1 = \frac{1}{4N}\frac{(N-1)(\omega^2+\delta_N)+2\,(N^2-N-1)\omega\delta_N}{(N-1)\,\omega+\delta_N}\,, \tag{10.49}$$

$$a_2 = \frac{1}{2N}\frac{(N-1)(\omega-\delta_N)^2}{(N-1)\omega+\delta_N}\,, \tag{10.50}$$

$$b_1 = \frac{1}{4N}\frac{(N-2)\omega^2+(3N-2)\,\delta_N^2+2\,(N^2-2N+2)\omega\,\delta_N}{(N-2)\omega+2\,\delta_N}\,, \tag{10.51}$$

$$b_2 = \frac{1}{2N}\frac{(N-2)\omega^2-(N+2)\,\delta_N^2+4\,\omega\delta_N}{(N-2)\omega+2\,\delta_N}\,, \tag{10.52}$$

$$b_3 = \frac{1}{2N}\frac{(N-2)(\omega-\delta_N)^2}{(N-2)\omega+2\,\delta_N}\,. \tag{10.53}$$

Potential and Kinetic Energy:

The parts of the total energy can be readily expressed as

$$\left\langle -\tfrac{1}{2}\sum_{i=1}^{N}\nabla_i^2 \right\rangle = \frac{3}{4}\{\omega+(N-1)\,\delta_N\}\,, \tag{10.54}$$

$$\left\langle \tfrac{1}{2}\omega^2\sum_{i=1}^{N} r_i^2 \right\rangle = \frac{3}{4}\frac{\omega}{\delta_N}\,\{(N-1)\,\omega+\delta_N\}\,, \tag{10.55}$$

$$\left\langle \tfrac{1}{2}\gamma^2\sum_{i=1}^{N} r_{ij}^2 \right\rangle = \frac{3}{4}\frac{\gamma^2}{\delta_N}\,N(N-1)\,. \tag{10.56}$$

Alternate Forms

The s-th order reduced density matrix can be expressed in different forms,

$$\rho_s(\mathbf{r}_1,\ldots,\mathbf{r}_s\,;\mathbf{r}'_1,\ldots,\mathbf{r}'_s) = \rho_s\left(\frac{\mathbf{r}_1-\mathbf{r}'_1}{2},\ldots,\frac{\mathbf{r}_s-\mathbf{r}'_s}{2}\right)$$

$$\times\exp\left[-\frac{1}{N}\,\{\omega+(N-1)\,\delta_N\}\left(\sum_{i=1}^{s}\frac{\mathbf{r}_i-\mathbf{r}'_i}{2}\right)^2+2\,\delta_N\sum_{i\leq j}^{s}\frac{\mathbf{r}_i-\mathbf{r}'_i}{2}\cdot\frac{\mathbf{r}_j-\mathbf{r}'_j}{2}\right]\,, \tag{10.57}$$

where the ρ appearing on the right hand side is the s particle density, that is

$$\rho_s(\mathbf{r}_1,\ldots,\mathbf{r}_s) = \rho_s(\mathbf{r}_1,\ldots,\mathbf{r}_s\,;\mathbf{r}_1,\ldots,\mathbf{r}_s)\,. \tag{10.59}$$

Also the reduced density matrix of order s can be expressed in terms of the one particle density,

$$\rho_s(\mathbf{r}_1,\dots,\mathbf{r}_s\,;\,\mathbf{r}'_1,\dots,\mathbf{r}'_s) = \frac{(N-1)\,!}{(N-s)\,!\,s\,!}\left(\frac{\delta_N}{\pi}\right)^{\frac{3(s-1)}{2}} \left\{\frac{(N-1)\,\omega+\delta_N}{(N-s)\,\omega+s\,\delta_N}\right\}^{\frac{3}{2}}$$
$$\times \exp\left[-\frac{1}{N}\left\{\omega+(N-1)\,\delta_N\right\}\left(\sum_{i=1}^{s}\frac{\mathbf{r}_i-\mathbf{r}'_i}{2}\right)^2 + \delta_N\sum_{i\le j}^{s}(\mathbf{r}_i\cdot\mathbf{r}_j+\mathbf{r}'_i\cdot\mathbf{r}'_j)\right]\rho_1\left(\sum_{i=1}^{s}\frac{\mathbf{r}_i-\mathbf{r}'_i}{2}\right) \tag{10.60}$$

Also, the kinetic energy can be expressed as an integral involving the one body density,

$$\left\langle -\tfrac{1}{2}\sum_{i=1}^{N}\nabla_i^2\right\rangle = \int\left\{C+\tfrac{1}{2}\frac{N\omega\,\delta_N}{(N-1)\,\omega+\delta_N}\ln\rho_1(\mathbf{r}\,,\mathbf{r})\right\}\rho_1(\mathbf{r}\,,\mathbf{r})\,d\mathbf{r}\,, \tag{10.61}$$

where C is a constant given by

$$\begin{aligned} C =& \frac{3}{4N}\,\frac{(N-1)\,\omega^2+(N-1)\,\delta_N^2+(2N^2-2N+2)\,\omega\,\delta_N}{(N-1)\,\omega+\delta_N} \\ &-\tfrac{1}{2}\frac{N\omega\,\delta_N}{(N-1)\,\omega+\delta_N}\ln\left[N\left(\frac{\delta_N}{\pi}\right)^{\frac{3}{2}}\left\{\frac{N\omega}{(N-1)\omega+\delta_N}\right\}^{\frac{3}{2}}\right]. \end{aligned} \tag{10.62}$$

10.3 Hartree Solution and its Reduced Density Matrices

Eq. (10.45) gives the reduced density matrices of arbitrary order. In this section we show that the Hartree solution for this problem can also be obtained exactly. Taking

$$\psi^H(\mathbf{r}_1,\dots,\mathbf{r}_N) = \prod_{i=1}^{N}\varphi(\mathbf{r}_i)\,, \tag{10.63}$$

the Hartree equation is

$$\epsilon\varphi(\mathbf{r}) = \left\{-\tfrac{1}{2}\nabla^2+\tfrac{1}{2}\,\omega^2r^2 \pm \sum_{k=2}^{N}\gamma^2\int\varphi^*(\mathbf{r}_k)(\mathbf{r}_k-\mathbf{r})^2\,\varphi(\mathbf{r}_k)\,d\mathbf{r}_k\right\}\varphi(\mathbf{r})\,. \tag{10.64}$$

Each of the terms in the summation is identical and evaluates to

$$\begin{aligned} \int\varphi^*(\mathbf{r}_k)(\mathbf{r}_k-\mathbf{r})^2\,\varphi(\mathbf{r}_k)\,d\mathbf{r}_k =& r^2+\int\varphi^*(\mathbf{r}_k)r_k^2\varphi(\mathbf{r}_k)\,d\mathbf{r}_k+2\int\varphi^*(\mathbf{r}_k)\mathbf{r}\cdot\mathbf{r}_k\varphi(\mathbf{r}_k)\,d\mathbf{r}_k \\ =& r^2+\int\varphi^*(\mathbf{r}_k)r_k^2\varphi(\mathbf{r}_k)\,d\mathbf{r}_k\,, \end{aligned} \tag{10.65}$$

where the last term in the middle step is zero due to symmetry. Eq. (10.64) then becomes

$$\epsilon\varphi(\mathbf{r}) = \{-\tfrac{1}{2}\nabla^2 + \tfrac{1}{2}\,\delta_{N-1}^2 \mathbf{r}^2 \pm \tfrac{1}{2}(N-1)\,\gamma^2\, I\}\varphi(\mathbf{r})\,, \tag{10.66}$$

or

$$(-\tfrac{1}{2}\nabla^2 + \tfrac{1}{2}\,\delta_{N-1}^2 \mathbf{r}^2)\varphi(\mathbf{r}) = \{\epsilon \mp \tfrac{1}{2}(N-1)\,\gamma^2\, I\}\,\varphi(\mathbf{r})\,, \tag{10.67}$$

where we have set

$$I = \int \varphi^*(\mathbf{r})\, r^2 \varphi(\mathbf{r})\, d\mathbf{r}\,. \tag{10.68}$$

Eq. (10.67) is identical to the standard one particle harmonic oscillator equation. The ground state solution is

$$\varphi(r) = \left(\frac{\delta_{N-1}}{\pi}\right)^{\frac{3}{4}} e^{-\frac{1}{2}\delta_{N-1} r^2}\,, \tag{10.69}$$

with energy

$$\epsilon \pm \tfrac{1}{2}\,(N-1)\,\gamma^2 I = \frac{3}{2}\,\delta_{N-1}\,. \tag{10.70}$$

To complete the solution we must evaluate I. Substituting Eq. (10.69) into Eq. (10.68),

$$I = \left(\frac{\delta_{N-1}}{\pi}\right)^{\frac{3}{2}} 4\pi \int_0^\infty r^4 e^{-\delta_{N-1} r^2}\, dr = \frac{3}{2}\delta_{N-1}\,. \tag{10.71}$$

Using Eq. (10.70) the orbital energies are therefore

$$\epsilon = \frac{3}{2}\delta_{N-1} \mp \frac{3}{4}\,\frac{(N-1)\gamma^2}{\delta_{N-1}}\,. \tag{10.72}$$

The total energy of the system is

$$\begin{aligned} E_H &= \sum_{i=1}^{N} \epsilon - \sum_{i=1}^{N}\sum_{i\leq j}^{N} \iint \mp\tfrac{1}{2}\gamma^2 (\mathbf{r}_i - \mathbf{r}_j)^2\, |\varphi(r_i)|^2 |\varphi(r_j)|^2\, d\mathbf{r}_i\, d\mathbf{r}_j \\ &= N\epsilon \pm \tfrac{1}{4}\, N(N-1)\,\gamma^2 \iint (\mathbf{r}_i - \mathbf{r}_j)^2\, |\varphi(r_i)|^2 |\varphi(r_j)|^2\, d\mathbf{r}_i\, d\mathbf{r}_j \\ &= \frac{3}{2} N \delta_{N-1}\,. \end{aligned} \tag{10.73}$$

The Hartree N-body wave function

$$\psi_N^H\,(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \left(\frac{\delta_{N-1}}{\pi}\right)^{\frac{3N}{4}} \exp\left(-\tfrac{1}{2}\delta_{N-1} \sum_{i=1}^{N} r_i^2\right)\,. \tag{10.74}$$

from which the reduced density matrices may be calculated straightforwardly as

$$\psi_s^H\,(\mathbf{r}_1, \ldots, \mathbf{r}_s\,;\, \mathbf{r}'_1, \ldots, \mathbf{r}'_s) = \binom{N}{s} \left(\frac{\delta_{N-1}}{\pi}\right)^{\frac{3s}{2}} \exp\left(-\tfrac{1}{2}\delta_{N-1} \sum_{i=1}^{s} (r_i^2 + r_i'^2)\right)\,. \tag{10.75}$$

We mention here that the various aspects of this model have been also considered by the different methods by Pruski[35] *et al.* and Sage[41].

Chapter 11

A STUDY OF THE COLLE-SALVETTI FUNCTIONAL FOR ρ_2

11.1 Colle and Salvetti Functional Scheme

As mentioned in Chapter 9, Colle and Salvetti have given a simple method for the calculation of the correlation energy by way of the second order reduced density matrix, which has given remarkably good results for a number of atoms and molecules[13]. Their method is based on the following ideas. First, that the full N body wave function is assumed to be well approximated by

$$\psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N) = \psi^{HF}(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)\prod_{i,j}^{N} f(\mathbf{r}_i,\mathbf{r}_j)\,, \tag{11.1}$$

where ψ^{HF} is the Hartree-Fock solution and f is a two body function to be determined. Assuming Eq. (11.1), they argue that the second order density matrix can be approximated by

$$\rho_2(\mathbf{r}_1,\mathbf{r}_2\,;\,\mathbf{r}'_1,\mathbf{r}'_2) = \rho_2^{HF}(\mathbf{r}_1,\mathbf{r}_2\,;\,\mathbf{r}'_1,\mathbf{r}'_2)f(\mathbf{r}_1,\mathbf{r}_2)f(\mathbf{r}'_1,\mathbf{r}'_2)\,. \tag{11.2}$$

They further assume that the exact ρ_1 can be approximated by the Hartree Fock density matrix

$$\rho_1(\mathbf{r}_1,\mathbf{r}'_1) \cong \rho_1^{HF}(\mathbf{r}_1,\mathbf{r}'_1)\,. \tag{11.3}$$

They also take for f the following expression

$$\begin{gathered} f(\mathbf{r}_1,\mathbf{r}_2) = 1 - e^{-\beta^2 r^2}\,\{1 - \Phi(\mathbf{R})\,(1 + \frac{r}{2})\}\,, \\ r = |\mathbf{r}_1 - \mathbf{r}_2| \qquad ; \qquad \mathbf{R} = \tfrac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)\,, \end{gathered} \tag{11.4}$$

where $\Phi(\mathbf{R})$ is to be determined. β is taken to be a function of the density

$$\beta = q\,\rho^{\frac{1}{3}}\,, \tag{11.5}$$

with q being a constant.

Using the equation connecting the first and second order density matrix

$$\int \rho_2^{HF}(\mathbf{r}_1,\mathbf{r}_2,;\mathbf{r}'_1,\mathbf{r}_2)f(\mathbf{r}_1,\mathbf{r}_2)f(\mathbf{r}'_1,\mathbf{r}_2)\,d\mathbf{r}_2 = \frac{N-1}{2}\,\rho_1(\mathbf{r}_1,\mathbf{r}'_1)\,, \tag{11.6}$$

then it can determine that

$$\Phi = \frac{\sqrt{\pi}\beta}{1+\sqrt{\pi}\beta}. \tag{11.7}$$

Note that no use is made of Schrödinger's equation. However, for the simple case of helium, this expression for Φ has also been derived directly from Schrödinger's equation[10].

By using the results which we obtained analytically in the previous chapter, we will study a number of aspects of the above assumptions of Colle-Salvetti functional scheme. In addition to having an exactly solution of ρ_2, this particular model has the significant advantage that the exact wave function happens to have the functional form given by Eq. (11.1). Therefore this is a particularly good model to study the approximation given by Eq. (11.2), which is one of the main ideas of the Colle Salvetti method, as the choice of f can be written exactly. As we are dealing with a boson problem we will use the Hartree solution instead of the Hartree-Fock one in the appropriate equations.

For convenience we repeat the exact an Hartree solution of our model problem. The exact wave function of Eq.(10.15) in the previous chapter is

$$\begin{aligned}\psi^E(\mathbf{r}_1,\ldots,\mathbf{r}_N) &= \left(\frac{\delta_N}{\pi}\right)^{\frac{3(N-1)}{4}}\left(\frac{\omega}{\pi}\right)^{\frac{3}{4}} \\ &\times \exp\left[-\frac{1}{2N}\{(N-1)\,\delta_N+\omega\}\sum_{i=1}^{N} r_i^2-\frac{1}{N}(\omega-\delta_N)\sum_{i\leq j}^{N}\mathbf{r}_i\cdot\mathbf{r}_j\right].\end{aligned} \tag{11.8}$$

The exact Hartree solution is

$$\psi^H(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \left(\frac{\delta_{N-1}}{\pi}\right)^{\frac{3N}{4}}\prod_{i=1}^{N} e^{-\frac{1}{2}\delta_{N-1}r_i^2}, \tag{11.9}$$

or

$$\psi^H(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \left(\frac{\delta_{N-1}}{\pi}\right)^{\frac{3N}{4}}\exp\left[-\tfrac{1}{2}\delta_{N-1}\sum_{i=1}^{N} r_i^2\right]. \tag{11.10}$$

We first show that the exact solution may be put in the form given by Eq. (11.1). Factoring the Hartree solution, Eq. (11.9) or Eq. (11.10), from the exact solution of Eq. (11.8)

$$\frac{\psi^E(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)}{\psi^H(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)} = \prod_{i,j}^{N} f(\mathbf{r}_i,\mathbf{r}_j), \tag{11.11}$$

we have

$$f(\mathbf{r}_i,\mathbf{r}_j) = k\,e^{-\frac{1}{2}(\xi_1-\delta_{N-1})(r_i^2+r_j^2)-\xi_2\,\mathbf{r}_i\cdot\mathbf{r}_j}, \tag{11.12}$$

where

$$k = \left(\frac{\delta_N^{N-1} \omega}{\delta_{N-1}^N} \right)^{\frac{3}{N(N-1)}} , \tag{11.13}$$

$$\xi_1 = \frac{N(N-1)\,\delta_{N-1} + (N-1)\delta_N + \omega}{N(N-1)} , \tag{11.14}$$

$$\xi_2 = \frac{1}{N} (\omega - \delta_N) . \tag{11.15}$$

For future use we note that

$$\xi_1 + \xi_2 = \frac{(N-2)\,\delta_{N-1} - \omega}{N-1} , \tag{11.16}$$

$$\xi_1 - \xi_2 = \frac{2(N-1)\,\delta_N + N(N-2)\,\delta_{N-1} - (N-2)\,\omega}{N(N-1)} . \tag{11.17}$$

If we specialize the f of Eq. (11.11) for $\mathbf{r}_1$ and $\mathbf{r}_2$, we have

$$f(\mathbf{r}_1,\mathbf{r}_2) = C^{\frac{2}{N(N-1)}} \exp\{ -\frac{a}{N-1}(r_1^2 + r_2^2) - \xi_2\, \mathbf{r}_1 \cdot \mathbf{r}_2 \} , \tag{11.18}$$

where

$$a = \tfrac{1}{2}\{ \delta_N - \delta_{N-1} + \frac{1}{N}(\omega - \delta_N) \} , \tag{11.19}$$

and

$$C = \left(\frac{\delta_N^{N-1} \omega}{\delta_{N-1}^N} \right)^{\frac{3}{4}} . \tag{11.20}$$

Then the second order reduced density matrix of Colle-Salvetti scheme can be written as

$$\rho_2^{CS}(\mathbf{r}_1,\mathbf{r}_2\,;\mathbf{r}'_1,\mathbf{r}'_2) = \binom{N}{2} \left(\frac{\delta_{N-1}}{\pi} \right)^3 C^{\frac{4}{N(N-1)}} \times \exp[-\tfrac{1}{2}(\delta_{N-1} + \frac{2a}{N-1}) (r_1^2 + r_1'^2 + r_2^2 + r_2'^2) - \xi_2\, (\mathbf{r}_1 \cdot \mathbf{r}_2 + \mathbf{r}'_1 \cdot \mathbf{r}'_2)] . \tag{11.21}$$

11.2 Calculation of Physical Quantities

We now calculate analytically different physical quantities using the exact and approximate density matrices. The subscripts E and H refer to the exact and Hartree case respectively, and the subscript C will refer to using the density matrix given by Eq. (11.21) and the f given by Eq. (11.18).

Kinetic Energy:

$$\left\langle -\tfrac{1}{2}\sum_{i=1}^{N} \nabla_i^2 \right\rangle_E = \frac{3}{4}\{\omega + (N-1)\,\delta_N\} \tag{11.22}$$

$$\left\langle -\tfrac{1}{2}\sum_{i=1}^{N} \nabla_i^2 \right\rangle_H = \frac{3}{4} N\,\delta_{N-1}\,, \tag{11.23}$$

$$\left\langle -\tfrac{1}{2}\sum_{i=1}^{N} \nabla_i^2 \right\rangle_C = \frac{3}{4} N k \delta_{N-1}^3\, \frac{\xi_1}{(\xi_1^2 - \xi_2^2)^{\frac{3}{2}}}\,. \tag{11.24}$$

Central Potential Energy:

$$\left\langle \tfrac{1}{2}\omega^2 \sum_{i=1}^{N} r_i^2 \right\rangle_E = \frac{3}{4}\frac{\omega}{\delta_N}\,\{(N-1)\,\omega + \delta_N\}\,, \tag{11.25}$$

$$\left\langle \tfrac{1}{2}\omega^2 \sum_{i=1}^{N} r_i^2 \right\rangle_H = \frac{3}{4} N \frac{\omega^2}{\delta_{N-1}}\,, \tag{11.26}$$

$$\left\langle \tfrac{1}{2}\omega^2 \sum_{i=1}^{N} r_i^2 \right\rangle_C = \frac{3}{4} N k\,\omega^2\,\delta_{N-1}^3\, \frac{\xi_1}{(\xi_1^2 - \xi_2^2)^{\frac{5}{2}}}\,. \tag{11.27}$$

Interparticle Potential Energy:

$$\left\langle \tfrac{1}{2}\gamma^2 \sum_{i=1}^{N} r_{ij}^2 \right\rangle_E = \frac{3}{4}\frac{\gamma^2}{\delta_N}\, N(N-1)\,. \tag{11.28}$$

$$\left\langle \tfrac{1}{2}\gamma^2 \sum_{i=1}^{N} r_{ij}^2 \right\rangle_H = \frac{3}{4}\frac{\gamma^2}{\delta_{N-1}}\, N(N-1)\,. \tag{11.29}$$

$$\left\langle \tfrac{1}{2}\gamma^2 \sum_{i=1}^{N} r_{ij}^2 \right\rangle_C = \frac{3}{4} N(N-1)\,\gamma^2 k\,\delta_{N-1}^3\, \frac{\xi_1 + \xi_2}{(\xi_1^2 - \xi_2^2)^{\frac{5}{2}}}\,. \tag{11.30}$$

Total Energy:

$$\langle H \rangle_E = \frac{3}{2}\{\omega + (N-1)\,\delta_N\}\,, \tag{11.31}$$

$$\langle H \rangle_H = \frac{3}{2} N\delta_{N-1}\,, \tag{11.32}$$

$$\langle H \rangle_C = \frac{3}{4} Nk\,\delta_{N-1}^3 \frac{\xi_1\{\xi_1^2 - \xi_2^2 + \omega^2 \pm (N-1)\gamma^2\} \pm \xi_2(N-1)}{(\xi_1^2 - \xi_2^2)^{\frac{5}{2}}}\,. \tag{11.33}$$

where ± refers to a attraction and repulsion, respectively.

Two particle distribution function and Correlation Hole

The two particle distribution function is given by

$$g(r_{12}) = \iint \delta\,(r_{12} - |\mathbf{r}_1 - \mathbf{r}_2|)\,\rho_2(\mathbf{r}_1,\mathbf{r}_2\,;\,\mathbf{r}_1,\mathbf{r}_2)\,d\mathbf{r}_1\,d\mathbf{r}_2\,, \tag{11.34}$$

and its reproducibility by an approximate density matrix is a measure of how well mutual interactions are taken into account. The correlation hole is defined as [15]

$$\Delta(r_{12}) = g(r_{12}) - g^H(r_{12})\,. \tag{11.35}$$

The two particle distribution functions for the density matrices given by Eqs. (10.50), (10.77), and (11.21) can be evaluated analytically. We give here only the final results:

$$g^E(r_{12}) = \sqrt{\frac{2}{\pi}}\,\delta_N^{\frac{3}{2}} r_{12}^2 e^{-\frac{1}{2}\delta_N r_{12}^2}\,, \tag{11.36}$$

$$g^H(r_{12}) = \sqrt{\frac{2}{\pi}}\,\delta_{N-1}^{\frac{3}{2}} r_{12}^2 e^{-\frac{1}{2}\delta_{N-1} r_{12}^2}\,, \tag{11.37}$$

$$g^C(r_{12}) = \sqrt{\frac{2}{\pi}}\,\frac{k\delta_{N-1}^3}{(\xi_1 + \xi_2)^{\frac{3}{2}}}\, r_{12} e^{-\frac{1}{2}(\xi_1 - \xi_2) r_{12}^2}\,. \tag{11.38}$$

11.3 Comparison of Exact and Approximate Solutions

We have numerically compared the above results for various ranges of the coupling constant and particles number. For clarity of presentation we give and discuss the results for a specific range of $\gamma^2 (= 0.1 \sim 0.15)$ and a specific value of $N (= 5)$ which we have found to be representative. ω is taken to be 1. The given results are for the attractive case.

The main objective of the Colle Salvetti method is to improve the correlationless wave function so that a better accounting of the mutual interaction of the particles is achieved. How well the density matrix takes into account these effects may be examined by studying the two particle distribution function. In Figure 8, we have plotted the difference between the exact and Hartree two particle distribution, that is, the correlation hole ($\gamma = 0.12$).

The approximate correlation hole is so close to that curve that no visible distinction could be made. We have therefore plotted on the same figure the difference between the exact and the g_C distribution as given by Eq. (11.38). The improvement is over 99.5% for the whole range of the two particle distribution. This close fit of the two particle distribution is reflected in the improvement of the interparticle potential energy, which is illustrated in Figure 9. The interparticle potential energy is improved significantly.

In Figures 10 and 11, we show the central potential energy and kinetic energies and although the approximate density matrix does give better answers the improvement is minimal. We should point out that in the procedure followed by Colle and Salvetti it is assumed that the first order matrix is well enough approximated by the Hartree-Fock density matrix and hence the one body properties would remain the same. Figure 12 gives the total energy. Since there has been improvement in all three components of the energy and indeed significant improvement in the interparticle potential energy, it certainly seems puzzling that a corresponding improvement in the total energy has not occurred. Apparently, the reason is that the density matrix given by Eq.(11.2) is not N-representable. The improvement in the interparticle potential energy has been "too good" without a corresponding improvement in the other energies. Hence, the total energy has overshot the exact energy since the exact energy is no longer a lower bound. We suggest possible ways that this can be circumvented. One possibility is to modify f so that there are corresponding improvements in the kinetic energy and central potential energy. Also, there is no inherent reason that the f appearing in Eq. (11.2) should necessarily be the same f which best approximates the exact wave function. Furthermore, for particular interactions or particular choices of f the improvement for two body properties may be of such magnitudes so as not to overshoot the total energy by such large amounts. Apparently that is the case for the Coulomb interaction and/or for the f chosen by Colle and Salvetti.

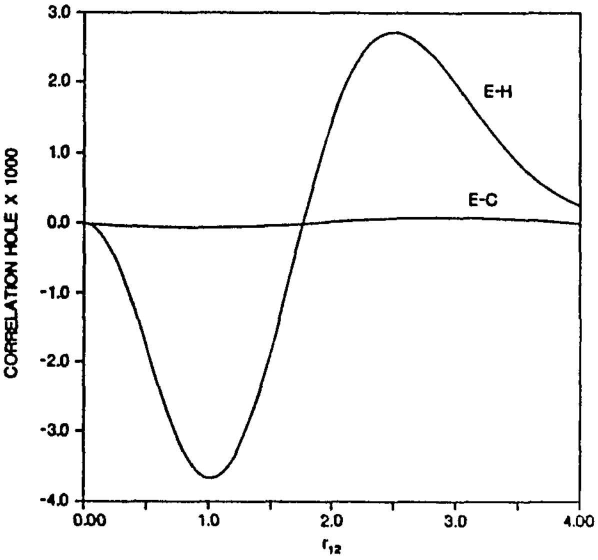


Figure 8. The Correlation Hole. The curve marked *E–H* is the difference between the exact and the Hartree two particle distribution. The figure marked *E–C* is the difference between the exact and the two particle distribution given by Eq. (11.38).

None the less the functional form for the second order density matrix as given by Eq. (11.2) appears to be an excellent approximation for obtaining two body properties.

11.4 Application to "Exact Density Determinant" Obtained from X-ray Scattering†

Recently a quantum mechanical method has been developed to construct orbitals from the experimental crystallographic data. The wave function obtained by this method is a Slater determinant orthonormal orbitals, but it is not a solution of the Hartree-Fock equations. The wave function reproduces to a very high degree the exact density for the crystal. Since the wave function is a single Slater determinant, the energy obtained from it must be worse than the Hartree-Fock energy, and contains no part of the correlation energy. We investigate whether the method of Colle and Salvetti's can be used to obtain the correlation energy from this experimentally derived wave function. We apply the method to the case of the beryllium atom.

We will not here describe the method for obtaining the single Slater determinant but limit ourselves to the issue as to whether we can use the scheme of Colle and Salvetti to

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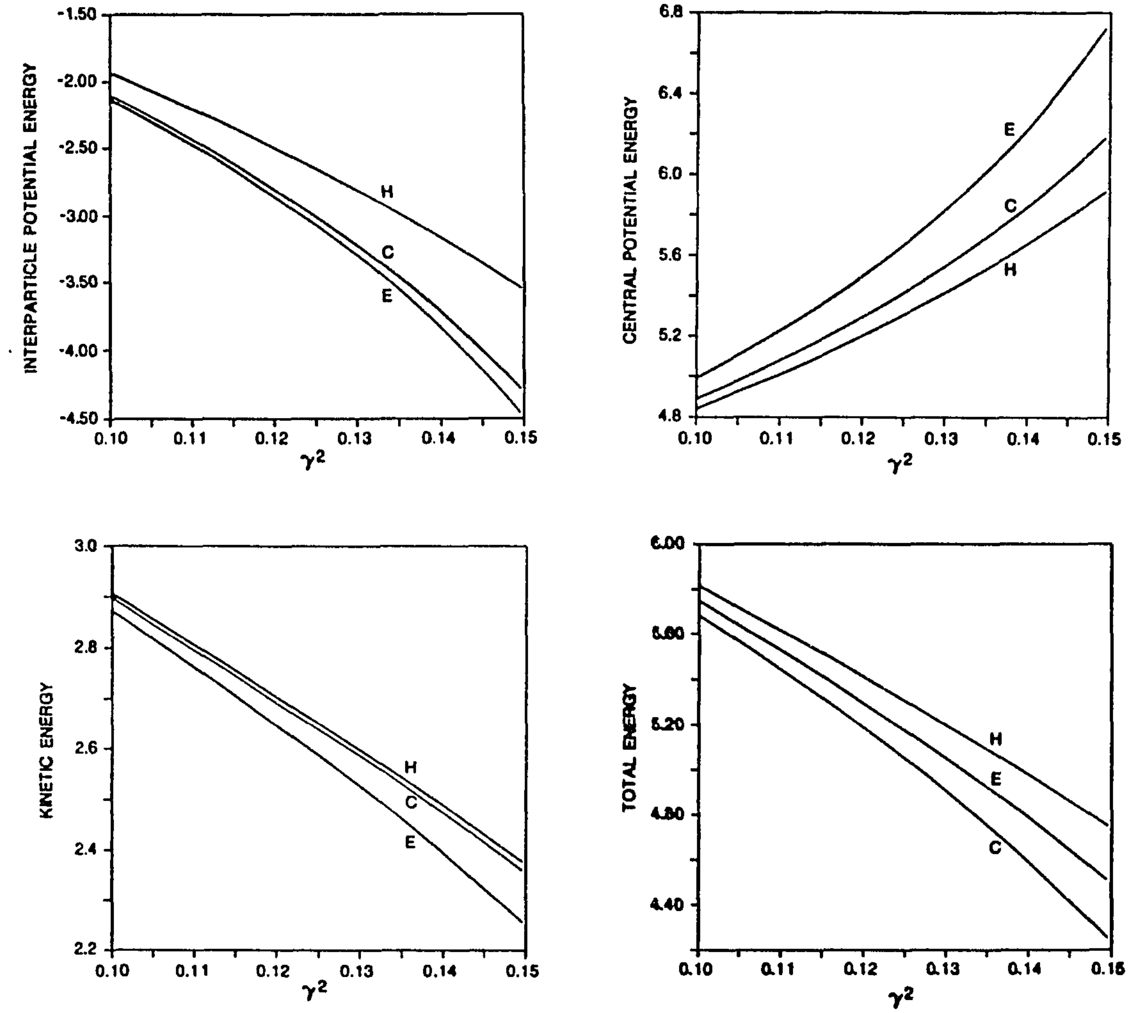
† This work was done with Dr. Massa and Dr. Frishberg.



Figures 9 – 12. The interparticle potential energy, the central potential energy, the kinetic energy and total energy for the exact wave function(E), for the Hartree solution (H) and the approximate density matrix (C).

improve it. The Colle-Salvetti functional for the approximate correlation energy can be written

$$E_c = -0.04918 \int \rho(\mathbf{R}) \frac{1 + 0.173\, W\, e^{-\frac{0.58}{\beta}}}{1 + \frac{0.8}{\beta}}\, d\mathbf{R}\,, \tag{11.39}$$

with

$$\beta = 2.29\, \rho^{\frac{1}{3}}(\mathbf{R}) \quad ; \quad W = 0.3814\, \rho^{-\frac{5}{3}} \left\{ \nabla_r^2 \rho_2^{HF} \left(\mathbf{R} - \frac{\mathbf{r}}{2} ; \mathbf{R} + \frac{\mathbf{r}}{2} \right) \right\}_{r=0} . \tag{11.40}$$

The numerical parameters were chosen by Colle and Salvetti so as to reproduce the correlation energy of helium.

We calculate the correlation energy, but will use the "exact density" determinant obtained from X-ray crystallographic data instead of the Hartree-Fock determinant. In the Colle Salvetti development it is a crucial part of the approximation that that the Hartree-Fock first order density matrix is close to the true first order density matrix. It is therefore reasonable to assume that the one particle density matrix based upon our "exact density" orbitals is also a good approximation to the true value. Formally the entire Colle-Salvetti formalism carries forward except that we substitute ED values for HF values. In addition we point out that in the derivation of Colle and Salvetti for $\Phi(\mathbf{R})$, the approximation that the exact first order density matrix is well enough approximated by the Hartree-Fock density matrix, is used only for the diagonal elements, i.e., $\rho_1(\mathbf{r},\mathbf{r}) = \rho_1^{HF}(\mathbf{r},\mathbf{r})$. For the situation that we are considering this assumption is no longer necessary since indeed $\rho_1^{ED}(\mathbf{r},\mathbf{r}')$ is by definition that single Slater determinant which gives the exact density.

We will not describe here the form of the wave function used for the Beryllium atom as it is described in detail in Reference 6.

For the calculation of energy, we have used a simple trapezoidal rule for the numerical integration. Since the wave function is expressed in terms of Slater type orbitals the following analytical formula for W was used

$$\begin{aligned}\nabla_r^2 &\left\{\left|\mathbf{R}-\frac{\mathbf{r}}{2}\right|^m \left|\mathbf{R}+\frac{\mathbf{r}}{2}\right|^n e^{-\alpha|\mathbf{R}-\frac{\mathbf{r}}{2}|-\beta|\mathbf{R}+\frac{\mathbf{r}}{2}|}\right\}\Bigg|_{\mathbf{r}=0} \\ &= \frac{1}{4R^2}\{(n-m)^2+(\alpha-\beta)^2R^2+2(n-m)(\alpha-\beta)R \\ &\quad +(n+m)-2(\alpha+\beta)R\}R^{n+m}e^{-(\alpha+\beta)R}\,.\end{aligned} \tag{11.41}$$

The energy for the integral given by Eq.(11.39) is −0.093618 a.u. which when added to the energy of the "exact density" determinant (−14.57145) results in a total energy of −14.665068 a.u. To examine how accurate this is we subtract the Hartree-Fock energy (−14.573014) which yields −0.0920 a.u. and differs from the exact correlation energy by only 2%. As a point of comparison, Colle and Salvetti[13] obtain −0.0926 a.u. for the correlation energy with an error of only 1.5%.

As the X-ray orthonormal orbital model of crystallography is based upon quantum mechanics, and is capable of yeilding high accuracy densities, it is likely to be increasingly used for interpreting the coherent diffraction data of crystalline solids. The correlation energy is an important quantity for many physical systems and the above indicates that the method of Colle and Salvetti can be used to calculate it from knowledge of "exact density" orbitals. The numerical test on the beryllium atom has given excellent results.

11.5 Generalization of Colle-Salvetti Method

As we have seen above, the Colle-Salvetti scheme works remarkably well for the various physical quantities. Now we want to find a systematic way of generalizing their method. Consider just an atomic system with at most two body operator. Since the correlation hole ie a two body physical quantity, a systematic improvement of Colle-Salvetti functional scheme should be possible by a systematic improvement of the fitting of the correlation hole. The most important consideration is to find an approximation to $f(\mathbf{r}_1,\mathbf{r}_2)$ which will lend itself to a high accuracy, and give the ability to have successive improvements in fitting the correlation hole. It is well known that one of the accurate schemes for the case is that of Hylleraas. Therefore we propose to approximate the second order density matrix by a Hylleraas type expansion. In another words, the $f(\mathbf{r}_1,\mathbf{r}_2)$ in Eq. (11.2) can be expanded in Hylleraas-like terms

$$f(\mathbf{r}_1,\mathbf{r}_2) \;=\; 1+e^{-ks/2}\sum_{lmn} c_{lmn}s^l u^m t^n \tag{11.42}$$

where s,t and u are the standard Hylleraas variables

$$s \;=\; \tfrac{1}{2}(r_1+\,r_2) \quad ; \quad t \;=\; \tfrac{1}{2}(r_1-r_2) \quad ; \quad u \;=\; |\mathbf{r}_1-\mathbf{r}_2| \tag{11.43}$$

and k is a constant. The fundamental idea is to obtain the coefficients c_{lmn}. We discuss three possible approaches.

The first method is to use the procedure of Colle and Salvetti. They only use the the constraint equation of Eq. (11.6) between the second and first order density matrices. In our case, we will use the constraint equations

$$\int \rho_2(\mathbf{r}_1,\mathbf{r}_2\,;\,\mathbf{r}_1',\mathbf{r}_2)\,d\mathbf{r}_2 = \frac{N-1}{2}\,\rho_1(\mathbf{r}_1,\mathbf{r}_1')\,, \tag{11.44}$$

$$\int \rho_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3\,;\,\mathbf{r}_1',\mathbf{r}_2',\mathbf{r}_3)\,d\mathbf{r}_3 = \frac{N-2}{3}\,\rho_2(\mathbf{r}_1,\mathbf{r}_2\,;\,\mathbf{r}_1',\mathbf{r}_2')\,, \tag{11.45}$$

instead of Eq. (11.6).

Another method of solution is the local energy method as developed by Frost[40] but applied to the reduced equation rather than the full N body wave function. The significant advantage of the Frost method is that it avoids the calculation of the many center integrals when applied to molecules. The main stumbling blocks of the Frost method is that due to the antisymmetry requirements the number of terms which must be considered increases as N factorial making the method impractical for large systems. However, this difficulty is overcome in the method proposed since the full N body wave function does not appear. What one does is define the local energy density matrix by

$$E(1,1') = \frac{F[\rho_1(1,1']}{\rho_1(1,1')} \tag{11.46}$$

where $F[\rho_1(1,1')]$ is the left hand side of Eq. (11.50) below. The basic idea, as in the Frost[40] method is to seek the coefficients which will make the right hand side of Eq. (11.46) as constant as possible. One achieves that by defining the variance of energy E and minimizing it with respect to the coefficients. This results in the best set of coefficients which keeps the local energy matrix as constant as possible in a global sense. The details of the method have been worked out by Massa and Cohen [42].

The third method is by way of the hierarchy equations which are exact equations for reduced density matrices. These equations have been derived by Cho[43], Nakatsuji[44] and Cohen and Frishberg[45]. Schlloser[46] has derived them for the MCSCF theory. We review the briefly the general idea. Writing Schrödinger's time independent equation for N particles in terms of the N body density matrix

$$H_N \rho_N(1,2,...N;1',2'...N') = E\rho_N \ , \tag{11.47}$$

one integrates out $N-s$ particles to obtain

$$\begin{aligned} H_s\rho_s + (s+1)\int \Big[\, \Omega_{s+1} \ + \sum_{i\,=\,1}^{N} \Omega_{i,s+1}\rho_{s+1} \,\Big]\, d(s+1) \\ + \frac{(s+1)(s+2)}{2}\int \Omega_{s+1,s+2}\rho_{s+2}\, d(s+1)\ d(s+2) = E\rho_s \ , \end{aligned} \tag{11.48}$$

where H_s is the reduced Hamiltonian defined by

$$H_s = \sum_{i=1}^{s}\Omega_i + \sum_{i,j=1}^{s}\Omega_{i,j} \ ; \ H_1 = \Omega_1 \tag{11.49}$$

and E is the total electronic energy. The first two equations of the hierarchy are:

$$H_1\rho_1 + 2\int(\Omega_2 + \Omega_{12})\rho_2 d2 + 3\int \Omega_{23}\rho_3\ d2\ d3 = E\rho_1 \ , \tag{11.50}$$

$$H_2\rho_2 + 3\int(\Omega_3 + \Omega_{13} + \Omega_{23})\rho_2 d3 + 6\int \Omega_{34}\rho_4\ d3\ d4 = E\rho_2 \ . \tag{11.51}$$

Now, although Eq. (11.51), for example, is an equation for ρ_2 it can not be solved independently since a knowledge of ρ_3 and ρ_4 is required. No one equation of the hierarchy can be solved since it is coupled to the others and hence no simplification is achieved until the chain of equations is decoupled at some stage. It is natural to first break the chain by taking

$$\rho_2(1,2,;1',2') \;=\; A\rho_1(1;1')\rho_1(2;2') \tag{11.52}$$

$$\rho_3(1,2,3;1',2',3') \;=\; A\rho_1(1;1')\rho_1(2;2')\rho_1(3;3') \tag{11.53}$$

where A is the antisymmetrized operator.

When Eqs. (11.52) and (11.53) are put into Eq. (11.50) we obtain an equation for ρ_1. It has been shown that the result is an equation for the Hartree-Fock density matrix and is equivalent to the Hartree-Fock equations for orbitals[42] . That is the Hartree-Fock density matrix satisfies

$$H_1\rho_1^{\mathrm{HF}} + 2\int(\Omega_2 \;+\Omega_{12})\rho_2^{\mathrm{HF}}\,d2 + 3\int\Omega_{23}\rho_3^{\mathrm{HF}}\;d2\;d3 \;=\; E^{\mathrm{HF}}\rho_1^{\mathrm{HF}}\;. \tag{11.54}$$

That the HF approximation energy naturally is very satisfying and can be thought as a first approximation to the density matrix.

The fact that the HF equation and the exact equation are identical in form allows one to obtain an equation for the correlated part of the density matrix as was done by Cohen[10] *et al.*. Defining F_1, F_2 and F_3 by

$$\rho_1(1;1') \;=\; \rho_1^{\mathrm{HF}}(1;1')\;\left[1+F_1(1;1')\right] \tag{11.55}$$

$$\rho_2(1,2;1',2') \;=\; \rho_2^{\mathrm{HF}}(1,2;1',2')\;\left[1+F_2(1,2;1',2')\right] \tag{11.56}$$

$$\rho_3(1,2,3;1',2',3') \;=\; \rho_3^{\mathrm{HF}}(1,2,3;1',2',3')\;\left[1+F_3(1,2,3;1',2',3')\right] \tag{11.57}$$

Subtracting Eq (11.50) from (11.54) we have

$$H_1\rho_1^{\mathrm{HF}}F_1 + 2\int(\Omega_2+\Omega_{12})\rho_2^{\mathrm{HF}}F_2d2 + 3\int\Omega_{23}\rho_3^{\mathrm{HF}}F_3d2d3 \;=\; \rho_1^{\mathrm{HF}}(EF_1 - E^{\mathrm{HF}}) \tag{11.58}$$

Various approximations for the F's have been considered[15]. If we make the approximation of Colle-Salvetti functionals

$$\left[1+F_1(1;1')\right] \;=\; 1 \tag{11.59}$$

$$\left[1+F_2(1,2;1',2')\right] \;=\; f(1,2)f(1',2') \tag{11.60}$$

$$\left[1+F_3(1,2,3;1',2',3')\right] \;=\; f(1,2)f(1',2')f(1,3)f(1',3')f(2,3)f(2',3') \tag{11.61}$$

we obtain

$$E_c\rho_1^{\mathrm{HF}}(1,1') = 2\int(\Omega_2+\Omega_{12})\rho_2{}^{\mathrm{HF}}\ \left[1-f(1,2)f(1',2')\right]\,d2$$
$$-3\int\Omega_{23}\rho_3^{\mathrm{HF}}\ \left[1-f(1,2)f(1',2)f(1,3)f(1',3)f^2(2,3)\right]\,d2\,d3 \qquad (11.62)$$

where E_c is the correlation energy

$$E_c \;=\; E_{\mathrm{exact}}-E_{\mathrm{HF}} \;=\; \int\Omega_{12}\rho_2{}^{\mathrm{HF}}\ \left[f^2(1,2)-1\right]\,d1\,d2\;. \qquad (11.63)$$

We are now ready to describe a possible scheme for obtaining the coefficients of c_{lmn} in Eq. (11.42). Substituting the Eq. (11.42) into Eq. (11.62) results in a set of algebraic equations for the coefficients c_{lmn}. We point out that one does not have to assume that F_1 is zero and the appropriate equation corresponding to Eq. (11.62) can readily be derived.

We also note that, for the case of helium, the approximation given by Eq. (11.60) with $f(\mathbf{r}_1,\mathbf{r}_2)$ given by Eq. (11.42) is N-representable and hence a variational calculation is also applicable. Although our aim is to develop a method for the general case, the form given by Eq. (11.60) has advantages over the standard Hylleraas solution because considerably fewer terms may have to be taken to achieve an equivalent accuracy.

Chapter 12

CORRELATION HOLE AND PHYSICAL PROPERTIES: A MODEL CALCULATION

12.1 Introduction

For Hamiltonians which contain at most two body interactions the second order density matrix determines all the relevant physical properties of the system. Since the second order density matrix is a function of twelve variables (four variables in three dimensions) Coulson and Nielson[15] introduced the concept of the correlation hole to study the difference between a correlated wave function and the Hartree-Fock wave function. It is defined as

$$\Delta(r_{12}) = f_e(r_{12}) - f_{HF}(r_{12}), \tag{12.1}$$

where $f_e(r_{12})$ and $f_{HF}(r_{12})$ are the probability distributions of the interparticle distance between any two electrons calculated using the exact and Hartree-Fock wave function respectively. In general the probability distribution for the interparticle distance can be calculated from the diagonal terms of the second order density matrix by

$$f(r_{12}) = \int \delta\left(r_{12} - |\mathbf{r}_1 - \mathbf{r}_2|\right) \rho_2(\mathbf{r}_1,\mathbf{r}_2\,;\,\mathbf{r}_1,\mathbf{r}_2)\, d\mathbf{r}_1\, d\mathbf{r}_2\,. \tag{12.2}$$

This concept was extended to momentum space by Banyard and Reed [2] where they defined the correlation hole in momentum space.

$$\Delta(p_{12}) = g_e(p_{12}) - g_{HF}(p_{12}), \tag{12.3}$$

where $g(p_{12})$ is the probability distribution for the relative momentum difference between any two particles.

The correlation hole is a function of one variable, and presumably gives a good criteria for the accuracy of a wave function. The idea being that the closer the approximate correlation hole is to the exact correlation hole the better the wave function. Because it is a function of one variable and because it is based on the physical idea that the Hartree Fock solution leaves out interparticle correlation, and hence the interparticle distance is particularly relevant, the correlation hole has been studied and applied with considerable profit[20].

We will use the exactly solvable boson model problem in Chapter 9 to study various aspects of the correlation hole. First we outline a new method to calculate the momentum correlation hole as introduced by Banyard and Reed. Our general aim is to study the correlation between the goodness of fit of the correlation hole with the accuracy of physical quantities.

12.2 Momentum Correlation Hole: Method of Calculation

We describe a method for calculation of the momentum hole which is the previously given method. The joint probability distribution for momentum of two particles is of course the diagonal terms of the second order momentum density matrix. If we define the second order momentum density matrix by $\gamma_2(\mathbf{p}_1.\mathbf{p}_2\,;\,\mathbf{p}'_1,\mathbf{p}'_2)$ then it can be obtained from the N-body momentum density function in the usual manner.

$$\gamma_2(\mathbf{p}_1.\mathbf{p}_2\,;\,\mathbf{p}'_1,\mathbf{p}'_2) = \binom{N}{2}\int \phi^*(\mathbf{p}'_1,\mathbf{p}'_2,\mathbf{p}_3,\dots,\mathbf{p}_N)\phi(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3,\dots,\mathbf{p}_N)\,d\mathbf{p}_3,\dots,\,d\mathbf{p}_N\,, \tag{12.4}$$

where $\phi(\mathbf{p}_1,\dots,\mathbf{p}_N)$ is the momentum wave function

$$\phi(\mathbf{p}_1,\dots,\mathbf{p}_N) = \left(\frac{1}{2\pi}\right)^{\frac{3N}{2}}\int \psi(\mathbf{r}_1,\dots,\mathbf{r}_N)\exp\{-i\sum_{k=1}^{N}\mathbf{p}_k\cdot\mathbf{r}_k\}\,d\mathbf{r}_1,\dots,\,d\mathbf{r}_N\,. \tag{12.5}$$

An alternative way to calculate $\gamma_2(\mathbf{p}_1.\mathbf{p}_2\,;\,\mathbf{p}'_1,\mathbf{p}'_2)$ is from the second order reduced density matrix in position space.

$$\gamma_2(\mathbf{p}_1.\mathbf{p}_2\,;\,\mathbf{p}'_1,\mathbf{p}'_2) = \left(\frac{1}{2\pi}\right)^{6}\int \rho_2(\mathbf{r}_1,\mathbf{r}_2\,;\,\mathbf{r}'_1.\mathbf{r}'_2)$$
$$\times\exp\{-i(\mathbf{p}_1\cdot\mathbf{r}_1+\mathbf{p}_2\cdot\mathbf{r}_2)+i(\mathbf{p}'_1\cdot\mathbf{r}'_1+\mathbf{p}'_2\cdot\mathbf{r}'_2)\}\,d\mathbf{r}_1\,d\mathbf{r}_2\,d\mathbf{r}'_1\,d\mathbf{r}'_2\,. \tag{12.6}$$

All these methods involve considerable labor and we have found the method to be described below much easier. The method is based on the characteristic function which in general is defined for a random variable x, say, by

$$M(\theta) = \langle\, e^{i\theta x}\,\rangle = \int e^{i\theta x}\,P(x)\,dx \tag{12.7}$$

where $P(x)$ is the probability distribution for x. Knowledge of $M(\theta)$ gives the probability distribution by fourier inversion.

$$P(x) = \frac{1}{2\pi} \int e^{-i\theta x} M(\theta)\, d\theta \tag{12.8}$$

In our case we are trying to obtain the probability distribution and hence we have to be able to obtain the characteristic function some other way[9]. Since the characteristic function is an expectation value we can calculate it by the usual rule of quantum mechanics.

$$\begin{aligned} M(\theta) &= \left\langle e^{i\theta\cdot(\mathbf{p}_2-\mathbf{p}_1)} \right\rangle & (12.9)\\ &= \left\langle e^{\theta\cdot(\nabla_2-\nabla_1)} \right\rangle & (12.10)\\ &= \int e^{\theta\cdot(\nabla_2-\nabla_1)}\, \rho_2(\mathbf{r}_1,\mathbf{r}_2\,;\,\mathbf{r}'_1,\mathbf{r}'_2)\big|_{\substack{\mathbf{r}_1=\mathbf{r}'_1\\ \mathbf{r}_2=\mathbf{r}'_2}}\, d\mathbf{r}_1\, d\mathbf{r}_2 & (12.11) \end{aligned}$$

Since ∇_1 and ∇_2 commute there is no ambiguity in breaking up the exponential and therefore

$$M(\theta) = \int e^{\theta\cdot\nabla_2}\, e^{-\theta\cdot\nabla_1}\, \rho_2(\mathbf{r}_1,\mathbf{r}_2\,;\,\mathbf{r}'_1,\mathbf{r}'_2)\big|_{\substack{\mathbf{r}_1=\mathbf{r}'_1\\ \mathbf{r}_2=\mathbf{r}'_2}}\, d\mathbf{r}_1\, d\mathbf{r}_2\,, \tag{12.12}$$

Now, $e^{\theta\cdot\nabla_r}$ is the translation operator,

$$e^{\theta\cdot\nabla_r} f(\mathbf{r}) = f(\mathbf{r}+\theta)\,, \tag{12.13}$$

and hence

$$M(\theta) = \int \rho_2(\mathbf{r}_1-\theta,\mathbf{r}_2+\theta\,;\,\mathbf{r}_1,\mathbf{r}_2)\, d\mathbf{r}_1\, d\mathbf{r}_2\,. \tag{12.14}$$

The probability distribution for the vector $\mathbf{p}_{21}$ is therefore

$$\begin{aligned} G(\mathbf{p}_{21}) &= \frac{1}{(2\pi)^3} \int e^{-i\theta\cdot\mathbf{p}_{21}} M(\theta)\, d\theta & (12.15)\\ &= \frac{1}{(2\pi)^3} \int e^{-i\theta\cdot\mathbf{p}_{21}}\, \rho_2(\mathbf{r}-\theta,\mathbf{r}_2+\theta\,;\,\mathbf{r}_1,\mathbf{r}_2)\, d\theta\, d\mathbf{r}_1\, d\mathbf{r}_2\,. & (12.16) \end{aligned}$$

To obtain the distribution for the scalar $p_{12} = |\mathbf{p}_{12}|$ we use

$$g(p_{12}) = \int G(\mathbf{p}'_{21})\, \delta(p_{21} - |\mathbf{p}'_{21}|)\, d\mathbf{p}'_{21}\,, \tag{12.17}$$

which for the case where $p_{12} = |\mathbf{p}'_{12}|$, reduces to

$$g(p_{12}) = 4\pi^2 p_{12}^2 G(|\mathbf{p}_{21}|)\,. \tag{12.18}$$

12.3 Model Problem: Exact, Hartree and Approximate Wave Functions

In Chapter 9, we have solved a model problem where the reduced density matrices can be calculated analytically for both the exact[35,12] and Hartree[12] wave functions. From the reduced density matrices we have calculated the correlation hole and other relevant physical quantities exactly. We now use this model to ascertain whether the goodness of fit of the correlation hole is directly related to the accuracy of the physical quantities predicted by the approximate wave function.

In this chapter, we consider an approximate wave function with two parameters A and B of the form

$$\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) = K_N \exp\left(-2A\sum_{i=1}^{N} r_i^2 - 4\,B\sum_{i\leq j}^{N} \mathbf{r}_i\cdot\mathbf{r}_j\right) \tag{12.19}$$

where the normalization factor is given by

$$K_N^2 = \left\{\frac{4(A-B)}{\pi}\right\}^{\frac{3N}{2}} \left\{\frac{A+(N-1)B}{A-B}\right\}^{\frac{3}{2}} . \tag{12.20}$$

The s order reduced density matrix can be calculated as in Reference 12

$$\rho_s^A(\mathbf{r}_1,\ldots,\mathbf{r}_s\,;\mathbf{r}'_1,\ldots,\mathbf{r}'_s) = \binom{N}{s}\left\{\frac{4(A-B)}{\pi}\right\}^{\frac{3s}{2}} \left\{\frac{A+(N-1)B}{A+(N-s-1)B}\right\}^{\frac{3}{2}}$$
$$\times \exp\{-2A\sum_{i=1}^{s}(r_i^2+r_i'^2) - 4B\sum_{i\leq j}^{s}(\mathbf{r}_i\cdot\mathbf{r}_j+\mathbf{r}'_i\cdot\mathbf{r}'_j) - C_s R_s^2\}\,, \tag{12.21}$$

where

$$\mathbf{R}_s = \sum_{i=1}^{s}(\mathbf{r}_i+\mathbf{r}'_i)\,, \tag{12.22}$$

$$C_s = \frac{-(N-s)B^2}{A+(N-s-1)B}\,. \tag{12.23}$$

In particular, the first and second order reduced density matrices are

$$\rho_1(\mathbf{r}_1,\mathbf{r}'_1) = \binom{N}{1}\left\{\frac{4(A-B)}{\pi}\right\}^{\frac{3}{2}} \left\{\frac{A+(N-1)B}{A+(N-2)B}\right\}^{\frac{3}{2}} \exp\{-a_1(r_1^2+r_1'^2)+a_2\mathbf{r}_1\cdot\mathbf{r}'_1\}\,, \tag{12.24}$$

$$\rho_2(\mathbf{r}_1,\mathbf{r}_2\,;\mathbf{r}'_1,\mathbf{r}'_2) = \binom{N}{2}\left\{\frac{4(A-B)}{\pi}\right\}^{3} \left\{\frac{A+(N-1)B}{A+(N-3)B}\right\}^{3}$$
$$\times \exp\{-b_1(r_1^2+r_1'^2+r_2^2+r_2'^2) - b_2\,(\mathbf{r}_1\cdot\mathbf{r}_2+\mathbf{r}'_1\cdot\mathbf{r}'_2)$$
$$+ b_3\,(\mathbf{r}_1\cdot\mathbf{r}'_2+\mathbf{r}'_1\cdot\mathbf{r}_2+\mathbf{r}_1\cdot\mathbf{r}'_1+\mathbf{r}_2\cdot\mathbf{r}'_2)\}\,, \tag{12.25}$$

where

$$a_1 = \frac{2A^2 + 2(N-2)AB - (N-1)B^2}{A + (N-2)B}, \tag{12.26}$$

$$a_2 = \frac{2(N-1)B^2}{A + (N-2)B}, \tag{12.27}$$

$$b_1 = \frac{2A^2 + 2(N-3)AB - (N-2)B^2}{A + (N-3)B} \tag{12.28}$$

$$b_2 = \frac{4AB + (2N-8)B^2}{A + (N-1)B}, \tag{12.29}$$

$$b_3 = \frac{2(N-2)B^2}{A + (N-3)B}. \tag{12.30}$$

Also the second order reduced density matrix in momentum space can be obtained exactly after a long calculation.

$$\gamma_1(\mathbf{p}\,;\mathbf{p}') = \binom{N}{1}\left(\frac{1}{4\pi A}\right)^{\frac{3}{2}} e^{-a_1(p^2+p'^2)+a_2\mathbf{p}\cdot\mathbf{p}'} \tag{12.31}$$

$$\begin{aligned}\gamma_2(\mathbf{p}_1,\mathbf{p}_2\,;\mathbf{p}'_1,\mathbf{p}'_2) = &\binom{N}{2}\left(\frac{1}{4\pi}\right)^3\left(\frac{1}{A^2-B^2}\right)^{\frac{3}{2}}\\ &\exp\{-b_1(p_1^1 + p_2^2 + p_1'^2 + p_2'^2) - b_2(\mathbf{p}_1\cdot\mathbf{p}_2 + \mathbf{p}'_1\cdot\mathbf{p}'_2)\\ &+ b_3(\mathbf{p}_1+\mathbf{p}_2)\cdot(\mathbf{p}'_1+\mathbf{p}'_2)\},\end{aligned} \tag{12.32}$$

where

$$a_1 = \frac{2A^2 + 2(N-2)AB + (N-1)B^2}{16A(A-B)\{A+(N-1)B\}}, \tag{12.33}$$

$$a_2 = \frac{(N-1)B^2}{8A(A-B)\{A+(N-1)B\}}, \tag{12.34}$$

$$b_1 = \frac{2A^2 + 2(N-1)AB(N-2)B^2}{16(A^2-B^2)\{A+(N-1)B\}}, \tag{12.35}$$

$$b_2 = \frac{B(2A+NB)}{8(A^2-B^2)\{A+(N-1)B\}}, \tag{12.36}$$

$$b_3 = \frac{(N-2)B^2}{8(A^2-B^2)\{A+(N-1)B\}}. \tag{12.37}$$

Energies

Here we show the various energies for the Exact, Hartree and approximation solution. For comparison, we list again the energies for the Exact and Hartree solution from Chapter 9.

Kinetic Energy:

$$\left\langle -\tfrac{1}{2}\sum_{i=1}^{N} \nabla_i^2 \right\rangle_E = \frac{3}{4}\{\omega + (N-1)\,\delta_N\} \tag{12.38}$$

$$\left\langle -\tfrac{1}{2}\sum_{i=1}^{N} \nabla_i^2 \right\rangle_H = \frac{3}{4} N\,\delta_{N-1}\,, \tag{12.39}$$

$$\left\langle -\tfrac{1}{2}\sum_{i=1}^{N} \nabla_i^2 \right\rangle_A = 3NA\,. \tag{12.40}$$

Central Potential Energy(CPE):

$$\left\langle \tfrac{1}{2}\omega^2\sum_{i=1}^{N} r_i^2 \right\rangle_E = \frac{3}{4}\frac{\omega}{\delta_N}\,\{(N-1)\,\omega + \delta_N\}\,, \tag{12.41}$$

$$\left\langle \tfrac{1}{2}\omega^2\sum_{i=1}^{N} r_i^2 \right\rangle_H = \frac{3}{4} N\frac{\omega^2}{\delta_{N-1}}\,, \tag{12.42}$$

$$\left\langle \tfrac{1}{2}\omega^2\sum_{i=1}^{N} r_i^2 \right\rangle_A = \frac{3}{16}\,\frac{N\,\omega^2\{A+(N-2)B\}}{(A-B)\{A+(N-1)B\}}\,. \tag{12.43}$$

Interparticle Potential Energy(IPE):

$$\left\langle \tfrac{1}{2}\gamma^2\sum_{i=1}^{N} r_{ij}^2 \right\rangle_E = \frac{3}{4}\frac{\gamma^2}{\delta_N}\,N(N-1)\,. \tag{12.44}$$

$$\left\langle \tfrac{1}{2}\gamma^2\sum_{i=1}^{N} r_{ij}^2 \right\rangle_H = \frac{3}{4}\frac{\gamma^2}{\delta_{N-1}}\,N(N-1)\,. \tag{12.45}$$

$$\left\langle \tfrac{1}{2}\gamma^2\sum_{i=1}^{N} r_{ij}^2 \right\rangle_A = \frac{3}{16}\frac{\gamma^2}{A-B}\,N(N-1)\,. \tag{12.46}$$

Total Energy:

$$\langle H \rangle_E = \frac{3}{2}\{\omega + (N-1)\,\delta_N\}\,, \tag{12.47}$$

$$\langle H \rangle_H = \frac{3}{2} N \delta_{N-1}\,, \tag{12.48}$$

$$\langle H \rangle_A = 3NA + \frac{3}{16} N \frac{\{\omega^2 - (N-1)\gamma^2\}A + \{(N-2)\omega^2 - (N-1)^2\gamma^2\}B}{(A-B)\{A + B(N-1)\}}\,. \tag{12.49}$$

We should point out that the exact and Hartree solution are special cases of the wave function given by Eq. (10.19). To obtain the exact solution one takes

$$A = \frac{1}{4N}\{(N-1)\delta_N + \omega\}\,, \tag{12.50}$$

$$B = \frac{1}{4N}(\omega - \delta_N)\,. \tag{12.51}$$

For the Hartree solution one takes

$$A = \tfrac{1}{4}\delta_{N-1}\,, \tag{12.52}$$

$$B = 0\,. \tag{12.53}$$

12.4 Correlation Hole

Position Correlation Hole

The distributions for the interparticle distance for the above wave functions can be calculated using the diagonal terms of the second order density matrix as given by Eq. (10.25).

$$f_E(r_{12}) = \sqrt{\frac{2}{\pi}}\,\delta_N^{\frac{3}{2}}\, r_{12}^2\, e^{-\frac{1}{2}\delta_N r_{12}^2} \tag{12.54}$$

$$f_H(r_{12}) = \sqrt{\frac{2}{\pi}}\,\delta_{N-1}^{\frac{3}{2}}\, r_{12}^2\, e^{-\frac{1}{2}\delta_{N-1} r_{12}^2} \tag{12.55}$$

$$f_A(r_{12}) = \sqrt{\frac{2}{\pi}}\,\{4(A-B)\}^{\frac{3}{2}}\, r_{12}^2\, e^{-2(A-B) r_{12}^2} \tag{12.56}$$

In Figure 13, we plot the correlation hole for various N.

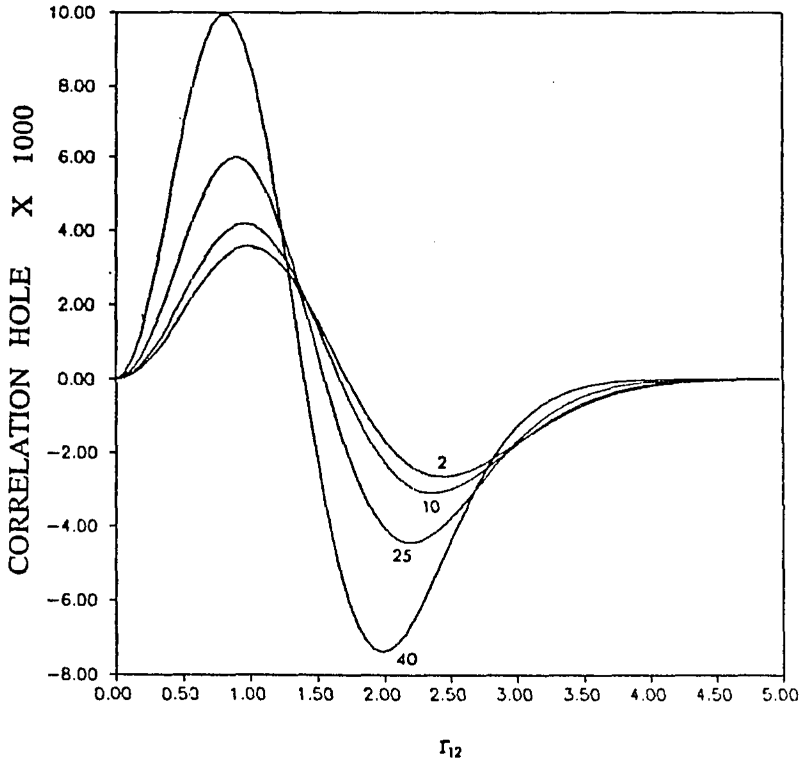


Figure 13. The position correlation hole for different particle numbers for the repulsive case. The constants are $\omega = 1$ and $\gamma = 0.12$.

Momentum Correlation Hole

To calculate the momentum correlation hole we will use the method described in the introduction. The moment generating function is, using Eq. (10.14) and the density matrix given by Eq. (10.25),

$$M(\theta) = \int \rho_2(\mathbf{r}_1 - \theta.\mathbf{r}_2 + \theta\,;\mathbf{r}_1,\mathbf{r}_2)\,d\mathbf{r}_1\,d\mathbf{r}_2 \tag{12.57}$$

$$\begin{aligned} &= \binom{N}{2}\left\{\frac{4(A-B)}{\pi}\right\}\left\{\frac{A+(N-1)B}{A+(N-3)b}\right\}^{\frac{3}{2}} \\ &\quad\times \int \exp\bigl[-b_1\{(\mathbf{r}_1-\theta)^2 + (\mathbf{r}_2+\theta)^2 + r_1^2 + r_2^2\} \\ &\qquad - b_2\{(\mathbf{r}_1-\theta)\cdot(\mathbf{r}_2-\theta) + \mathbf{r}_1\cdot\mathbf{r}_2\} \\ &\qquad + b_3(\mathbf{r}_1-\theta+\mathbf{r}_2+\theta)\cdot(\mathbf{r}_1+\mathbf{r}_2)\bigr]\,d\mathbf{r}_1\,d\mathbf{r}_2 \end{aligned} \tag{12.58}$$

$$\begin{aligned} &= \binom{N}{2}\left\{\frac{4(A-B)}{\pi}\right\}\left\{\frac{A+(N-1)B}{A+(N-3)B}\right\}^{\frac{3}{2}} \\ &\quad\times \int \exp\{-(2b_1-b_3)(r_1^2+r_2^2) - 2(b_2-b_3)\mathbf{r}_1\cdot\mathbf{r}_2 \\ &\qquad - (b_2-2b_1)\,\theta\cdot(\mathbf{r}_1-\mathbf{r}_2)\}\,d\mathbf{r}_1\,d\mathbf{r}_2\,. \end{aligned} \tag{12.59}$$

Using the following general integral where $\mathbf{C}_1$ and $\mathbf{C}_2$ are two arbitrary vectors

$$\int \exp\{-A(r_1^2+r_2^2)-2B\mathbf{r}_1\cdot\mathbf{r}_2-2\mathbf{C}_1\cdot\mathbf{r}_1-2\mathbf{C}_2\cdot\mathbf{r}_2\}\,d\mathbf{r}_1\,d\mathbf{r}_2 = \left(\frac{\pi}{A^2-B^2}\right)^{\frac{3}{2}}\exp\left\{\frac{A(C_1^2+C_2^2)-2B\mathbf{C}_1\cdot\mathbf{C}_2}{A^2-B^2}\right\} \tag{12.60}$$

we have for the generating function

$$M(\theta)=\left(\frac{1}{\pi}\right)^{\frac{3}{2}} e^{-2(A-B)\theta^2} \tag{12.61}$$

The probability distribution for the $\mathbf{p}_{21}$ vector is then

$$P(\mathbf{p}_{21})=\left(\frac{1}{2\pi}\right)^3\int M(\theta)\,e^{-i\theta\cdot\mathbf{p}_{21}}\,d\theta \tag{12.62}$$

$$=\left(\frac{1}{4\pi^3}\right)\int e^{-2(A-B)\theta^2-i\theta\cdot\mathbf{p}_{21}}\,d\theta \tag{12.63}$$

$$=\left\{\frac{1}{8\pi^2(A-B)}\right\}^{\frac{3}{2}} e^{-\frac{p_{12}^2}{8(A-B)}} \tag{12.64}$$

where we have used

$$\int e^{-a\theta^2-b\theta\cdot\mathbf{J}}\,d\theta=\left(\frac{\pi}{a}\right)^{\frac{3}{2}} e^{\frac{b^2J^2}{4a}} \tag{12.65}$$

The probability distribution for the scalar distance is

$$g(p_{12})=4\pi p_{12}^2 P(|p_{12}|) \tag{12.66}$$

$$=\left(\frac{4}{\pi^2}\right)\left\{\frac{1}{8(A-B)}\right\}^{\frac{3}{2}} p_{12}^2\,e^{-\frac{p_{12}^2}{8(A-B)}} \tag{12.67}$$

In Figure 14, we plot the momentum correlation hole for various N.

12.5 Numerical Results

Our aim is to study the correlation between the fitting of the correlation hole and the closeness of the physical quantities for an approximate wave function. We therefore need a measure as to how well the correlation hole of an approximate wave function is to the exact correlation hole. We have chosen the following measure

$$\epsilon_r^2=\int\{f_c(r_{12})-f_A(r_{12})\}^2\,dr_{12}\,, \tag{12.68}$$

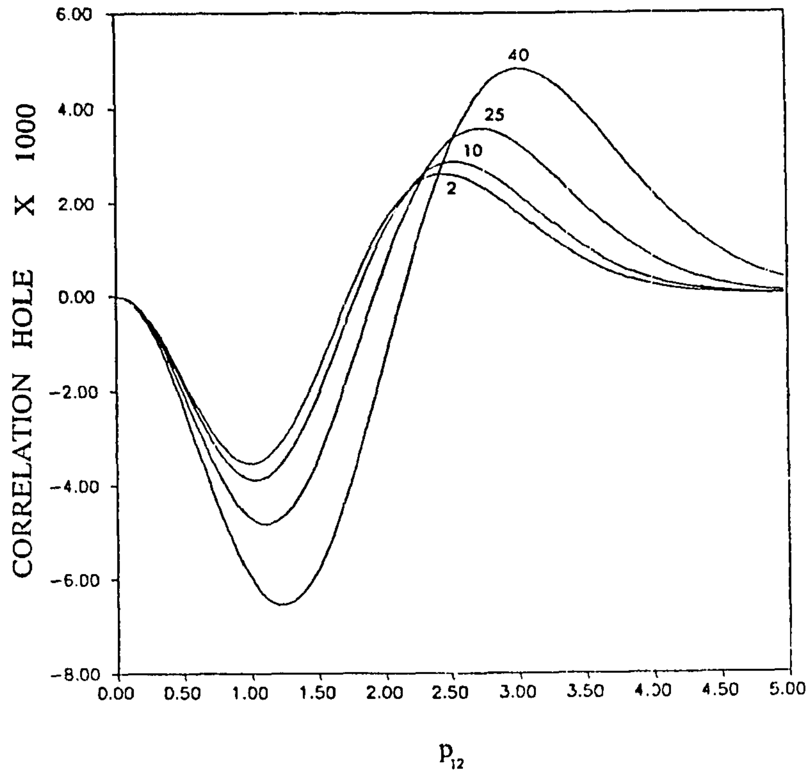


Figure 14. The momentum correlation hole for different particle numbers for the repulsive case. The constants are $\omega = 1$ and $\gamma = 0.12$.

and a similar definition for the momentum correlation hole

$$\epsilon_p^2 = \int \{f_e(p_{12}) - f_A(p_{12})\}^2 \, dp_{12} \,. \tag{12.69}$$

We worked these out and they are

$$\epsilon_r^2 = \frac{3}{4\sqrt{\pi}} \left\{ p\overline{\delta_N} + 2\sqrt{A-B} - \frac{64\sqrt{2}\delta_N^{\frac{3}{2}}(A-B)^{\frac{3}{2}}}{(\delta_N + 4A - 4B)^{\frac{5}{2}}} \right\} \tag{12.70}$$

$$\epsilon_p^2 = \frac{3}{4\sqrt{\pi}} \left\{ \frac{1}{\sqrt{\delta_N}} + \frac{1}{2\sqrt{A-B}} + \frac{32\sqrt{2}\delta_N(A-B)}{(\delta_N + 4A - 4B)^{\frac{5}{2}}} \right\} . \tag{12.71}$$

In Figures 15 and 16, we have plotted the various energies for different values of the deviations as measured by Eqs. (12.70) and (12.71). This was done in the following way. We varied the value of A and B by one percent on both sides of the value which produces the exact solution and for each of those values the deviation and the energies was calculated an plotted. The figures represent 625 points, 25 points for each variation of A and B.

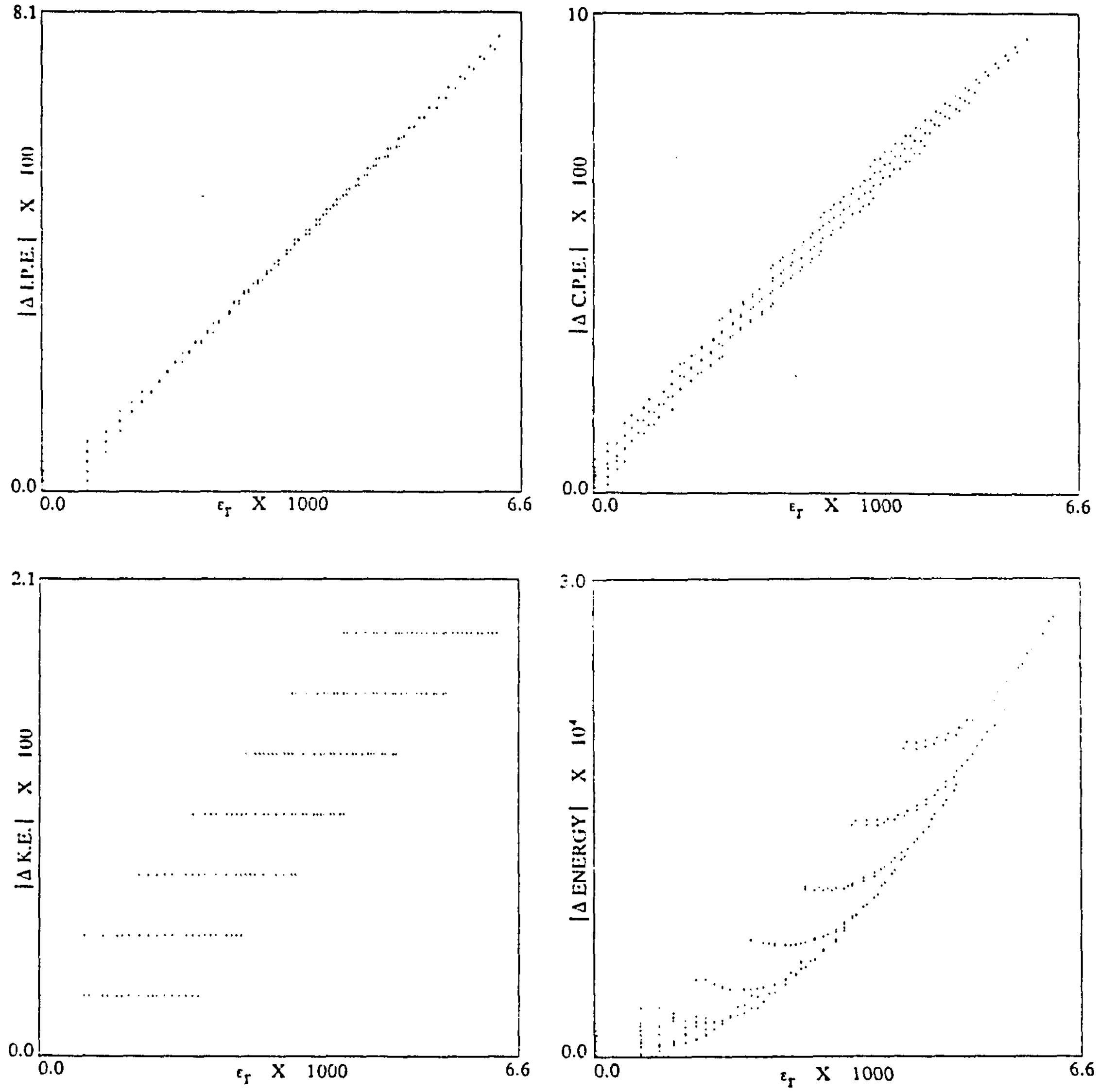


Figure 15. Deviations in interparticle potential energy (I.P.E.), central potential energy (C.P.E.), kinetic energy (K.E.) and total energy (ENERGY) versus ϵ_r.

As can be seen from the figures it is generally true that the smaller the deviation of the approximate correlation hole to the exact one the closer will be the energies to their exact values. Non the less it is also clear that there are a considerable number of exceptions. In all the cases there are points which have a larger deviation but smaller energy deviation then some other point. This can also be seen from the analytical expression since it depends only on $A - B$ but the energies do not only depend on $A - B$.

12.6 Phase Space Correlation Hole

In this section we generalize the correlation hole concept of Coulson and Nielson in position and extended by Banyard and Reed[2] to momentum by defining the correlation hole in the pseudo phase space of position and momentum. We do this in the phase space formulation of quantum mechanics and show that the phase space distribution correlation hole has as its marginals the distributions of Coulson and Nielson in position space and that of Banyard and Reed in momentum space.

Although position and momentum do not commute in quantum mechanics one can still define a joint distribution of position and momentum which is very close to the classical distribution in phase space. What one seeks is a phase space function $F(\mathbf{r},\mathbf{p})$ of position and momentum which satisfies

$$\int F_N(\mathbf{r},\mathbf{p})\, d\mathbf{p} = |\psi_N(\mathbf{r})|^2 \tag{12.72}$$

$$\int F_N(\mathbf{r},\mathbf{p})\, d\mathbf{r} = |\phi_N(\mathbf{p})|^2 \tag{12.73}$$

Wigner[39] was the first to have found such a function and others have been found since that time. All of quantum mechanics can be formulated in terms of these joint distributions and is usually called the phase space formulation of quantum mechanics. For a review of the phase space formulation of quantum mechanics references[1,24,11] may be consulted. We emphasize that we are not discussing any notions of hidden variables and indeed the phase space formulation gives the identical result as the operator formalism.

All bilinear distribution functions which satisfy conditions (12.72) and (12.73) can be generated from

$$\begin{aligned} F_N(\mathbf{r},\mathbf{p}) = \left(\frac{1}{2\pi}\right)^{6N} \int \exp\left\{ i\left[\sum_{i=1}^{N} \theta_i \cdot (\mathbf{u}_i - \mathbf{r}_i) - \tau_i \cdot \mathbf{p}_i\right]\right\} \\ \times\, \psi_N^*(\mathbf{u}_i - \tfrac{1}{2}\tau_i)\psi_N(\mathbf{u}_i + \tfrac{1}{2}\tau_i)\, f_N(\theta_i, \tau_i) \prod_{i=1}^{N} d\theta_i\, d\tau_i\, d\mathbf{u}_i\, , \end{aligned} \tag{12.74}$$

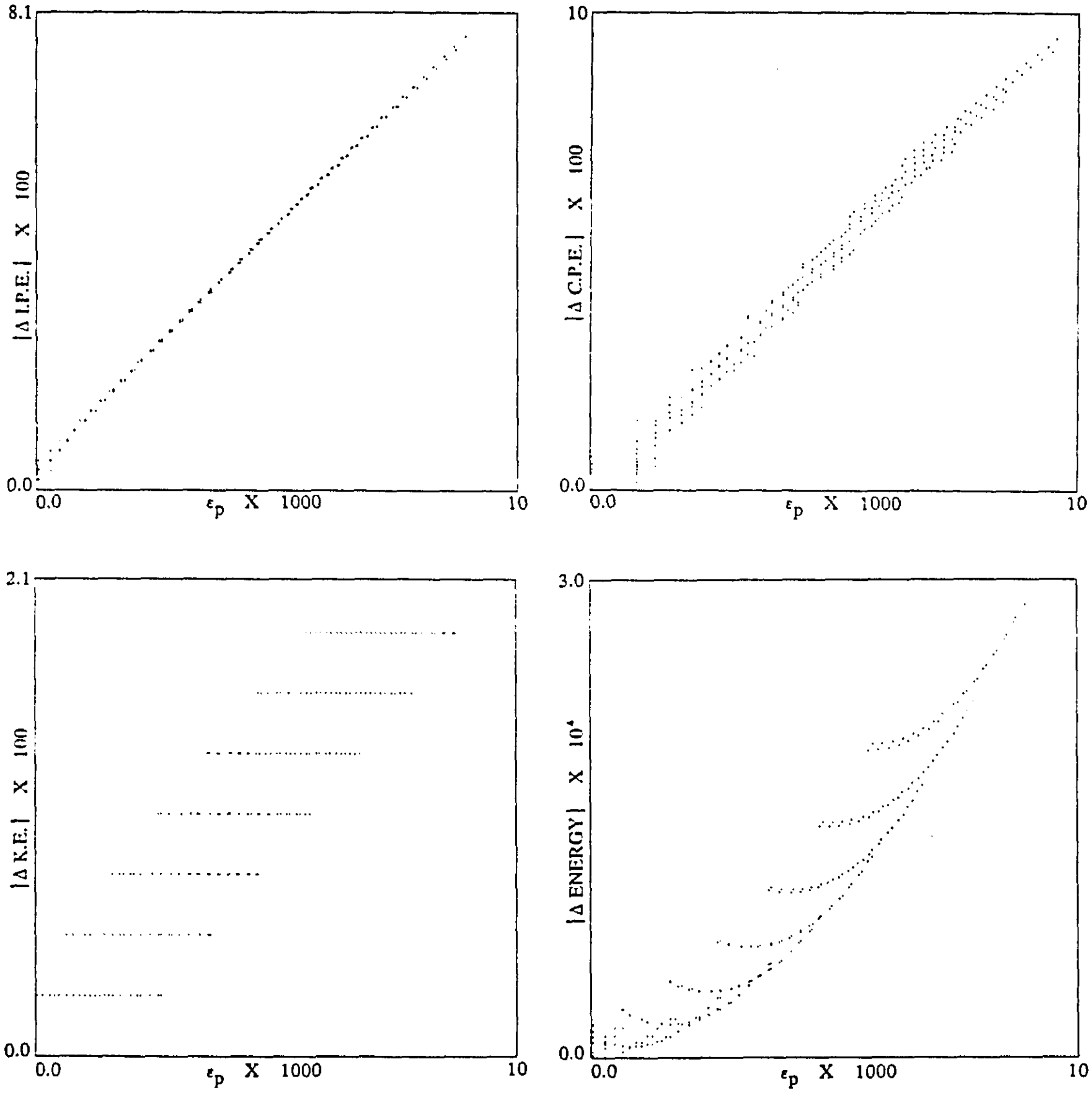


Figure 16. Deviations in interparticle potential energy (I.P.E.), central potential energy (C.P.E.), kinetic energy (K.E.) and total energy (ENERGY) versus ϵ_p.

which is the N dimensional generalization of Eq. (2.4) in Chapter 2. We define the phase space correlation hole. We first define the joint distribution of r_{12} and r_{21}.

$$h(r_{12},p_{12}) = \int \delta(r_{12}-|\mathbf{r}_1-\mathbf{r}_2|)\,\delta(p_{12}-|\mathbf{p}_1-\mathbf{p}_2|)F_2(\mathbf{r}_1,\mathbf{r}_2\,;\,\mathbf{p}_1,\mathbf{p}_2)\,d\mathbf{r}_1\,d\mathbf{r}_2\,d\mathbf{p}_1\mathbf{p}_2 \quad (12.75)$$

where F_2 is the reduced two particle distribution of position and momentum. It is obtained from the N body distribution by

$$F_2(\mathbf{r}_1,\mathbf{r}_2,\mathbf{p}_1,\mathbf{p}_2) = \binom{N}{2}\int F_N(\mathbf{r}_1,\ldots,\mathbf{r}_N,\mathbf{p}_1,\ldots,\mathbf{p}_N)\,d\mathbf{r}_3,\ldots,\,d\mathbf{r}_N\,d\mathbf{p}_3,\ldots,\,d\mathbf{p}_N\,. \quad (12.76)$$

The phase space correlation hole is defined by

$$\Delta(r_{12},p_{12}) = h_e(r_{12},p_{12}) - h_{HF}(r_{12},p_{12}) \quad (12.77)$$

It can be shown that the phase space distribution correlation hole has as its marginals the distributions of Coulson and Nielson[15] in position space and that of Banyard and Reed[2] in momentum space. That is

$$\int h(r_{12},p_{12})\,dp_{12} = f(r_{12}) \quad (12.78)$$

$$\int h(r_{12},p_{12})\,dr_{12} = g(p_{12}) \quad (12.79)$$

We now generalize the correlation hole relative to an operator, that is a physical observable. Consider observable represented by the operator A. We define the correlation hole for that observable by

$$\Delta(a) = \eta_e(a) - \eta_{HF}(a) \quad (12.80)$$

where $\eta(a)$ is the quantum mechanical probability distribution for that observable in the state ψ. If the density matrix in known in the "A" representation, then $\eta(a)$ can be calculated from the diagonal elements of that density matrix. Usually of course one does not have, nor desires to calculate that density matrix and therefore the method described previously can be used to calculate the distribution for A. Suppose for example that A is a one body operator, then its characteristic function is calculated from the first order density matrix

$$M_a(\theta) = \int e^{i\theta a(1)}\rho(1,1')\,d1 \quad (12.81)$$

and the distribution is then given by

$$\eta(a) = \int e^{-i\theta a}M_a(\theta)\,d\theta\,. \quad (12.82)$$

For two body operators we calculate the characteristic function from the second order reduced density matrix

$$M_a(\theta) = \int e^{i\theta A(1,1')}\rho_2(1,2\,;\,1',2')\,d1\,d2\,, \quad (12.83)$$

and again find the joint distribution from Eq.(10.83)

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