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Screening effect in semiconductor superlattices

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City University of New York, 1992

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Screening Effect in Semiconductor Superlattices

by
Buu-Kao Chen

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

1992

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Table of Contents

Chapter I: Introduction

Since the development of the molecular beam epitaxy crystal growth method, many new semiconductor devices have been made in the past few years. One example is a superlattice made by sandwiching two different kinds of thin crystals (the thickness of a crystal layer is from 10 to a few hundred Å) alternately with GaAs and $Al_xGa_{1-x}As$. This ultra-thin multilayer heterostructure semiconductor device has many characteristics such as an ultra-high mobility (above 200,000 $cm^2/v\text{–}sec$)[1] in the direction parallel to the layers (transverse direction) and a high sensitivity Gunn-effect in the layer's direction. For this reason, superlattices have attracted wide attention among physicists and electronic engineers.

The band gap of $Al_xGa_{1-x}As$ (if $x = .3$) is approximately 0.4 ev greater than that of GaAs. Experiments show that 85% of this difference is associated with the conduction band[2]. The conduction band in the GaAs layer is 0.34 ev lower than that in the $Al_xGa_{1-x}As$ layer. If ionized donors are present, conduction electrons will be available to occupy the lower conduction band in the GaAs layer. A similar effect holds if ionized acceptors are present. Either one of these will cause strong band bending. Therefore, using a simple sine or cosine wave function, single square well wave function or Kronig-Penney wave function[3] to calculate the transport coefficient of the superlattice is not adequate.

When GaAs or $Al_xGa_{1-x}As$ is heavily doped (doping > $10^{17}/cm^3$), the mean separation between carriers, r_0 [$r_0 = (3/4\pi\rho)^{1/3}$] is comparable to the solid state Bohr radius $a_{\mathrm{H}} = \varepsilon_b \hbar^2 / m^* e^2$. For this reason, many-body effects of carrier-carrier interaction should be important and calculation for the transport coefficients must include screening effects. However, because the r_s ($r_s = r_0 / a_H$) is not much smaller than 1, the Random Phase Approximation (R. P. A.) screening theory will not be adequate to solve the problem. This means that exchange and correlation effects in the periodic medium have to be taken into consideration.

Studies of superlattice properties have been made in the past few years. However, very few of the investigators considered the periodic medium screening effect. Some of them used a highly simplified wave function for the superlattice, while some used the two dimension electron gas to explain the phenomenon of the superlattice (see the detailed discussion in chapter V). But if the $\mathrm{Ga}_x\mathrm{Al}_{1-x}\mathrm{As}$ layer is thin, the electron wave in the superlattice is far different from the single well particle wave (please refer to chapter V). If the GaAs layer is a few hundred Å thick and/or the $\mathrm{Ga}_x\mathrm{Al}_{1-x}\mathrm{As}$ layer is thin (like 25 Å) the electrons in the superlattice do not actually have a two dimensional behavior. Treating the electron in the superlattice as a two dimensional electron gas will not be adequate for all superlattice crystals. The purpose of this thesis is to derive a method to solve for superlattice screening which includes exchange and correlation effects. A computerized self-consistent method is proposed. This will be described in the following two sections.

A): Since the bent band potential is symmetrical, for $k = 0$ or $k = \pi / L$ (L is the width of GaAs layer plus the width of $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ layer) the wave function will be either symmetrical or antisymmetrical. The eigenenergy and eigenfunction can be easily obtained by Numerov's[4] method (to be described later). Some approaches to get the eigenenergy of $k \neq 0$ and π/L eigenfunction equation will be presented. Hill's procedure[5] is a good method for finding the k value at other energies. The k is then given by

$$k_zL = (\frac{\pi}{2}) \sin^{-1}\left[\prod_n \frac{E_n(k=0)-E}{\frac{\hbar^2}{2m}(nK)^2 - E} \sin^2\left\{\frac{nL}{2}\left[\frac{2m^*}{\hbar^2}\right]^{\frac{1}{2}}\right\}\right]^{\frac{1}{2}} \qquad \text{for} \quad E \geq 0$$

$$k_zL = (\frac{\pi}{2}) \sin^{-1}\left[\prod_n \frac{E_n(k=0)-E}{\frac{\hbar^2}{2m}(nK)^2 - E} \sinh^2\left\{\frac{nL}{2}\left[\frac{2m^*}{\hbar^2}\right]^{\frac{1}{2}}\right\}\right]^{\frac{1}{2}} \qquad \text{for} \quad E < 0$$

in terms of the energies $E_n(k = 0)$ at the zone center. Here $K = 2\pi/L$.

We also want to obtain the numerical value of the matrix element $< i \mid e^{i q_z z} \mid j>$ in order to calculate the polarization Π. We need to find the eigenfunctions. It is difficult to use Hill's procedure to obtain the eigenfunctions in a superlattice. The tight binding approximation is one of the methods that can be used to find eigenfunctions and these eigenfunctions can be used to calculate the numerical values of the matrix element $< i \mid e^{i q_z z} \mid j>$ conveniently. Comparisons between the momentum obtained by the tight binding approximation and Kronig-Penney equations for different eigenenergies in a periodic square well potential will be discussed in chapter V. The comparisons will show that the tight binding approximation often applies well in a superlattice.

B): There are two restrictions in solving for the screening effect. First, because of potential change (the carrier distribution will cause the conduction band bending), the analytical result is not easy to obtain. Use of a numerical self-consistency method to solve the problem is therefore needed (please refer to chapter II). Second, the exchange and correlation effects in screening must be considered (please refer to chapter II). In this thesis, a solution by a self-consistent computer calculation is adopted. The Hartree wave function is replaced by the Hartree-Fock wave function in the Green's function. This Green's function is used to get the zeroth order perturbation polarization function Π^0 and one of the first order perturbation functions Π^A (the exchange polarization term). By this method, many higher order polarization terms will be automatically included in these low order polarization terms. Also, the exchange potential in the Hartree-Fock wave equation needs to be modified by these polarizations. The above mentioned procedure will be discussed in detail later (part of this idea evolved from the paper of D. J. W. Geldart and Roger Taylor[6]. For references, see the historical survey in chapter II).

We believe, by using the above approach, the screening coefficients can be obtained by an iterative self-consistent numerical calculation.

The steps are as follows:

A): The starting point of each iteration is to obtain the single square well potential's eigenenergy and eigenfunction for each sub-band. In the first iteration, the potential is a square well potential. The eigenenergy and eigenfunction can be solved easily. For later iterations, the Numerov-method is used to obtain the eigenfunction and eigenenergy for single potential well for each sub-band. As discussed above, the wave function is a Hartree-Fock wave function. Thus the potential used in the Numerov-method has to be adjusted for exchange and correlation effects (please refer to Section III.4).

B): Equations of a higher order tight binding approximation method are used to get eigenenergies $E_n(\mathbf{k})$, for the wave function which have different wave vector $\mathbf{k}$ and different sub-bands n.

C): From the $E_n(\mathbf{k})$, the doping concentration, and the two dimensional Fermi distribution equation, the Fermi level E_f of the superlattice is obtained.

D): The equations of the higher order tight binding approximation method and the data obtained above (eigenfunction, $E_n(\mathbf{k})$, E_f, etc.) are used to get the real space carrier distribution function (assuming a thermal equilibrium).

E): The real space carrier distribution function is applied to Poisson's equations to obtain the potential (band bending). If the potential change is below a certain limit, the computer calculation is terminated.

From the final computer calculation, a set of data describing the polarization functions Π^0 and Π^A (from step F) can be obtained. These will be self-consistent data.

F): Acquisition of the polarization functions Π^0, Π^A, can be used in determining the screening effect. Also, the exchange potential has to be obtained (please refer to Eq. (3.4.6)). This set of data is needed in step A) Hartree-Fock wave equation. After step F), step A) will be applied again for the next iteration.

I have previously calculated the conducting band bending with the sub-conductor band shift based on the one electron wave function and the electron potential has been adjusted for the effect of non-uniform carrier concentration (a self-consistent method, similar method to that used in this paper except for the omission of screening). The results are shown in Chapter V. These results prove that not only is the band bending appreciable but also the shift of the sub-bands is different for different sub-bands. An obvious effect is that the transformation coefficients are dependent on the energy difference between the sub-bands. Therefore the transformation coefficients are heavily dependent on the difference of the sub-band shifts. In a heavily doped superlattice the screening effect is strong and the potential well is deep and periodically varying. Therefore a simple wave function is not adequate for studying the superlattice characteristics. For the same reason, the homogeneous medium screening function is not suitable for this kind of medium. An accurate screening theory and eigenfunction of a superlattice will enable much better transport coefficients to be obtained.

In chapter II, I will describe some important studies in screening theory. Most of them involve the study of the homogeneous medium. Some important studies on superlattices in recent years and the conceptual difference will also be discussed in that chapter. In Chapter III, theories for this screening calculation will be presented. These include: The Fourier transformation of a two point variable function in a periodic medium; the relationship between the screened electric potential and the external electric potential at the superlattice; the reason for using the Hartree-Fock wave function instead of the Hartree wave function in the Green's function and the polarization function which automatically includes the higher order terms; the polarization function of the superlattice; the two-dimensional Fermi-Dirac distribution and high order tight binding theory.

In Chapter IV, programming procedures are discussed. These include the formulation of Numerov's method, the treatment of singularities by our program, the application of the effective mass concept to simplify the calculation, the approximation of the Π^A result by use of Π^0's data and other necessary formulas for this calculation. Lastly in Chapter V, some numerical results will be presented. These results are obtained by my method in a square well potential or a homogeneous medium. Also, I have applied my method to calculate the screening effect in homogeneous media to compare the results with that of other people. My results compare well with others. The reason for presenting these results is to prove that my proposed method to solve the screening effect in a superlattice is an effective one.

Chapter II Historical Survey

In this chapter, some of the contributions of the screening effect will be described. I will also show that the method used in this thesis to determine the screening effect in a superlattice is an effective one. At present there are just a few papers about the effect of screening on the periodic potential[7,8,9]. Before moving to discuss my method of solving the screening problem in a superlattice, I will describe, in the first section, some important studies of the screening effect in a homogeneous medium with a uniform and a non-uniform background potential. In the second section, I will discuss the reasons why the foregoing studies can not be applied to a superlattice. Explanation as to why my method is a proper one is given (the detailed derivation of the equations of the screening in a superlattice will appear in chapter III). In addition, I will show the comparison between my method and other screening theories as applied to a homogeneous medium.

Section II.1 Screening Theory for a Homogeneous Medium[10] .

The first important theory of screening may be the localized response theory (the Thomas-Fermi Approximation)[11] for a static external field. The starting point of the theory is that the Fermi-level is uniform over the whole medium. A non-screened potential of an impurity charge $\rho_{\mathrm{ext}}(\mathbf{x}) = - \mid e \mid \delta(\mathbf{x})$ is $V_{\mathrm{ext}}(\mathbf{x}) = -\frac{e^2}{\varepsilon_0 x}$ in real space and $V_{\mathrm{ext}}(\mathbf{q}) = \frac{4\pi e^2}{\varepsilon_0 q^2}$ in momentum space. Here ε_0 is the background dielectric constant. The potential already interacts with the background medium and the screening calculated is an additional dielectric response. The Thomas-Fermi screened potential is $V_{\mathrm{sc}}(\mathbf{x}) = \frac{-e^2 e^{-\lambda_{\mathrm{TF}} x}}{x}$ and $V_{\mathrm{sc}}(\mathbf{q}) = \frac{-4\pi e^2}{q^2 + \lambda_{\mathrm{TF}}^2}$ in real space and momentum space respectively; λ_{TF} is the Thomas-Fermi screening length and is independent of $\mathbf{q}$,

$$\lambda_{\mathrm{TF}}^2 = \frac{6\pi n_0 e^2}{E_f} = \frac{4\left(\frac{3}{\pi} n_0\right)^{\frac{1}{3}}}{a_{\mathrm{H}}} \tag{2.1.1}$$

here E_f is the Fermi level , n_0 is the electron concentration and a_{H} is the solid state Bohr radius.

The screening dielectric function can be defined by the relation between an external potential V_{ext} and a screened potential V_{sc}:

$$V_{\mathrm{ext}}(\mathbf{x}) = \int d\mathbf{x}'\, \varepsilon_{\mathrm{sc}}(\mathbf{x}, \mathbf{x}')\, V_{\mathrm{sc}}(\mathbf{x}') \tag{2.1.2}$$

For a homogeneous medium the screening dielectric equation becomes

$$V_{\mathrm{ext}}(\mathbf{x}) = \int d\mathbf{x}'\, \varepsilon_{\mathrm{sc}}(\mathbf{x} - \mathbf{x}')\, V_{\mathrm{sc}}(\mathbf{x}') \tag{2.1.3}$$

in real space and

$$\varepsilon_{sc}(\mathbf{q}) = \frac{V_{ext}(\mathbf{q})}{V_{sc}(\mathbf{q})} \tag{2.1.4}$$

in momentum space. The dielectric function for the Thomas-Fermi approximation is simply

$$\varepsilon_{sc}(\mathbf{q}) = 1 + \frac{\lambda_{TF}^2}{q^2} \tag{2.1.5}$$

We can define some notation here[12]. An external distribution function $\rho_{ext}(\mathbf{x})$ (with units of volume^{-1}) will generate an induced charge distribution $e\ \rho_{indu}(\mathbf{x})$ and the total charge distribution function

$$e\ \rho_{tot}(\mathbf{x}) = e\ \rho_{sc}(\mathbf{x}) = e\ \rho_{ext}(\mathbf{x}) + e\ \rho_{indu}(\mathbf{x}) \tag{2.1.6}$$

In a homogeneous medium the polarization function $\Pi(\mathbf{q})$ and the proper polarization function $\Pi^*(\mathbf{q})$ are defined by

$$\rho_{indu}(\mathbf{q}) \equiv \Pi^*(\mathbf{q})V_{sc}(\mathbf{q}) \equiv \Pi(\mathbf{q})V_{ext}(\mathbf{q}) \tag{2.1.7}$$

These polarization functions differ from the term polarization used in electrostatics. Some books or papers use the opposite sign convention: $\rho_{indu} = -\,\Pi V$.

The Lindhard[13] polarization function (see also Bardeen[14]) obtained by combining the linear electromagnetic response and the Boltzmann transport equation is:

$$\mathrm{Re}\,\Pi_{LH}(\mathbf{q},\,\omega) = -\,\frac{m^*k_f}{\pi\hbar^2} \times \left\{ \frac{1}{2} + \frac{1}{4q}\left[1 - \left(\frac{\omega - q^2}{2q}\right)^2\right] \ln \left| \frac{\omega - 2q + q^2}{\omega - 2q - q^2} \right| + \right.$$

$$\left. \frac{1}{4q}\left[1 - \left(\frac{\omega + q^2}{2q}\right)^2\right] \ln \left| \frac{\omega + 2q + q^2}{\omega - 2q + q^2} \right| \right\} \tag{2.1.8a}$$

$$\mathrm{Im}\,\Pi_{LH}(\mathbf{q},\omega) = \begin{cases} \dfrac{m^* k_f}{4\hbar}\,\dfrac{\omega}{q} & \omega \le |\,2q - q^2\,| \\ \dfrac{m^*}{4\hbar}\,\dfrac{\omega}{q}\left\{1 - \left(\dfrac{\omega - q^2}{2q}\right)^2\right\} & |\,2q - q^2\,| \le \omega \le 2q + q^2 \\ 0 & \omega \ge 2q + q^2 \end{cases} \qquad (2.1.8b)$$

here q is the wave vector in units of q_f, ω is in units of $\frac{E_f}{\hbar}$, where q_f and E_f are the Fermi Momentum and Fermi Energy.

The same results can be obtained by using perturbation theory of one particle Quantum Mechanics or by calculating to the lowest order polarization function in many body theory. We know that in a homogeneous medium the potential in momentum space can be expressed by

$$V(\mathbf{q}) = \Phi(\mathbf{q})\,\rho(\mathbf{q}) \qquad (2.1.9)$$

here $\Phi(\mathbf{q}) = \frac{4\pi e^2}{q^2}$ is the Coulomb potential in momentum space and $\rho(\mathbf{q})$ is the momentum space density function. From Eq. (2.1.4), (2.1.6) and (2.1.7) we can get

$$\varepsilon_{sc}(\mathbf{q}) = 1 - \Pi^*(\mathbf{q})\,\Phi(\mathbf{q}) \qquad (2.1.10)$$

$$\varepsilon_{sc}(\mathbf{q}) = \frac{1}{1 + \Pi(\mathbf{q})\,\Phi(\mathbf{q})} \qquad (2.1.11)$$

Eq. (2.1.7) and (2.1.10) can be interpreted by[15,16,17]

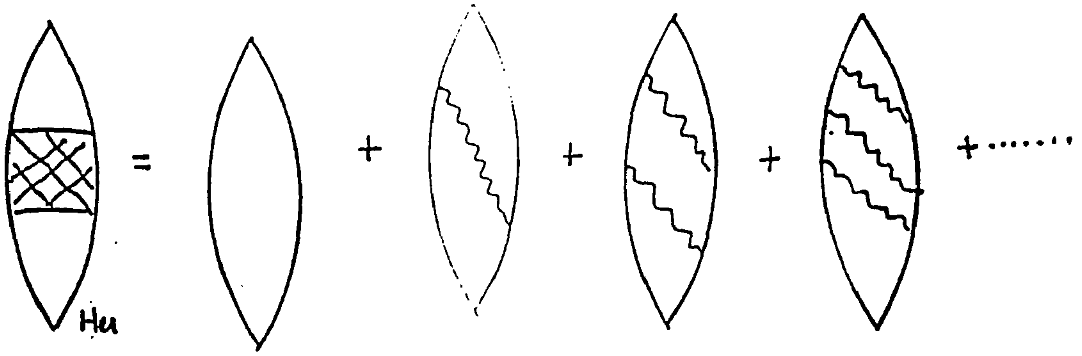
$$\rho_{indu}(\mathbf{q}) = \Pi^*(\mathbf{q}) V_{sc}(\mathbf{q}) = \Pi^*(\mathbf{q})[\, V_{ext}(\mathbf{q}) + V_{indu}(\mathbf{q})\,]$$

$$= \Pi^*(\mathbf{q})[\, V_{\mathrm{ext}} + \Phi(\mathbf{q})\rho_{\mathrm{indu}}(\mathbf{q}) \,] \tag{2.1.12}$$

which can be solved iteratively. The R.P.A. (Random Phase Approximation) screening equation[15,16,17] is to use $\Pi_{LH}(\mathbf{q})$ instead of the $\Pi^*(\mathbf{q})$ in Eq. (2.1.12). The R.P.A. may be the most accurate screening equation if the exchange and correlation interaction can be omitted. Also, when $\omega = 0$ and $| q | << 1$ the R.P.A. screening equation is an approximation to the Thomas-Fermi approximation.[18]

Adler[7] uses electromagnetic response and the single particle Louville equation to solve the screening problem in a periodic medium. M. H. Cohen and his co-worker[8,9] solve the many-body problem for a self-consistent Hartree crystal potential. If we omit exchange and correlation interactions and apply a suitable superlattice's eigenenergies and eigenfunctions to the equations in those papers, the screening problem can be resolved. The equations which I will derive in chapter III have similar characteristics. In addition, I have considered higher order perturbation term, but only for static external potential.

Hubbard[19] was the first one to consider the exchange contribution to screening. His Feynman diagram of polarization function is



and he made an approximation that the major contribution of the exchange interaction occurs for momentum equal to $\mathbf{k} + \mathbf{q}_f$ (here $\mathbf{k}$ is the momentum of the polarization function and $\mathbf{q_f}$ is the Fermi momentum of electron). He got the relation between the polarization function with the exchange interaction and the polarization function without the exchange interaction is

$$\Pi_{\mathrm{HU}}(k) = \frac{\Pi^0(k)}{1 + \frac{1}{2}\frac{k^2}{k^2 + q_f^2}\,\Phi(\mathbf{k})\,\Pi^0(k)} \tag{2.1.13}$$

(see Appendix A, which shows how Hubbard derived this equation and why this equation can not be applied to a superlattice medium). For this reason, we can, without approximation, express the polarization function that includes exchange and correlation in terms of the one that omits exchange and correlation in the form:

$$\Pi_{\mathrm{xc}}(\mathbf{q},\omega) = \frac{\Pi_{\mathrm{no,\,xc}}(\mathbf{q},\,\omega)}{1 + G(\mathbf{q})\,\Phi\,(\mathbf{q})\Pi_{\mathrm{no,\,xc}}(\mathbf{q},\,\omega)} \tag{2.1.14}$$

where $G(\mathbf{q})$ is to be found. The $G(\mathrm{q})$ of Hubbard's exchange term is simply

$$G_{\mathrm{Hu}}(\mathbf{q}) = \frac{1}{2}\,\frac{q^2}{q^2 + q_f^2} \tag{2.1.15}$$

Singwi[20] discovered that $G(\mathrm{q})$ is related to the two point distribution function. The real space two particle distribution function $f(\mathbf{r}_1,\,\mathbf{r}_2)$ can be approximated as

$$f(\mathbf{r}_1,\,\mathbf{r}_2) = f(\mathbf{r}_1)\,f(\mathbf{r}_2)\,g(\mathbf{r}_1 - \mathbf{r}_2) \tag{2.1.16}$$

here $f(\mathbf{r})$ is a one particle distribution function. The Fourier transformation of $g(\mathbf{r}) - 1$ is $\frac{1}{n_0}\,[S(\mathbf{q}) - 1]$, where $S(\mathbf{q})$ is dynamic form factor and n_0 is the electron density in the absence of an external potential. Moreover, $S(\mathbf{q})$ is related to $\varepsilon_{\mathrm{xc}}(\mathbf{q},\,\omega)$ by a sum rule (see D. Pine[15] p129-131)

$$S(\mathbf{q}) = -\frac{\hbar^2 q^2}{4\pi e^2 n_0}\int_0^\infty \mathrm{Im}\,[\,\varepsilon_{xc}(\mathbf{q},\,\omega)\,]^{-1}\,d\omega \tag{2.1.17}$$

Singwi[20] derived the following relation between $G(\mathbf{q})$ and $S(\mathbf{q})$:

$$G(\mathbf{q}) = -\frac{1}{n_0}\int \frac{\mathbf{q}\cdot\mathbf{q}'}{q^2}\,[S(\mathbf{q}-\mathbf{q}') - 1\,]^{-1} d^3q' \tag{2.1.18}$$

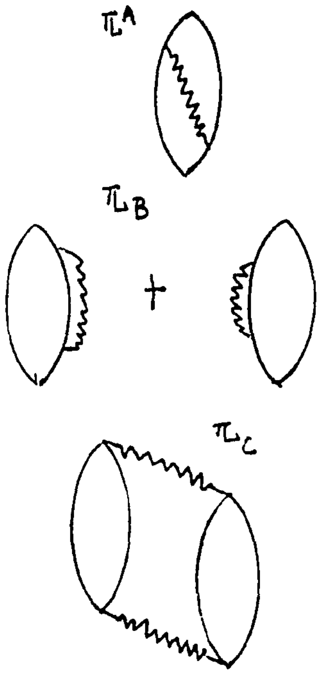
within the approximation Eq. (2.1.16). The dielectric function which takes into account exchange and correlation interaction can be expressed (see Eq.(2.1.10)) by

$$\varepsilon_{xc}(\mathbf{q},\,\omega) = 1 - \Pi_{xc}(\mathbf{q},\,\omega)\Phi(\mathbf{q}) \tag{2.1.19}$$

Eq.s (2,1,14), (2,1,17), (2.1.18) and (2.1.19) have to be solved simultaneously to satisfy self-consistency.

From the above discussion, we know that the functions $\varepsilon_{xc}(\mathbf{q},\,\omega)$, $g(\mathbf{r})$ and $G(\mathbf{q})$ are related to each other. Since $g(\mathbf{r})$ has definite limiting values ($g(0) = 0$ and $g(\infty) = 1$), we can determine whether an $\varepsilon_{xc}(\mathbf{q},\,\omega)$ is good or not from $G(\mathbf{q})$ ($g(\mathbf{r})$) or obtain $\varepsilon_{xc}(\mathbf{q},\,\omega)$ from $G(\mathbf{q})$ ($g(\mathbf{r})$). Singwi and his co-workers[20] and Shaw[21] have shown that $g(\mathbf{r})$ derived from Hubbard's $G(\mathbf{q})$ or modified Hubbard's $G(\mathbf{q})$ (modified by Sham[22]) is negative when $q_f r$ is < 1 with $r_s > 2$, where q_f is Fermi momentum, r_s having been described in chapter I. This is due to an overestimation of the short range correlations between particles. Shaw[21], Toigo and Woodruff[23], Singwi and his co-workers[20,24,25] and Brosens, Lemmens and DeVreese[26–28] have tried different methods to improve the value of $G(\mathbf{q})$. Most of them have the value of $g(\mathbf{r})$ still slightly negative when $r\, q_f \approx 0$ and r_s is large.

Geldart and Vosko[30] and Geldart and Taylor[6] obtained the polarization function by including polarization terms of the lowest exchange, the lowest Hartree-Fock and an approximation Π_c (lowest figure in the left, Geldart and Toylar call it Π^c). Singwi and his co-worker[31] showed that their "two particle distribution function" can be comparable with those of Geldart and Taylor[6] and Brosens, Lemmens and DeVreese's[26-28] $G(\mathbf{q}, \omega)$.



Section II.2 Reasons for Using the Self-Consistency Method To Solve the Screening Effect in a Superlattice

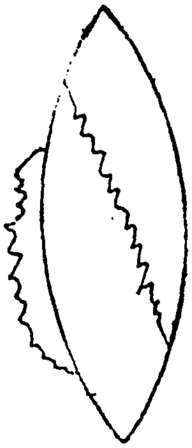
The major problem in obtaining the screening effect in a superlattice is that the lattice width (thickness of the layers) is of the same order or smaller than the Thomas-Fermi screening length and the reciprocal of the Fermi momentum (In most cases the thickness of the GaAs or $Al_xGa_{1-x}As$ layer is from 25 Å to 250 Å; when the doping is 10^{17} then $1/\lambda_{TF} = 88$ Å; $1/k_f = 69.6$ Å; $r_s = r_0/a_H = 1.22$; when the doping is 10^{19} then $1/\lambda_{TF} = 34$ Å; $1/k_f = 15$ Å; $r_s = 0.26$), and the potential well is deep (.3 ev).

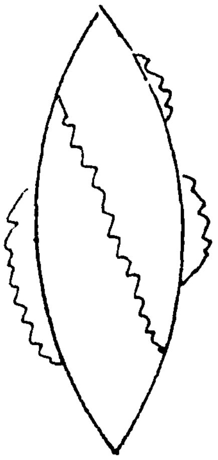
Kohn and Sham[32, 33] have derived the screening equations for a slowly varying potential. However, they are not suitable when applied to a periodically rapidly varying potential like that in a superlattice. Stern and Howard[34] have derived the screening at an inversion layer. It is inadequate to simplify the superlattice potential to that of a single well potential.

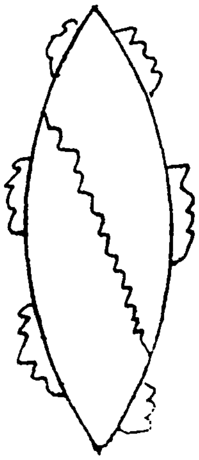
The potential in a superlattice is periodically varying and r_s is not much smaller than 1. The effects of exchange and correlation in screening of the periodic potential must also be considered. We should use a method similar to that of Singwi, et al, to obtain a polarization function which includes the exchange and correlation interaction. We have to obtain a good value of $G(\mathbf{q})$, then substitute it into Eq. (2.1.12) to adjust the polarization function when the exchange and correlation interaction has not been considered. Problems arise when this method is used to solve the screening effect in a superlattice. Since the convolution theorem for the Fourier transformation is not applicable to a non-uniform medium, all equations which are required in this method (especially Eq. (2.1.12), see Appendix.A) have to be modified, and these modifications are not simple.

Since the electron potential is changed by the carrier distribution, analytical results can not be easily obtained (example: the eigenfunction and Fermi level, etc.). Therefore, computer calculations must be used. In such calculations, it is as easy to use the Hartree-Fock wave function as the Hartree wave function in the polarization function calculation. The Hartree-Fock wave function instead of the Hartree wave function is used in calculating the zeroth order polarization function Π^0. This Π^0 will automatically include the Hartree-Fock polarization function (please refer to chapter III. Geldart and Taylor[6] has only the lowest order Hartree-Fock polarization function). In other words, our Π^0 automatically includes some of the exchange and correlation effects.

On the other hand, if we use $G(\mathbf{q})$ to adjust a no exchange and correlation polarization function to obtain a polarization function which includes the exchange and correlation interaction, the lowest order polarization function must still be calculated. Yet the G in a non-homogeneous periodic medium (no longer a function of just $\mathbf{q}$) is not as easy to obtain. From the above discussion, we know that using Singwi's[20,21,24-29] method of handling the screening problem is not convenient in a superlattice. This is the major reason why a new self-consistency method is required. The Hartree-Fock wave function is used to calculate the exchange polarization function Π^B (the Π^A, Π^B, Π^C, as defined by Geldart and Taylor[6]). Our Π^B will automatically include a lot of Hartree-Fock polarization functions and exchange polarization functions (some of those Feynman diagrams are:







etc). In this thesis, the Geldert and Taylor's[6] Π^c polarization function is not calculated. Instead, I include many higher order Hartree-Fock polarization functions and use the interaction potential to calculate the exchange polarization function which is the screened potential (instead of the bare electron-electron interacting potential or the Thomas-Fermi potential, as used in most calculations). I feel confident that my screening theory is better than that of Geldart and Taylor[6]. Many investigators used the two particle distribution function $G(\mathbf{q})$ ($g(\mathbf{r})$) to determine whether the screening equation has involved a proper exchange and correction adjustment or not. Here I use my method (which will be used to find the screening effect in a superlattice) to calculate the screening effect in the homogeneous medium. Comparing my $G(\mathrm{q})$ with the $G(\mathbf{q})$ of other screening theories (Singwi and his co-worker[31], Geldart and Taylor[6] and Brosens, Lemmens and DeVreese's[26–28]) in homogeneous medium as shown in chapter V, Figure 5-9, my $G(\mathbf{q})$ compares well with others[28] (my curve is between "Hubbard" and "Toigo and Woodruff"). This proves that my proposed method involves the exchange and correlation effects and has also considered periodicity characteristics.

Chapter III The Equations of Screening Theory and The Tight Binding Approximation in a Superlattice

Section III.1 Fourier Representation of Superlattice Properties

In order to find the relationship between the Fourier component of the screened electric potential and the Fourier component of the external electric potential in a superlattice, I will try first to obtain the Fourier transformation of a two point function (two position variable) in a medium which is homogeneous in two dimensions and periodic in the third dimension.

An arbitrary two point function $f(\mathbf{x}_1, \mathbf{x}_2)$ in any medium has a Fourier component $A(\mathbf{k}_1, \mathbf{k}_2)$ which is given by

$$A(\mathbf{k}_1, \mathbf{k}_2) = \int d\mathbf{x}_1 \int d\mathbf{x}_2 f(\mathbf{x}_1, \mathbf{x}_2)\, e^{-i\,\mathbf{k}_1 \cdot \mathbf{x}_1} e^{i\,\mathbf{k}_2 \cdot \mathbf{x}_2} \tag{3.1.1}$$

Let $\mathbf{y}_1 = \dfrac{\mathbf{x}_1 + \mathbf{x}_2}{2}$, $\mathbf{y}_2 = \mathbf{x}_1 - \mathbf{x}_2$, then

$$A(\mathbf{k}_1, \mathbf{k}_2) = \int d\mathbf{y}_1 d\mathbf{y}_2\, f(\mathbf{y}_1, \mathbf{y}_2)\, e^{-i\,\mathbf{y}_1 \cdot (\mathbf{k}_1 - \mathbf{k}_2)} e^{-i\,\frac{1}{2}\,\mathbf{y}_2 \cdot (\mathbf{k}_1 + \mathbf{k}_2)} \tag{3.1.2}$$

Where the Jacobin $J\left[\dfrac{\mathbf{y}_1, \mathbf{y}_2}{\mathbf{x}_1, \mathbf{x}_2}\right] = 1$, can be omitted.

If a substance is homogeneous in $\mathbf{x}$ space, translation invariance requires $f(\mathbf{y}_1, \mathbf{y}_2)$ to be independent of $\mathbf{y}_1$, so that

$$A(\mathbf{k}_1,\ \mathbf{k}_2) = (2\pi)^{3/2}\ \delta(\mathbf{k}_1 - \mathbf{k}_2) \int d\mathbf{y}_2\ f(\mathbf{y}_2)\ e^{-i\frac{1}{2}\mathbf{y}_2\cdot(\mathbf{k}_1+\mathbf{k}_2)} \tag{3.1.3}$$

Multiplying both sides by $\int \frac{d\mathbf{k}_2}{(2\pi)^3}$, the Fourier transfer of $f(\mathbf{x}_1 - \mathbf{x}_2)$ is dependent only upon $\mathbf{k}_1$.

$$B(\mathbf{k}_1) = \int \frac{d\mathbf{k}_2}{(2\pi)^3} A(\mathbf{k}_1,\ \mathbf{k}_2) = \int d\mathbf{x}_2\ f(\mathbf{x}_1,\ \mathbf{x}_2)\ e^{-i\mathbf{k}_1\cdot(\mathbf{x}_1-\mathbf{x}_2)} \tag{3.1.4}$$

This is a formula commonly found in most text books. On the other hand, we know that the Fourier component in a periodic medium exists only when $\mathbf{k}_1 - \mathbf{k}_2 = m_i\mathbf{k}_i + m_j\mathbf{k}_j + m_k\mathbf{k}_k = \mathbf{K}$, where $(\mathbf{k}_i,\ \mathbf{k}_j,\ \mathbf{k}_k)$ are, respectively, unit vectors of a periodic structure.

$$A(\mathbf{k}_1,\ \mathbf{k}_2) = \int d\mathbf{y}_1\ d\mathbf{y}_2 f(\mathbf{y}_1,\ \mathbf{y}_2)\ e^{-i\mathbf{y}_1\mathbf{K}}\ e^{-i\frac{1}{2}\mathbf{y}_2\cdot(\mathbf{k}_1+\mathbf{k}_1+\mathbf{K})}$$

$$= \int d\mathbf{x}_1\ d\mathbf{x}_2 f(\mathbf{x}_1,\ \mathbf{x}_2)\ e^{-i\mathbf{k}_1\cdot\mathbf{x}_1} e^{i(\mathbf{k}_1+\mathbf{K})\cdot\mathbf{x}_2} \tag{3.1.5}$$

For a superlattice which has periodic structure in the z direction and is homogeneous in the $\mathbf{x}$ and $\mathbf{y}$ directions (it is assumed throughout this thesis that the layer's direction is the z direction), we have

$$A(\mathbf{k}_1,\ \mathbf{k}_1 + m\frac{2\pi}{L}\hat{z}) = \int d\mathbf{x}_1 d\mathbf{x}_2 f(\mathbf{x}_1,\ \mathbf{x}_2)\ e^{-i\mathbf{k}_1\cdot\mathbf{x}_1} e^{i(\mathbf{k}_1+m\frac{2\pi}{L}\hat{z})\cdot\mathbf{x}_2} \tag{3.1.6}$$

where L is the width of GaAs layer plus the width of $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ layer; $\hat{z}$ is a unit vector in z direction.

Section III.2 The Equation of Electrostatics for a Superlattice

In this section, I would like to discuss the relationship between the external electric potential and the screened electric potential in a superlattice. The electric field $\mathbf{E}(\mathbf{x})$ can be expressed by

$$\mathbf{E}(x) = -\nabla \int dx' \left[\frac{e\rho_{\text{ext}}(\mathbf{x})}{|\mathbf{x}-\mathbf{x}'|} + \mathbf{P}(\mathbf{x}') \cdot \nabla' \frac{1}{|\mathbf{x}-\mathbf{x}'|} \right] \tag{3.2.1}$$

The external charge density $e\rho_{\text{ext}}(\mathbf{x})$ is the electron distribution function and $\mathbf{P}(\mathbf{x}')$ is the polarization vector of electrostatics. $e\rho_{\text{ext}}(\mathbf{x})$ is also called the free charge density or test charge density. Here we define the induced charge density as $e\rho_{\text{indu}}(\mathbf{x}) = -\nabla' \cdot \mathbf{P}(\mathbf{x}')$. (Others call ρ_{indu} the polarization charge density). After integration by parts Eq. (3.2.1) becomes:[35]

$$\mathbf{E}(\mathbf{x}) = -\nabla \left\{ \int dx' \frac{e\rho_{\text{ext}}(\mathbf{x}') + e\rho_{\text{indu}}(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} + \int dS \frac{\mathbf{P}(\mathbf{x}) \cdot \hat{\rho}}{|\mathbf{x}-\mathbf{x}'|} \right\} \tag{3.2.2.}$$

The integration region is very large. The surface only locates at the position which $|\mathbf{x}-\mathbf{x}'|$ is very large. The integration $\int \frac{d\mathbf{x}'}{|\mathbf{x}-\mathbf{x}'|}$ is much larger than the integration $\int \frac{d\mathbf{S}}{|\mathbf{x}-\mathbf{x}'|}$, the last term can be omitted. Eq. (3.2.2.) can be simplified to:

$$E(\mathbf{x}) = -\nabla \int dx' \frac{e\rho_{\text{tot}}(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} \tag{3.2.3a}$$

here $\rho_{\text{tot}}(\mathbf{x}) = \rho_{\text{sc}}(\mathbf{x}) = \rho_{\text{ext}}(\mathbf{x}) + \rho_{\text{indu}}(\mathbf{x})$. The displacement field $\mathbf{D}(\mathbf{x})$ is defined by

$$\mathbf{D}(\mathbf{x}) = -\nabla \int dx' \frac{e\rho_{\text{ext}}(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} \tag{3.2.3b}$$

In a non-homogeneous medium the relation between $\mathbf{D}(\mathbf{x})$ and $\mathbf{E}(\mathbf{x})$ in a superlattice should be expressed by

$$\mathbf{D}(\mathbf{x}) = \int d\mathbf{x}' \; \bar{\bar{\varepsilon}}(\mathbf{x}, \mathbf{x}') \cdot \mathbf{E}(\mathbf{x}') \tag{3.2.4}$$

rather than by $\mathbf{D}(\mathbf{x}) = \bar{\bar{\varepsilon}} \cdot \mathbf{E}(\mathbf{x})$, as used in homogeneous substances. Therefore, the dyadic $\bar{\bar{\varepsilon}}(\mathbf{x}, \mathbf{x}')$ is not just a function of the difference $\mathbf{x} - \mathbf{x}'$. Here we restrict ourselves to consider the linear response in the screening effect. It is convenient to calculate the screening effect on the electric potential, since the potential is a scalar. It is better to replace Eq. (3.2.4.) by a scalar relation

$$\Phi_{\mathrm{ext}}(\mathbf{x}) = \int d\mathbf{x} \; \eta(\mathbf{x}, \mathbf{x}')\Phi_{\mathrm{sc}}(\mathbf{x}') \tag{3.2.5}$$

where $\eta(\mathbf{x}, \mathbf{x}')$ is an inverse potential response function, $\Phi_{\mathrm{sc}}(\mathbf{x})$ is the screened electric potential $\mathbf{E}(\mathbf{x}) = -\nabla\Phi_{\mathrm{sc}}(\mathbf{x})$ and $\Phi_{\mathrm{ext}}(\mathbf{x})$ is the external electric potential $\mathbf{D}(\mathbf{x}) = -\nabla\Phi_{\mathrm{ext}}(\mathbf{x})$. The corresponding equation in wave-vector space can be written as

$$\Phi_{\mathrm{ext}}(\mathbf{k}) = \int \frac{d\mathbf{k}'}{(2\pi)^3}\eta(\mathbf{k}, \mathbf{k}')\Phi_{\mathrm{xc}}(\mathbf{k}') \tag{3.2.6}$$

where $\eta(\mathbf{k}, \mathbf{k}') \equiv \int \eta(\mathbf{x}, \mathbf{x}') \, e^{-i\mathbf{k}\cdot\mathbf{x}} e^{i\mathbf{k}'\cdot\mathbf{x}'} d\mathbf{x} \, d\mathbf{x}'$. The relationship between $\bar{\bar{\varepsilon}}$ and η is

$$\eta(\mathbf{x}, \mathbf{x}') = \sum_{i,j} \int \frac{d\mathbf{x}}{|\mathbf{x} - \mathbf{x}'|} \frac{\partial}{\partial x_i'} \frac{\partial}{\partial x_j'} \varepsilon_{i,j}(\mathbf{x}', \mathbf{x}') \frac{1}{4\pi} \tag{3.2.7}$$

in real space, and

$$\eta(\mathbf{k}', \mathbf{k}) = \sum_{i,j} \frac{\mathrm{k_I} \cdot \mathrm{k'_j}}{(\mathrm{k_j}')^2} \varepsilon_{i,j}(\mathbf{k}', \mathbf{k}) \tag{3.2.8}$$

in momentum space. We define the direct response function $\chi(\mathbf{k}', \mathbf{k})$ by

$$\Phi_{\mathrm{sc}}(\mathbf{k}) = \int \frac{d\mathbf{k}}{(2\pi)^3} \chi(\mathbf{k}, \mathbf{k}')\Phi_{\mathrm{ext}}(\mathbf{k}) \tag{3.2.9}$$

The reciprocal of this equation can exist if we can find a function of $\chi(\mathbf{k}', \mathbf{k})$ such that

$$\frac{\int d\mathbf{k}'}{(2\pi)^3}\,\eta(\mathbf{k}',\,\mathbf{k}')\,\chi(\mathbf{k}',\,\mathbf{k}) = (2\pi)^3\delta(\mathbf{k}-\mathbf{k}') \qquad (3.2.10)$$

For a superlattice

$$\eta(\mathbf{k},\,\mathbf{k}') = (2\pi)^3\eta(\mathbf{k}_\perp,\,k_z;\,\mathbf{k}_\perp',\,k_z{}') \cdot \delta\,(\mathbf{k}_\perp-\mathbf{k}_\perp')\;\delta\,(\mathbf{k}_z-\mathbf{k}_z{}'+nK) \qquad (3.2.11)$$

where $K = 2\pi\,/L$, $\mathbf{k}_\perp = k_x\hat{x} + k_y\,\hat{y}$ and $\hat{z}$ is the layer's direction.

$$\Phi_{\text{ext}}(\mathbf{k}_\perp,\,k_z) = \int\frac{d\mathbf{k}'}{(2\pi)^3}\,\eta(\mathbf{k},\,\mathbf{k}')\,\Phi_{\text{xc}}(\mathbf{k}_\perp{}',\,k_z{}')$$

$$= \sum_N \eta(\mathbf{k}_\perp,\,k_z;\,\mathbf{k}_\perp,\,k_z+nK)\,\Phi_{\text{sc}}(\mathbf{k}_\perp,\,\mathbf{k}_z+nK) \qquad (3.2.12)$$

Let $k_z = k_z{}' + mK$, $|\,k_z{}'\,| \le K/2 = \pi\,/L$ and $m+n=m'$ Then

$$\Phi_{\text{ext}}(\mathbf{k}_\perp,\,k_z{}''+mK) = \sum_{m'}\eta(\mathbf{k}_\perp,\,k_z{}''+mK;\,\mathbf{k}_\perp,\,k_z{}''+m'K)\,\Phi_{\text{sc}}(\mathbf{k}_\perp,\,k_z{}''+m'K) \qquad (3.2.13)$$

Let $\Phi\,(\mathbf{k}_\perp,\,k_z)$ be a column vector, with m^{th} element $\Phi(\mathbf{k}_\perp,\,k_z+mK)$ and $\overline{\overline{\Lambda}}(\mathbf{k}_\perp,\,k_z)$ a matrix, and its element $\Lambda_{m,\,m'}$ is $\eta(\mathbf{k}_\perp,\,k_z+mK;\,\mathbf{k}_\perp,\,k_z+m'\,K)$. Then Eq. (3.2.12) can be expressed as

$$\Phi_{\text{ext}}(\mathbf{k}_\perp,\,k_z) = \overline{\overline{\Lambda}}\,(\mathbf{k}_\perp,\,k_z)\,\Phi_{\text{sc}}(\mathbf{k}_\perp,\,k_z) \qquad (3.2.14)$$

Similarly, we can define matrix a $\overline{\overline{X}}(\mathbf{k}_\perp,\,k_z)$ in such a way that $\overline{\overline{X}}(\mathbf{k}_\perp,\,k_z) = [\overline{\overline{\Lambda}}(k_\perp,\,k_z)]^{-1}$. Then the screened potential vector is $\Phi_{\text{sc}}(\mathbf{k}_\perp,\,k_z) = \overline{\overline{X}}(\mathbf{k}_\perp,\,k_z)\,\Phi_{\text{ext}}\,(\mathbf{k}_\perp,\,k_z)$.

An example of an application of the above equations follows:

Example: $V(\mathbf{x}_1,\,\mathbf{x}_2)$ is the interaction energy for two electrons at $\mathbf{x}_1$ and $\mathbf{x}_2$. $V(\mathbf{x}_1,\,\mathbf{x}_2)$ is equal to that of an electric charge $-\,|\,e\,|$ located at $\mathbf{x}_1$ interacting with a potential which is generated by an electric charge $-\,|\,e\,|$ located at $\mathbf{x}_2$. $\Phi_{\text{sc}}(\mathbf{k}_\perp,\,k_z+mK)$ is the

Fourier component of the screened potential which is generated by electric charge located at $\mathbf{x}_2$. And we know that the Fourier component of the non-screened potential which is generated by the electric charge located at $\mathbf{x}_2$ is $\frac{-4\pi\ |e|}{k_\perp^2 + (k_z + m'K)^2}$ then

$$V(\mathbf{x}_1,\, \mathbf{x}_2) = -\ |e|\int \frac{d\mathbf{k}_\perp}{(2\pi)^2}\int_{-\frac{\pi}{L}}^{\frac{\pi}{L}} \frac{dk_z}{(2\pi)} \sum_m \Phi_{sc}(\mathbf{k}_\perp,\, k_z + mK)\ \exp[\, i\ (k_\perp \cdot \rho_1 + (k_z + mK)\cdot z_1)\,]$$

$$= \int \frac{d\mathbf{k}_\perp}{(2\pi)^2}\int_{-\frac{\pi}{L}}^{\frac{\pi}{L}} \frac{dk_z}{2\pi} \sum_m \sum_{m'} \frac{4\pi e^2}{k_\perp^2 + (k_z + m'k)^2} X(\mathbf{k}_\perp,\, k_z + mK;\, \mathbf{k}_\perp,\, k_z + m'K)$$

$$\times \exp[i\ (\mathbf{k}_\perp \cdot \rho_1 + (k_z + mk)\cdot z_1)]\ \exp[-\, i\ (\mathbf{k}_\perp \cdot \rho_2 + (k_z + m'K)\cdot z_2)\,] \qquad (3.2.15)$$

This can be rewritten as a "Fourier Series"

$$V(\mathbf{x}_1,\, \mathbf{x}_2) = \int \frac{d\mathbf{k}_\perp}{(2\pi)^2}\int_{-\frac{\pi}{L}}^{\frac{\pi}{L}} \frac{dk_z}{(2\pi)} \sum_m \sum_{m'} \exp[\, i\ (\ \mathbf{k}_\perp \cdot \rho_1 + (k_z + mK)\cdot z_1)\,]$$

$$\times\, V(\mathbf{k}_\perp,\, k_z + mK;\, \mathbf{k}_\perp,\, k_z + m'K)\cdot \exp\,[\, -\, i\ (\ \mathbf{k}_\perp \cdot \rho_2 + (k_z + m'K)\cdot z_2)\,] \qquad (3.2.16)$$

Eq. (3.2.15) and (3.2.16) will be used in the later section.

III.3 The Linear Response Theory

In this section many-body theory will be used to describe the polarization function of a superlattice. Explanation will also be provided of the use of the Hartree-Fock wave function instead of the Hartree wave in Green's function and of the application of this Green's function method to evaluate the low order perturbation polarization function. This low order perturbation polarization function will automatically include some of the higher order perturbation polarization corrections.

Before deriving the relevant equations to explain the polarization function for a superlattice, I would like to explain the difference between the "potential" used in the electric field and that used in the Schrodinger equation. In an electric field the potential refers to how much energy a charged particle will have, the dimension is energy/(charge unit). In the Schrodinger equation, the potential means how much energy a particle possesses so it has the dimension of energy. The calculations in this thesis deal with electrons. For this reason, $U(\mathbf{x})$ will be used to denote the Schrodinger potential, since $U(\mathbf{x}) = -|e|\Phi(\mathbf{x})$. Also, for the convenience of later calculations, $\rho(\mathbf{x})$ is the electron distribution function which does not have a charge unit. The potential functions are

$$U_{\text{ext}}(\mathbf{x}) = \int d\mathbf{x}' \frac{e^2 \rho_{\text{ext}}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} \tag{3.3.1a}$$

$$U_{\text{sc}}(\mathbf{x}) = \int d\mathbf{x}' \frac{e^2 \rho_{\text{sc}}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} \tag{3.3.1b}$$

$$U_{\text{ext}}(\mathbf{x}) = \int d\mathbf{x}' \eta(\mathbf{x}, \mathbf{x}') U_{\text{sc}}(\mathbf{x}) \tag{3.3.1c}$$

where the self-consistent potential is the sum of external and induced potential since $\rho_{\text{sc}}(\mathbf{x}) = \rho_{\text{ext}}(\mathbf{x}) + \rho_{\text{indu}}(\mathbf{x})$. The polarization function $\Pi(\mathbf{x}, \mathbf{x}')$ and proper polarization function $\Pi^*(\mathbf{x}, \mathbf{x}')$ are defined by

$$\rho_{\mathrm{indu}}(\mathbf{x}) = \int d\mathbf{x}'\Pi^*(\mathbf{x}, \mathbf{x}')U_{\mathrm{sc}}(\mathbf{x}') = \int d\mathbf{x}'\Pi(\mathbf{x}, \mathbf{x}')U_{\mathrm{ext}}(\mathbf{x}') \tag{3.3.2}$$

In a Feynman diagram presentation, the proper polarization $\Pi^*(\mathbf{x}, \mathbf{x}')$ only includes linked and no repetition (no iteration) diagrams. From Eq. (3.3.1c) and (3.3.2) we get

$$\eta(\mathbf{x}, \mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}') - \int \frac{e^2\Pi^*(\mathbf{x}'', \mathbf{x}')}{|\mathbf{x} - \mathbf{x}''|}d\mathbf{x}'' \tag{3.3.3}$$

In the three dimensional homogeneous case, the Fourier representation of this equation is

$$\eta(\mathbf{k}, \mathbf{k}') = (2\pi)^3\, \delta_{\mathbf{k},\, \mathbf{k}'}\left(1 - \frac{4\pi e^2}{k^2}\Pi^*(\mathbf{k},\mathbf{k}') \right) \tag{3.3.4}$$

For a superlattice, we have

$$\eta(\mathbf{k}_\perp,\, k_z + mK;\, \mathbf{k}_\perp,\, k_z + m'K) =$$

$$\delta(m, m') - \frac{4\pi e^2}{[k_\perp^2 + (k_z + mK)^2]} \cdot \Pi^*(\mathbf{k}_\perp,\, k_z + mK;\, \mathbf{k}_\perp,\, k_z + m'K) \tag{3.3.5}$$

From linear response theory an arbitrary operator $\hat{O}(t)$ can be defined as (please refer to Fetter and Walecka[12], where linear response is discussed in Section 13 and linked diagrams in Section 9):

$$< \hat{O}(t)> \equiv < \Psi_s(t) \,|\, \hat{O}(t) \,|\, \Psi_s(t)>_{\text{linked diag}} = < \psi_H(0) \,|\, \hat{O}(t) \,|\, \psi_H(0)> +$$

$$i\hbar^{-1}< \psi_H(0) \,|\, \int_{t_0}^{t} dt'[\, \hat{H}_H^{\,\mathrm{ex}}(t),\, \hat{O}_H(t)] \,|\, \psi_H(0)>_{\text{linked diag}} + \ldots\ldots\ldots\ldots \tag{3.3.6}$$

where $|\Psi_s(t)>$ is a Schrodinger picture eigenfunction after the perturbation (external) Hamiltonian H^{ex} is turned on (at time t_0). $|\psi_H(0)>$ is the Heisenberg picture eigenfunction. If we only take the first (linear) term then

$$\delta < \hat{O}(t) > \equiv < \hat{O}(t) >_{ext} - < \hat{O}(t) > =$$

$$i\hbar^{-1} \int_{t_0}^{t} dt' < \psi_H(0) \,|\, [\, \hat{H}_H^{ext}(t'), \hat{O}_H(t)] \,|\, \psi_H(0) >_{\text{linked diag}} \tag{3.3.7}$$

To calculate the screening effect, the perturbation Hamiltonian can be expressed by

$$\hat{H}_H^{ext}(t) = \int d\mathbf{x}\, \hat{\rho}_H(\mathbf{x}, t) U_{ext}(\mathbf{x}', t') \tag{3.3.8}$$

where t_0 is the time when the perturbation is turned on, and t_0 is taken to be $-\infty$. The change of electron density (same as induced electron density) is

$$\delta < \hat{\rho}(\mathbf{x}, t) > = i\hbar^{-1} \int_{t_o}^{t} dt' \int dx'\, U_{ext}(\mathbf{x}', t') < \psi_H(0) \,|\, [\hat{\rho}_H(\mathbf{x}'t'), \hat{\rho}_H(\mathbf{x}, t)] \,|\, \psi_H(0) > \tag{3.3.9}$$

Let $\tilde{n}_H(\mathbf{x},t) = \hat{\rho}_H(\mathbf{x}, t) - < \hat{\rho}_H(\mathbf{x}, t) >$. The retarded polarization function (please refer to Fetter and Walecka[12], Section 14)

$$iD^R(\mathbf{x}, t; \mathbf{x}'t') = \theta(t - t') \frac{< \Psi_0 \,|\, [\tilde{n}_H(\mathbf{x}, t), \tilde{n}_H(\mathbf{x}', t')] \,|\, \Psi_0 >}{< \Psi_0 \,|\, \Psi_0 >} \tag{3.3.10}$$

is defined so that the induced charge density equation is

$$\delta < \hat{\rho}(\mathbf{x}, t) > = \hbar^{-1} \int_{-\infty}^{\infty} dt' \int d^3x'\, D^R(\mathbf{x}, t; \mathbf{x}', t')\, U_{ext}(\mathbf{x}', t') \tag{3.3.11}$$

where $D^R(\mathbf{x}, t; \mathbf{x}', t')$ is the retarded function of the polarization function $D(\mathbf{x}, t; \mathbf{x}', t')$. The latter polarization function is defined by

$$iD(\mathbf{x}, t; \mathbf{x}'t') = \frac{< \Psi_0 \,|\, T\, [\tilde{n}_H(\mathbf{x}, t), \tilde{n}_H(\mathbf{x}', t')] \,|\, \Psi_0 >}{< \Psi_0 \,|\, \Psi_0 >} \tag{3.3.12}$$

Taking the Fourier transformation of its time coordinate

$$D(\mathbf{x}, \mathbf{x}', \omega) =$$

$$\sum_{\Psi_0' \neq \Psi_0} \frac{<\Psi_0 \,|\hat{\rho}_H(\mathbf{x})\,|\Psi_0'><\Psi_0'\,|\hat{\rho}_H(\mathbf{x}')\,|\Psi_0>}{\omega - (E' - E)/\hbar + i\,\eta} + \frac{<\Psi_0\,|\hat{\rho}_H(\mathbf{x})\,|\Psi_0''><\Psi_0''\,|\hat{\rho}_H(\mathbf{x}')\,|\Psi_0>}{\omega + (E'' - E)/\hbar + i\,\eta} \tag{3.3.13}$$

The Fourier transformation of the retarded polarization function is

$$D^R(\mathbf{x}, \mathbf{x}', \omega) =$$

$$\sum_{\Psi_0' \neq \Psi_0} \frac{<\Psi_0 \,|\hat{\rho}_H(\mathbf{x})\,|\Psi_0'><\Psi_0'\,|\hat{\rho}_H(\mathbf{x}')\,|\Psi_0>}{\omega - (E' - E)/\hbar + i\,\eta} + \frac{<\Psi_0\,|\hat{\rho}_H(\mathbf{x})\,|\Psi_0''><\Psi_0''\,|\hat{\rho}_H(\mathbf{x}')\,|\Psi_0>}{\omega + (E'' - E)/\hbar - i\,\eta} \tag{3.3.14}$$

Since $\eta \approx 0$ then

$$\frac{1}{\omega \pm i\,\eta} = P(1\,/\,\omega\,) \mp i\,\pi\,\delta(\omega)$$

we get Re D^R = Re D and Im $D^R = \frac{\omega}{|\,\omega\,|}$Im D. Considering only the static perturbation potential from Eq.(3.3.13), we will obtain Im $D(\mathbf{x}, \mathbf{x}', \omega = 0) = 0$. The polarization function

$$\Pi(\mathbf{x}, t; \mathbf{x}', t') = \hbar^{-1}\, D(\mathbf{x}, t; \mathbf{x}', t')$$

The induced charge density distribution

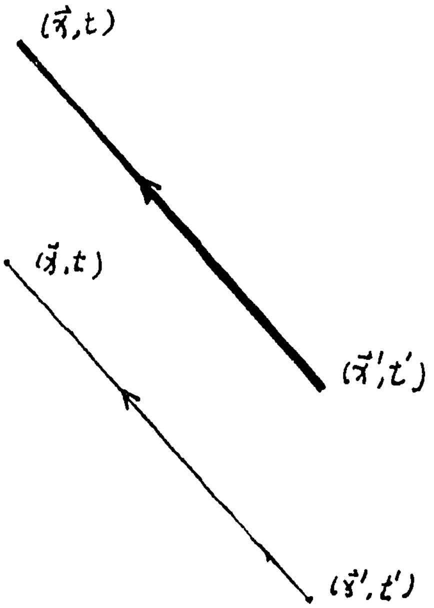
$$\delta< \hat{\rho}(\mathbf{x},t) > = \int_{-\infty}^{\infty} dt \int d^3\mathbf{x}'\,\Pi(\mathbf{x}, t; \mathbf{x}', t\,)U_{\text{ext}}(\mathbf{x}', t') \tag{3.3.15}$$

Subsection: Green's Function and The Hartree-Fock Equation in a Superlattice

the perturbation theory method is used to determine the expectation value in many-body theory by calculating Green's functions. The Green's function is defined

$$i\,G_{\alpha\beta}(\mathbf{x}, t; \mathbf{x}', t') = \frac{<\Psi_0 \mid T[\hat{\psi}_{H\,\alpha}(\mathbf{x}, t)\, \hat{\psi}^{+}_{H\,\beta}(\mathbf{x}', t')] \mid \Psi_0>}{<\Psi_0 \mid \Psi_0>} \tag{3.3.16}$$

Here T is the time ordering operator, α and β are spin indices, $\mid \Psi_0>$ is the Heisenberg picture ground state wave function (with $e-e$ interaction) and $\hat{\psi}_{H\,\alpha}(\mathbf{x}, t)$ is a Heisenberg operator and is equal to $e^{i\hat{H}/\hbar}\hat{\psi}_{\alpha}(\mathbf{x})e^{-i\hat{H}/\hbar}$. Here $\hat{\psi}_{\alpha}(\mathbf{x})$ is a field operator defined by $\hat{\psi}_{\alpha}(\mathbf{x}) \equiv \sum_{K}\psi_K(\mathbf{x})C_K$ where C_K is the creation operator (when $E_K > E_f$) or annihilation operator (when $E_K \leq E_f$), $\psi_K(\mathbf{x})$ is a single particle wave function and K is the eigenstate label for the single particle wave equation. Thus we know that Green's function is related to the single particle wave functions. The expectation value is related to a Green's function, therefore the expectation value is related to the single particle wave function. We claim that any theory of the many-body problem in a homogeneous medium can be extended to the case of a superlattice. In real space this requires only the use of superlattice's single particle function instead of the homogeneous medium single particle wave function. In momentum space, because the medium is not homogeneous, the equation needs to be modified.



The Green's function can be interpreted as a function that creates a particle (or hole if $t < t'$) at $(\mathbf{x}', t')$, travels to $(\mathbf{x}, t)$ then annihilates. It can be expressed by a Feynman diagram (a thick line). Let $G^0(\mathbf{x}, t; \mathbf{x}', t')$ be a non-interacting Green's function. This means that Hamiltonians will not include the interacting terms such as direct or exchange electron-electron coupling. The $G^0(\mathbf{x}, t; \mathbf{x}', t')$ is expressed by the Feynman diagram (a thin line). From Eq. (3.3.16) the time coordinate Fourier component of the non-interacting Green's function can be expressed as

$$G^0(\mathbf{x}, \mathbf{x}', \omega) = \sum_j \psi_j^0(\mathbf{x})\, \psi_j^{0*}(\mathbf{x}') \left[\frac{\theta\,(\varepsilon_j^0 - \varepsilon_f^0)}{\omega - \hbar^{-1}\,\varepsilon_j^0 + i\eta} + \frac{\theta\,(\varepsilon_f^0 - \varepsilon_j^0)}{\omega - \hbar^{-1}\,\varepsilon_f^0 - i\eta} \right] \qquad (3.3.17)$$

Here $\eta \to 0^+$, ε_f^0 is the Fermi level of the non-interacting ground state. ε_j^0 is the electron energy and the Heaviside step function $\theta(x)$ defined as

$$\theta(x) = \begin{cases} 1 & \text{if} \quad x > 0 \\ 0 & \text{if} \quad x \le 0 \end{cases} \qquad (3.3.18)$$

enforces the Fermi distribution. The $\psi_j^0(\mathbf{x})$ are the eigenfunctions of the Hartree wave equation

$$\left[\frac{-\hbar^2 \nabla^2}{2m^*} + U(\mathbf{x}) \right] \psi_j^0(\mathbf{x}) = \varepsilon_j^0 \psi_j^0(\mathbf{x}) \qquad (3.3.19)$$

Here $U(\mathbf{x})$ is the superlattice potential.

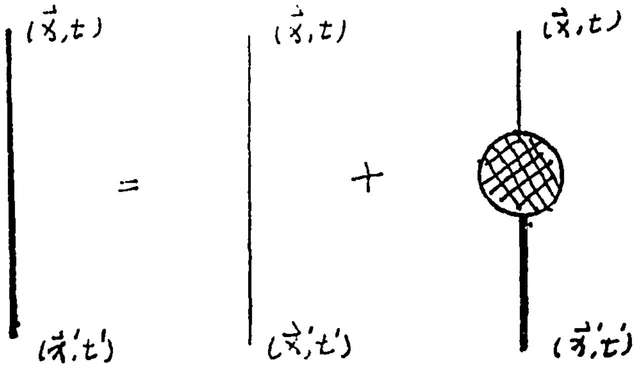
Let $\sum(\mathbf{x}_1, t_1; \mathbf{x}_1', t_1')$ be the self energy operator. The relationship between

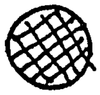
$G(\mathbf{x}, t; \mathbf{x}', t)$ and $G^0(\mathbf{x}, t; \mathbf{x}', t')$ can be expressed by the equation (please refer to Reference 9, Section 9)

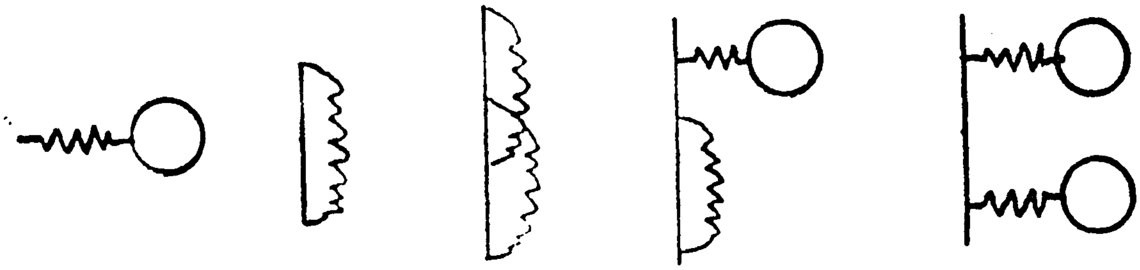
$$G(\mathbf{x}, t; \mathbf{x}', t') = G^0(\mathbf{x}, t; \mathbf{x}', t') +$$

$$\int d\mathbf{x}_1' \, dt_1' \int d\mathbf{x}_1 \, dt_1 G^0(\mathbf{x}, t; \mathbf{x}_1, t_1) \sum(\mathbf{x}_1, t_1; \mathbf{x}_1', t_1') G(\mathbf{x}_1', t_1'; \mathbf{x}', t') \qquad (3.3.20)$$

or by the Feynman diagram



The  represents the self energy. The first few terms of the latter can be expressed by



If the self energy includes only the first two terms (direct and exchange electron interaction) the Green's function can be written (please refer to Fetter and Walecka[12], Section 8)

$$G(\mathrm{x}, \mathrm{x}', \omega) = \sum_j \psi_j(\mathrm{x})\psi_j^*(\mathrm{x}') \left[\frac{\theta(\varepsilon_j - \varepsilon_f)}{\omega - \hbar^{-1}\varepsilon_j + i\eta} + \frac{\theta(\varepsilon_f - \varepsilon_j)}{\omega - \hbar^{-1}\varepsilon_j - i\eta} \right] \qquad (3.3.21)$$

here ε_j, $\psi_j(\mathrm{x})$ is the eigenenergy and eigenfunction of the Hartree-Fock wave equation

$$\varepsilon_j \, \psi_j(\mathrm{x}) = \left[\frac{-\hbar^2 \nabla_1^2}{2m^*} + U(\mathrm{x}_1) \right] \psi_j(\mathrm{x}_1) +$$

$$\int d\mathrm{x}_2 \left[V(\mathrm{x}_1 - \mathrm{x}_2)\, n(\mathrm{x}_2) - V(\mathrm{x}_1 - \mathrm{x}_2) \sum_i \psi_i(\mathrm{x}_1)\, \psi_i^*(\mathrm{x}_2)\, \theta(\varepsilon_f - \varepsilon_i) \right] \psi_j(\mathrm{x}_2) \qquad (3.3.22)$$

Here $n(\mathrm{x}_2)$ is the electron concentration at x_2 and $V(\mathrm{x}_1 - \mathrm{x}_2)$ is the electron-electron interaction energy.

The polarization function $\Pi(\mathrm{x}, t; \mathrm{x}', t') \equiv D(\mathrm{x}, t; \mathrm{x}', t)/\hbar$, is defined by Eq. (3.3.12)

$$\Pi(\mathrm{x}, t; \mathrm{x}', t') = \frac{-i}{\hbar}$$

$$\times \left\{ < \Psi_0 \mid T[\, \hat{\psi}^{+}_{\mathrm{H}\,\alpha}(\mathrm{x}, t)\, \hat{\psi}_{\mathrm{H}\,\alpha}(\mathrm{x}, t)\, \hat{\psi}^{+}_{\mathrm{H}\,\beta}(\mathrm{x}', t')\, \hat{\psi}_{\mathrm{H}\,\beta}(\mathrm{x}', t') \mid \Psi_0 > - < \hat{\rho}(\mathrm{x}, t) > < \hat{\rho}(\mathrm{x}', t') > \right\}_{\text{linked diag}}$$

$$= \frac{-i}{\hbar} < \Phi_0 \mid \sum_{\nu=0}^{\infty} \left(\frac{-i}{\hbar} \right)^{\nu} \frac{1}{\nu\,!} T \left[\int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \, \ldots\ldots\ldots\ldots \int_{-\infty}^{\infty} dt_\nu \right.$$

$$\left. \times H_I(t_1)\, H_I(t_2) \ldots\ldots\ldots\ldots H_I(t_\nu)\; \hat{\psi}^{+}_{I\,\alpha}(\mathrm{x}, t) \hat{\psi}_{I\,\alpha}(\mathrm{x}, t) \hat{\psi}^{+}_{I\,\beta}(\mathrm{x}', t') \hat{\psi}_{I\,\beta}(\mathrm{x}', t') \right] \mid \Phi_0 > -$$

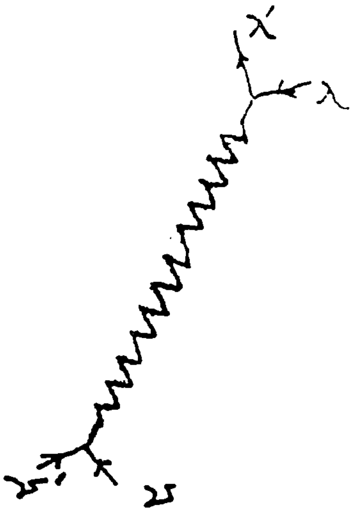
$$< \hat{\rho}(\mathrm{x}, t) > < \hat{\rho}(\mathrm{x}', t') >_{\text{linked diag}} \qquad (3.3.23)$$

Here $\mid \Phi_0 >$ is the ground state of the non-interacting system, $\hat{\psi}_{I\,\alpha}(\mathrm{x}, t)$ is an interaction operator and is equal to $e^{i\hat{\mathrm{H}}_0/\hbar}\hat{\psi}_\alpha(\mathrm{x})e^{-i\hat{\mathrm{H}}_0/\hbar}$ where $\hat{H} = \hat{H}_0 + \hat{H}_I$. The interaction

Hamiltonian

$$\hat{H}_I(t_i) = \frac{1}{2}\int d\mathbf{x}_i\, dt_i \int d\mathbf{x}_j\, dt_j\, \delta\,(\,t_i - t_j) \sum_{\lambda,\,\lambda',\,\nu,\,\nu'} V(\mathbf{x}_i,\, \mathbf{x}_j)_{\lambda,\,\lambda',\,\nu,\,\nu'}$$

$$\times\, \hat{\psi}^{+}_{I\,\lambda}(\mathbf{x})\; \hat{\psi}_{I\,\lambda}(\mathbf{x})\; \hat{\psi}^{+}_{I\,\nu}(\mathbf{x}\,')\; \hat{\psi}_{I\,\nu}(\mathbf{x}\,') \qquad (3.3.24)$$



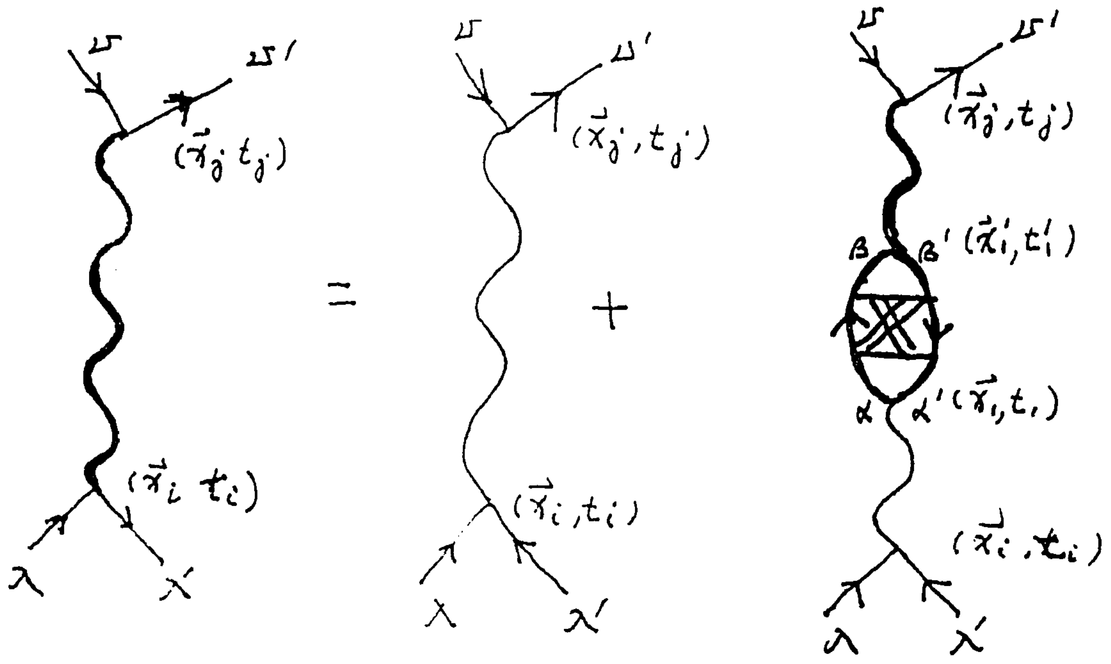
The $V(x_i,\, x_j)_{\lambda,\,\lambda',\,\nu,\,\nu'}$ is the electron-electron interaction potential. It can also be expressed by the Feynman diagram on the left. Here λ, λ', ν, ν' are spin indices. Because the electron-electron interaction does not change the spin direction, λ must be equal to λ' and ν must be equal to ν'. Usually we use a thick wavy line to express the screened interaction $V(x_i,\, x_j)_{\lambda,\,\lambda',\,\nu,\,\nu'}$ and a thin wave line to express the bare electric interaction $V_0\,(x_i,\, x_j)_{\lambda,\,\lambda',\,\nu,\,\nu'}$.

The relationship between $V(x_i,\, x_j)_{\lambda,\,\lambda',\,\nu,\,\nu'}$ and $V_0\,(x_i,\, x_j)_{\lambda,\,\lambda',\,\nu,\,\nu'}$ can be expressed by equation

$$V(x_i,\, x_j)_{\lambda,\,\lambda',\,\nu,\,\nu'} = V_0\,(x_i,\, x_j)_{\lambda,\,\lambda',\,\nu,\,\nu'} +$$

$$\int d\mathbf{x}_1'\, dt_1' \int d\mathbf{x}_1\, dt_1 V_0(x_i,\, x_1)_{\lambda,\,\lambda',\,\alpha,\,\alpha'}\, \Pi(\mathbf{x}_1\; t_1;\, \mathbf{x}_1',\, t_1')\, V(x_1',\, x_j)_{\beta,\,\beta',\,\nu,\,\nu'} \qquad (3.3.25)$$

or by the Feynman diagram



The proposed method in this thesis is to use the Hartree-Fock wave function to obtain the polarization function. For this reason, the exchange term in the Hartree-Fock equation and the potential used to calculate the exchange energy in this Hartree-Fock equation (Eq. (3.3.6)) use the screened electron-electron interaction potential instead of the bare interaction potential. For this reason, the exchange term in this Hartree-Fock equation not only calculates the exchange energy but also involves the correlation energy. For the exchange polarization function, this thesis use the Hartree-Fock wave function and the screened potential instead of the Hartree wave function and the bare electron-electron interaction potential. Many high order perturbation polarization functions are then included automatically. A further discussion follows in the next subsection.

Subsection: A Discussion of The Polarization Function $\Pi(\mathbf{x}, t; \mathbf{x}', t')$

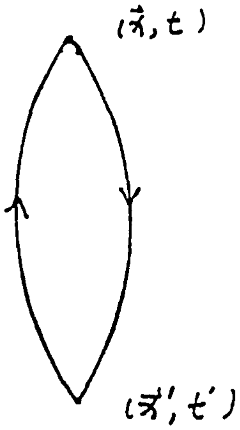
The unperturbed polarization function $\Pi(\mathbf{x}, t; \mathbf{x}', t')$ is

$$\Pi^0(\mathbf{x}, t; \mathbf{x}', t') = \frac{-i}{\hbar} < \Phi_0 \mid T\,[\, \hat{\psi}^{+}_{l\alpha}(\mathbf{x}, t)\, \hat{\psi}_{l\alpha}(\mathbf{x}, t)\, \hat{\psi}^{+}_{l\beta}(\mathbf{x}', t')\hat{\psi}_{l\beta}(\mathbf{x}', t')\,] \mid \Phi_0 >$$

$$- < \hat{\rho}(\mathbf{x}, t)>< \hat{\rho}(\mathbf{x}', t')> \qquad (3.3.26)$$

here T is the time ordering operator and l and α, β have been described under Eq. (3.3.24). Let N be the normal ordering operator and let $\hat{A}^{\cdot}\ \hat{B}^{\cdot}$ denote the contractor (please refer to Fetter and Walecka[12] section 8).

$$\hat{A}^{\cdot}\ \hat{B} \equiv T[\hat{A}\ \hat{B}] - N[\hat{A}\ \hat{B}] \qquad (3.3.27)$$



Because

$$N[\hat{A}^{\cdot\cdot}\ \hat{B}^{\cdot\cdot}\ \hat{C}\ \hat{D}] = \hat{A}^{\cdot\cdot}\ \hat{B}^{\cdot\cdot}\ N\,[\hat{C}\ \hat{D}]\,, \qquad (3.3.28)$$

$$\hat{\psi}^{+\cdot}_{l\alpha}(\mathbf{x}, t)\ \hat{\psi}^{+\cdot}_{l\beta}(\mathbf{x}', t') = \hat{\psi}^{\cdot}_{l\alpha}(\mathbf{x}, t)\ \hat{\psi}^{\cdot}_{l\beta}(\mathbf{x}', t') = 0 \qquad (3.3.29)$$

and $< \Phi_0 \mid \hat{\psi}^{+\cdot}_{l\alpha}(\mathbf{x}, t)\ \hat{\psi}^{\cdot}_{l\alpha}(\mathbf{x}, t) \mid \Phi_0 > = < \hat{\rho}(\mathbf{x}, t)>$.

From Wick's Theorem[36]

$$T[\hat{A}\ \hat{B}\ \hat{C}\ \hat{D}\ ] = N[\hat{A}^{\cdot}\ \hat{B}^{\cdot}\ \hat{C}\ \hat{D}\ ] + N[\hat{A}^{\cdot\cdot}\ \hat{B}\ \hat{C}^{\cdot\cdot}\ \hat{D}\ ] + N[\hat{A}^{\cdot\cdot}\ \hat{B}\ \hat{C}\ \hat{D}^{\cdot\cdot}\ ] + N[\hat{A}\ \hat{B}^{\cdot\cdot}\ \hat{C}^{\cdot\cdot}\ \hat{D}\ ] +$$

$$N[\hat{A}\ \hat{B}^{\cdot\cdot}\ \hat{C}\ \hat{D}^{\cdot\cdot}\ ] + N[\hat{A}\ \hat{B}\ \hat{C}^{\cdot\cdot}\ \hat{D}^{\cdot\cdot}\ ] + N[\hat{A}^{\cdot}\ \hat{B}^{\cdot}\ \hat{C}^{\cdot\cdot}\ \hat{D}^{\cdot\cdot}\ ] + N[\hat{A}^{\cdot}\ \hat{B}^{\cdot\cdot}\ \hat{C}^{\cdot}\ \hat{D}^{\cdot\cdot}\ ] + N[\hat{A}^{\cdot}\ \hat{B}^{\cdot\cdot}\ \hat{C}^{\cdot\cdot}\ \hat{D}^{\cdot}\ ]$$

$$(3.3.30)$$

the $\Pi^0(\mathbf{x}, t; \mathbf{x}', t')$ becomes

$$\Pi^0(\mathbf{x}, t; \mathbf{x}', t') = \frac{-i}{\hbar}(-1) \times 2 \times\ i\,G^0(\mathbf{x}', t'; \mathbf{x}, t)\ i\,G^0(\mathbf{x}, t; \mathbf{x}', t') \qquad (3.3.31)$$

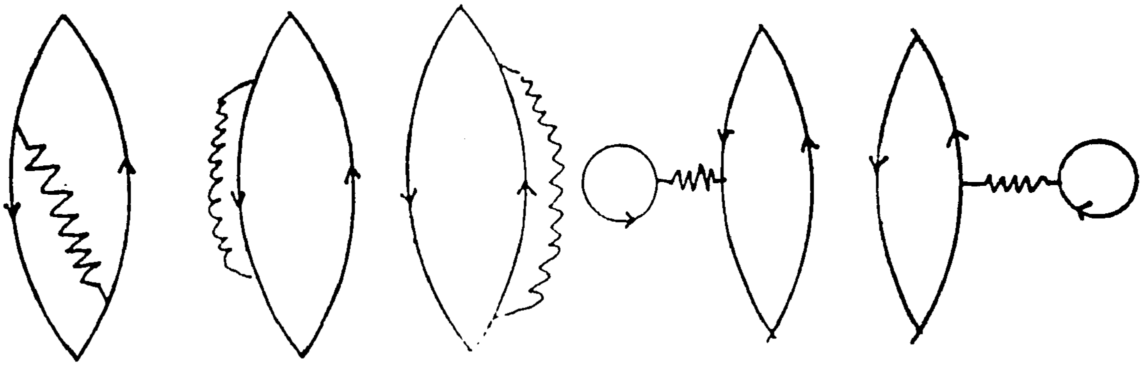
here 2 indicates the spin eigen state. The Feynman diagram of $\Pi^0(\mathbf{x}, t; \mathbf{x}', t')$ is shown on the last page.

To find the perturbation corrections to $\Pi(\mathrm{x}, t; \mathrm{x}', t')$ and to simplify the process, we use the following arguments:

A) One higher order means adding one more particle-particle interaction potential and four particle fields (in a Feynman diagram add a two particle propagator line) into the time order brackets and then multiplication by $(\frac{-i}{\hbar})$.

B) The Feynman diagram must be linked.

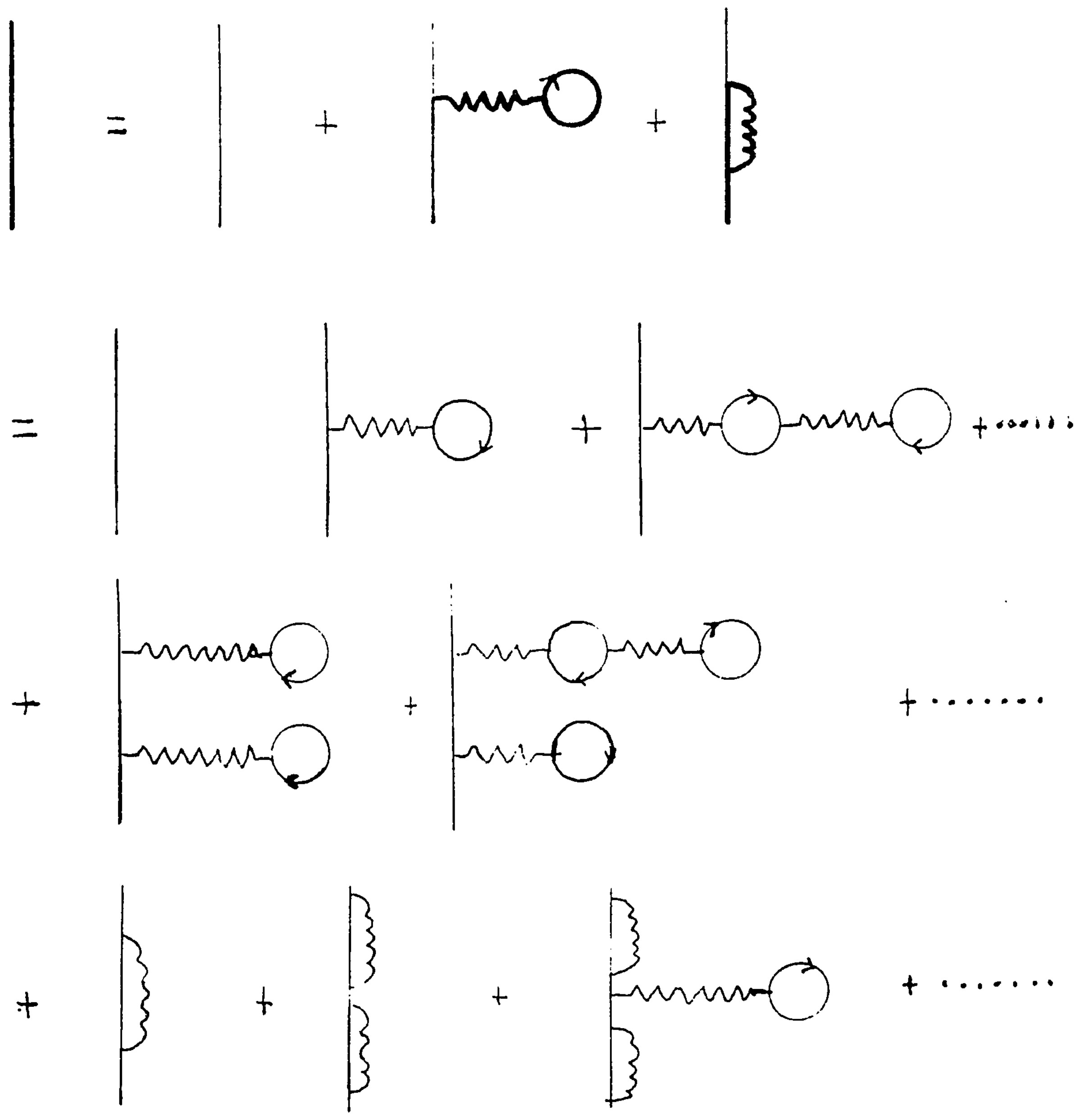
C) Because the variable of the interaction potential is neither (x, t) nor (x', t'), the Feynman diagram must be linked and normal ordering terms with contraction $\hat{\psi}^{+\cdot}_{l\alpha}(\mathrm{x}, t)\hat{\psi}^{+\cdot}_{l\alpha}(\mathrm{x}, t)$ or $\hat{\psi}^{+\cdot}_{l\beta}(\mathrm{x}, t)\hat{\psi}^{+\cdot}_{l\beta}(\mathrm{x}, t)$ will not be present. The possible Feynman diagrams for the polarization function Πs with first order perturbation are



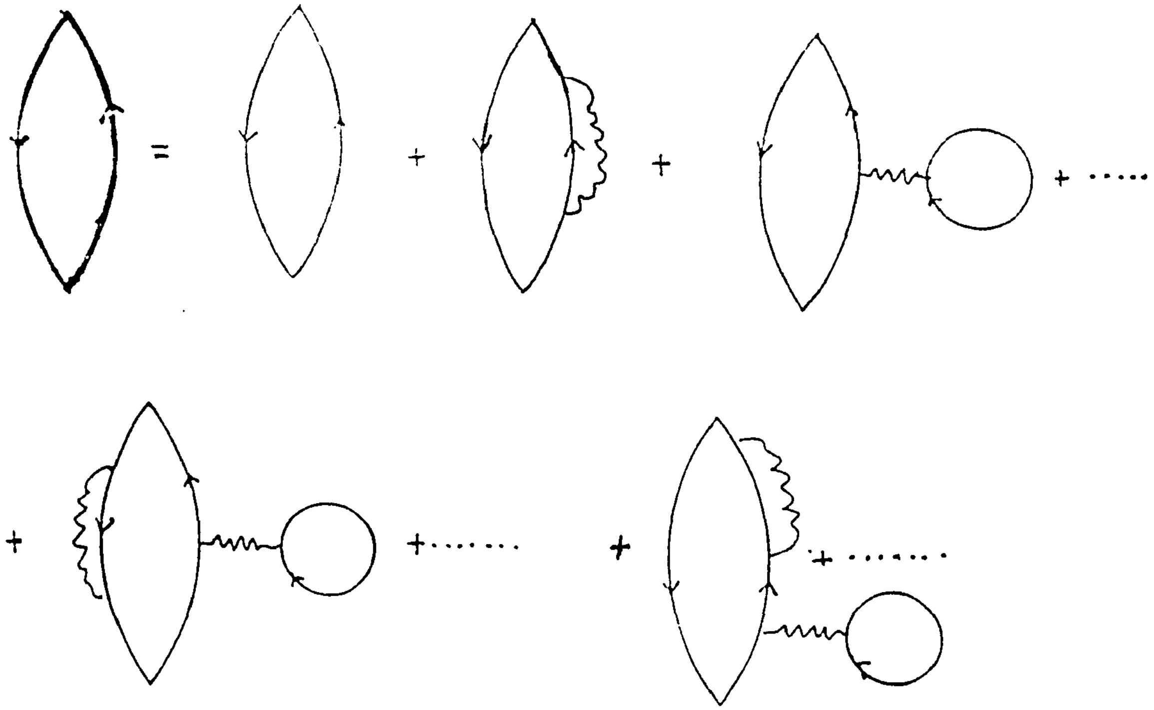
Derivation of a formula for any one of these diagrams is complicated (see the next section). Moreover, the single particle wave function for a superlattice is not analytic and the exchange and correlation effects of screening are also needed. To solve the screening problem, the following method is used. Instead of the Hartree single wave function (non-interacting ground state single particle wave function), the Hartree-Fock single wave function is used. This wave function will be inserted into

$\Pi^0(x, t; x', t')$ and the first Feynman diagram of the first order perturbation terms of the $\Pi(x, t; x', t')$ (let us call it $\Pi^A(x, t; x', t')$).

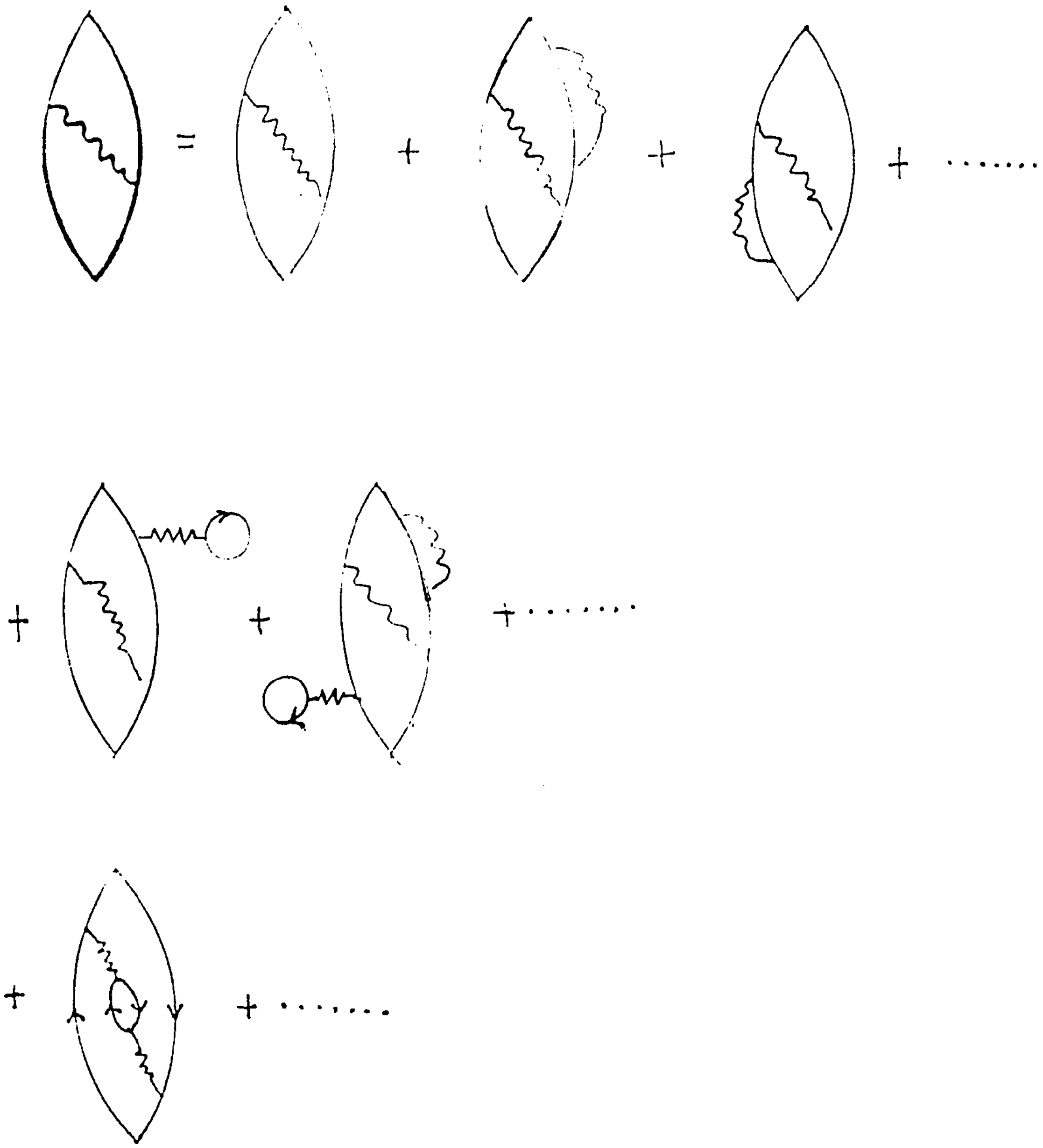
The Feynman diagram of the Green's function (in which the Hartree-Fock single wave function is used; please see discussion in Eq. (3.3.21)) is



If this Green's function replaces the non-interacting ground state Green's function in the polarization function of Π^0 , the Feynman diagram of the polarization function will be



Similarly, the diagram of the polarization function $\Pi^A(\mathbf{x}, t; \mathbf{x}', t')$



Section III.4 Hartree-Fock Equation and Polarization Function in a Superlattice

In this section, the equation of a single particle wave Hartree-Fock equation, the polarization function $\Pi^0(\mathbf{x}, t; \mathbf{x}', t')$ and the polarization function $\Pi^A(\mathbf{x}, t; \mathbf{x}', t')$ of the superlattice will be derived.

The Hartree-Fock wave equation obeys:

$$-\frac{\hbar^2}{2m^*}\nabla_1^2\psi_i(\mathbf{r}_1) + U(z)\psi_i(\mathbf{r}_1) + e\,\phi_{\text{dir}}(z_1)\psi_i(\mathbf{r}_1) -$$

$$\int d\mathbf{r}_2 V(\mathbf{r}_2, \mathbf{r}_1)\sum_j f_0(E_j)\psi_j(\mathbf{r}_1)\psi_j^*(\mathbf{r}_2)\psi_i(\mathbf{r}_2) = E_i\psi_i(\mathbf{r}_1) \tag{3.4.1}$$

Here the "dir" subscript means the function does not include the exchange and correction interactions between electrons, $\mathbf{r} = \rho + z\,\hat{z}$, $U(z)$ is the potential of the superlattice (the potential is independent of x and y direction), $V(\mathbf{r}_2, \mathbf{r}_1)$ is the electron-electron interaction potential, $f_0(E_i)$ is the finite temperature Fermi-Dirac distribution function and $e\,\phi_{\text{dir}}(z)$ is the potential generated by a non-uniform charge distribution. Since the charge distribution is uniform in the x and y directions, ϕ_{dir} depends on z only. If the screening adjustment is omitted, $e\,\phi_{\text{dir}}(z)$ obeys Poisson's equation.

If the medium is homogeneous in x and y, the single particle wave function can be expressed as

$$\psi_i(\mathbf{r}) = e^{i\,\mathbf{k}_{\perp i}\cdot\rho_i}F_{n_i,\,k_{z_i}}(z) \tag{3.4.2}$$

where n_i is the sub-band index. Multiplying both sides of Eq. (3.4.1) by $\frac{1}{(2\pi)^2}\int d^2\rho_1 e^{-i\,\mathbf{k}_{\perp i}\cdot\rho_1}$, Eq. (3.4.1) becomes

$$\left\{ \left[-\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial z_1^2} + \frac{\hbar^2}{2m^*}(\mathbf{k}_{\perp i})^2 \right] + U(z_1) + e\,\phi_{\mathrm{dir}}(z_1) \right\} F_{n_i,\,k_{z_i}}(z_1)$$

$$+ \text{exchange term} = E(k_i,\,k_{z_i},\,\mathbf{k}_{\perp i}) F_{n_i,\,k_{z_i}}(z_1) \qquad (3.4.3)$$

The exchange term is

$$-\sum_j \int d^3\mathbf{r}_2\, f_0(E_i) e^{i(\mathbf{k}_{\perp i} - \mathbf{k}_{\perp j}) \cdot \rho_2} F_{n_i,\,k_{z_i}}{}^*(z_2) F_{n_j,\,k_{z_j}}(z_2)$$

$$\times \frac{1}{(2\pi)^2} \int d\rho_1 e^{i(\mathbf{k}_{\perp j} - \mathbf{k}_{\perp i}) \cdot \rho_1} F_{n_j,\,k_{z_j}}{}^*(z_1)\; V(\mathbf{r}_1,\,\mathbf{r}_2) \qquad (3.4.4)$$

where

$$V(\mathbf{r}_1,\,\mathbf{r}_2) = \sum_{m_1} \sum_{m_2} \sum_{k_z,\,\mathbf{k}_\perp} V(k_z,\,\mathbf{k}_\perp;\,m_1,\,m_2) e^{i\mathbf{k}_\perp \cdot \rho_1 + i(k_z + m_1 K) z_1} e^{-i\mathbf{k}_\perp \cdot \rho_2 - i(k_z + m_2 K) z_2}$$

$$(3.4.5)$$

The eigenenergy contributed by the exchange term is

$$E_{\mathrm{xc}}(k_i,\,k_{z_i},\,\mathbf{k}_{\perp i}) = -\sum_j f_0(E_j) \sum_{m,\,m'} < n_j,\,k_{z_j} \mid e^{i(k_{z_i} - k_{z_j}(\pm K) + mK) \cdot z_1} \mid n_i,\,k_{z_i} >$$

$$\times < n_i,\,k_{z_i} \mid e^{-i(k_{z_i} - k_{z_j}(\pm K) + mK) \cdot z_2} \mid n_j,\,k_{z_j} > V(k_{z_i} - k_{z_j}(\pm K),\,\mathbf{k}_{\perp i} - \mathbf{k}_{\perp j};\,m,\,m') \qquad (3.4.6)$$

where $k_{z_i} - k_{z_j}(\pm K)$ means that if $k_{z_i} - k_{z_j} < -K/2$ or $k_{z_i} - k_{z_j} > K/2$ a value of $K = 2\pi/L$ will be added or subtracted such that $k_{z_i} - k_{z_j}$ will be within first Brillouin zone and $\mid n_i,\,k_{z_i}>$ is the eigenvector for the one dimensional single particle wave function. The eigenenergy can be separated into two parts.

$$E_{\mathrm{dir}}(k_i,\,k_{z_i},\,\mathbf{k}_{\perp i}) + E_{\mathrm{xc}}(k_i,\,k_{z_i},\,\mathbf{k}_{\perp i}) \qquad (3.4.7)$$

The $E_{\mathrm{dir}}(k_i,\,k_{z_i},\,\mathbf{k}_{\perp i})$ is a direct part and equals

$$E_{\mathrm{dir}}(k_i,\ k_{z_i},\ \mathbf{k}_{\perp_i} = 0) + \frac{\hbar^2}{2m^*}\, k_{\perp i}^2 \tag{3.4.8}$$

The $E_{xc}(k_i,\ k_{z_i},\ \mathbf{k}_{\perp_i})$ the exchange and correlation part was given by Eq.(3.4.6) and $V(k_{z_i} - k_{z_j}(\pm K),\ \mathbf{k}_{\perp_i} - \mathbf{k}_{\perp_j};\ m,\ m')$ must consider the screening effect (please refer to Eq. (3.3.25) and (3.4.5)).

The wave to be used to calculate the screening effect in a superlattice must have the characteristics of periodic potential well. The tight binding approximation wave function is proposed in this thesis. The tight binding wave function is constructed using a single potential well wave function. If the single well Hartree-Fock wave function is applied to the tight binding approximation equation (to be developed in the next section), this wave function will have the characteristics of a periodic potential with exchange and correlation effects.

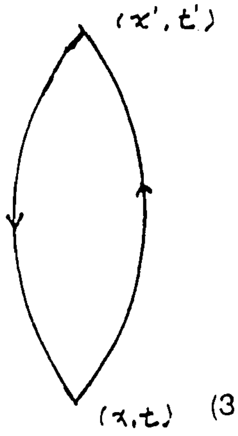
The polarization functions Π^0 and Π^A will be derived in the following manner. Here only the zero temperature case and the Fermi-Dirac distribution function will be considered (the reason for using the Fermi-Dirac distribution is discussed in Appendix C). Any single wave function in this section will be a Hartree-Fock wave function. For example, the equation used to derive the zeroth order perturbation function $\Pi^0(\mathbf{x},\ t;\ \mathbf{x}',\ t')$ uses the Hartree-Fock single particle wave function.

$$\Pi^0(\mathbf{x},\ t;\ \mathbf{x}',\ t') = \frac{1}{i\,\hbar} - 2\, i\, G^0(\mathbf{x},\ t;\ \mathbf{x}',\ t')\ i\, G^0(\mathbf{x},\ t;\ \mathbf{x}',\ t') \tag{3.4.9}$$

where the Green's function $G^0(\mathbf{x},\ t;\ \mathbf{x}',\ t')$ is equal to

$$-\, i \sum_i \psi_i(\mathbf{x})\psi_i^*(\mathbf{x}')\, e^{-i\frac{E_i}{\hbar}(t - t')}\left[\, \theta(t - t')\,(1 - f_0(E_i)\,) - \theta(t' - t)\, f_0\,(E_i)\,\right] \tag{3.4.10}$$

Here E_i is the eigenenergy and at zero temperature the Fermi-Dirac distribution function $f_0(E_i) = 1 - \theta(E_i - E_f)$, E_f is the Fermi level. The time coordinate Fourier component of this Green's function



$$G^0(\mathrm{x}, \mathrm{x}', \omega) = \int d(t-t')\, G^0(\mathrm{x}, t; \mathrm{x}', t')\, e^{i\omega(t-t')} =$$

$$\sum_i \psi_i(\mathrm{x})\, \psi_i^*(\mathrm{x}') \left[\frac{\theta(E_i - E_f)}{\omega - \frac{E_i}{\hbar} + i\eta} + \frac{\theta(E_f - E_i)}{\omega - \frac{E_i}{\hbar} - i\eta} \right] \qquad (3.4.11)$$

From Eq. (3.4.9) and by using the convolution theorem of Fourier transformation

$$\Pi^0(\mathrm{x}, \mathrm{x}', \omega) = \frac{2i}{\hbar} \int \frac{d\omega}{2\pi} G^0(\mathrm{x}, \mathrm{x}', \omega')\, G^0(\mathrm{x}', \mathrm{x}, \omega - \omega') =$$

$$\frac{-2i}{\hbar} \sum_i \sum_j \psi_i(\mathrm{x})\psi_i^*(\mathrm{x}')\psi_j(\mathrm{x}')\psi_j^*(\mathrm{x}) \int \frac{d\omega'}{2\pi}$$

$$\times \left[\frac{\theta(E_i - E_f)\, \theta(E_f - E_j)}{(\omega' - \frac{E_i}{\hbar} + i\eta)(\omega - \omega' - \frac{E_j}{\hbar} - i\eta)} + \frac{\theta(E_j - E_f)\, \theta(E_f - E_i)}{(\omega' - \frac{E_i}{\hbar} - i\eta)(\omega - \omega' - \frac{E_j}{\hbar} + i\eta)} \right].$$

When $\omega = 0$, the result is

$$\Pi^0(\mathrm{x}, \mathrm{x}', \omega = 0) = 2 \sum_i \sum_j \psi_i(\mathrm{x})\psi_i^*(\mathrm{x}')\psi_j(\mathrm{x}')\psi_j^*(\mathrm{x}) \frac{\theta(E_f - E_i) - \theta(E_f - E_j)}{E_i - E_j} \qquad (3.4.12)$$

The polarization function in momentum space is

$$\Pi^0(\mathbf{k}_1,\ \mathbf{k}_2) = 2 \sum_i \sum_j < i \mid e^{i\,\mathbf{k}_2 \cdot \mathbf{r}'} \mid j >< j \mid e^{-i\,\mathbf{k}_1 \cdot \mathbf{r}} \mid i > \frac{\theta(E_f - E_i) - \theta(E_f - E_j)}{E_i - E_j} \tag{3.4.13}$$

Because only the static electric field is considered, the notation of $\omega = 0$ will be omitted in this thesis. In a superlattice the Fourier component of $\Pi(\mathbf{k}_1,\ \mathbf{k}_2)$ can exist only if $\mathbf{k}_{\perp 1} = \mathbf{k}_{\perp 2}$ and $k_{z_1} = k_{z_2} + NK$. Let $k_{z_1} = k_z + m_1 K$, $\mid k_z \mid \leq K/2 = \pi/L$ and $m_1 + N = m_2$. Because

$$\sum_i \equiv \frac{1}{(2\pi)^3} \int d^2 k_{\perp_i} \sum_{n_i} \int_{-\frac{\pi}{L}}^{\frac{\pi}{L}} dk_{z_i}$$

Eq. (3.4.13) becomes

$$\Pi^0(\mathbf{k}_\perp,\ k_z;\ m_1,\ m_2) = \frac{2}{(2\pi)^3} \sum_{n_i,\ n_j} \int d^2 k_{\perp_i} \int_{-\frac{\pi}{L}}^{\frac{\pi}{L}} dk_{z_i}$$

$$\times \frac{f_0(E(k_i,\ k_{z_i},\ \mathbf{k}_{\perp_i}) - E(n_j,\ k_{z_j} = k_{z_i} - (\pm K),\ \mathbf{k}_{\perp_j} = \mathbf{k}_{\perp_i} - \mathbf{k}_\perp)\ )}{E_i - E_j}$$

$$\times < k_i,\ k_{z_i},\ \mathbf{k}_{\perp_i} \mid e^{i\,(m_2 K + k_z) \cdot z} \mid n_j,\ k_{z_j} = k_{z_i} - (\pm K),\ \mathbf{k}_{\perp_j} = \mathbf{k}_{\perp_i} - \mathbf{k}_\perp) >$$

$$\times < j \mid e^{-i\,(m_1 + k_z) \cdot z} \mid i > \tag{3.4.14}$$

here $f_0(E) = 1$ when $E \geq 0$ otherwise $f_0(E) = 0$, $k_{z_i} - (\pm K)$ has been explained under Eq. (3.4.6).

From the Feynman diagram, we know that the lowest exchange polarization term

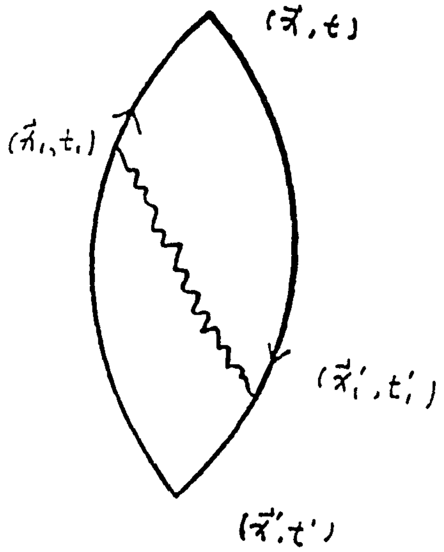
$$\Pi^A(\mathbf{x}, t; \mathbf{x}', t') = (-1)\frac{-i}{\hbar}(i)^4 \sum_{\alpha,\alpha'}\sum_{\lambda,\lambda'}\sum_{\mu,\mu'}\sum_{\beta,\beta'}$$

$$\delta_{\alpha',\lambda}\,\delta_{\lambda,\lambda'}\,\delta_{\lambda',\beta}\,\delta_{\beta,\beta'}\,\delta_{\beta',\mu}\,\delta_{\mu,\mu'}\,\delta_{\mu',\alpha}\,\delta_{\alpha,\alpha'}$$

$$\times \int d\mathbf{x}_1\, dt_1 d\mathbf{x}_1{}'\, dt_1{}' \, \frac{1}{2}\, \frac{-i}{\hbar}\, V(\mathbf{x}_1, t_1; \mathbf{x}_1{}', t_1{}')$$

$$\times\, \delta(t_1 - t_1{}') G^0_{\alpha,\lambda}(\mathbf{x}, t; \mathbf{x}_1, t_1) G^0_{\lambda',\beta}(\mathbf{x}_1, t_1; \mathbf{x}', t')$$

$$\times\, G^0_{\beta',\mu}(\mathbf{x}', t'; \mathbf{x}_1{}', t_1{}') G^0_{\mu',\alpha'}(\mathbf{x}_1{}', t_1{}'; \mathbf{x}, t) \tag{3.4.15}$$



where the notation Π^A is defined by Geldart and Taylor[6], α, α′, λ, λ′, μ, μ′, β, β′ are the spin indices. Let $f_i(\omega) = \left[\frac{\theta(E_i - E_f)}{\omega - E_i/\hbar + i\,\eta} - \frac{\theta(E_i - E_f)}{\omega - E_i/\hbar - i\,\eta} \right]$ then

$$\Pi^A(\mathbf{x}, \mathbf{x}', \omega = 0) = \hbar^{-2} \int d^3x_1 dt_1 \int d^3x_1{}' dt_1{}' \, \delta(t_1 - t_1{}')\, V(\mathbf{x}_1, t_1; \mathbf{x}_1{}', t_1{}')$$

$$\times \sum_i \sum_j \sum_k \sum_l \psi_i(\mathbf{x})\, \psi_i{}^*(\mathbf{x}_1)\, \psi_j(\mathbf{x}_1)\, \psi_j{}^*(\mathbf{x}')\, \psi_k(\mathbf{x}')\, \psi_k{}^*(\mathbf{x}_1{}')\, \psi_l(\mathbf{x}_1{}')\, \psi_l{}^*(\mathbf{x})$$

$$\times \int \frac{d\omega_1}{2\pi}\, e^{-i\,\omega_1(t - t_1)}\, f_i(\omega_1) \int \frac{d\omega_2}{2\pi}\, e^{-i\,\omega_2(t_1 - t')}\, f_j(\omega_2)$$

$$\times \int \frac{d\omega_3}{2\pi}\, e^{-i\,\omega_3(t' - t_1{}')}\, f_k(\omega_3) \int \frac{d\omega_4}{2\pi}\, e^{-i\,\omega_4(t_1{}' - t')}\, f_l(\omega_4) \tag{3.4.16}$$

The time part of this equation becomes

$$\int \frac{d\omega_2}{2\pi}\, f_j(\omega_2)\, f_k(\omega_2) \left[\frac{\theta(E_j - E_f)\,\theta(E_f - E_k)}{E_k - E_j + i\,\eta} - \frac{\theta(E_k - E_f)\,\theta(E_f - E_j)}{E_k - E_j - i\,\eta} \right]$$

$$\times \int \frac{d\omega_1}{2\pi} f_i(\omega_4)\, f_l(\omega_4) \left[\frac{\theta(E_i - E_f)\, \theta(E_f - E_l)}{E_l - E_i + i\,\eta} - \frac{\theta(E_l - E_f)\, \theta(E_f - E_i)}{E_l - E_i - i\,\eta} \right] \tag{3.4.17}$$

The polarization function in momentum space is then

$$\Pi^A(k_z, \mathbf{k}_\perp; m_1, m_2) = \int d^3x \int d^3x' e^{-i\,(\mathbf{k}_\perp \cdot \rho + (k_z + m_1 K)\, z)}\, \Pi^A(\mathbf{x}; \mathbf{x}')\, e^{i\,(\mathbf{k}_\perp \cdot \rho' + (k_z + m_2 K)\, z')} \tag{3.4.18}$$

From Eq. (3.4.2) we can get

$$\sum_{n_i} \psi_i(\mathbf{x}) = \sum_{n_i} \int \frac{d^2\, k_{\perp i}}{(2\pi)^2} \int_{-\frac{\pi}{L}}^{\frac{\pi}{L}} dk_{z_i} e^{i\,\mathbf{k}_{\perp i} \cdot \rho} F_{n_i,\, k_{z_i}}(z) \tag{3.4.19}$$

where $F_{n_i,\, k_{z_i}}(z)$ is the one dimensional single particle wave function of a superlattice. The electron-electron interaction potential is

$$V(\mathbf{x}_1, \mathbf{x}_1') = \sum_{m_1',\, m_2'} \int d^2k_\perp' \int_{-\frac{\pi}{L}}^{\frac{\pi}{L}} V(\mathbf{k}_\perp', k_z'; m_1, m_2)$$

$$\times\, e^{i\,(\mathbf{k}_\perp' \cdot \rho_1 + (k_z' + m_1' K)\, z_1)}\, e^{-i\,(\mathbf{k}_\perp' \cdot \rho_1' + (k_z + m_2 K)\, z_1')} \tag{3.4.20}$$

Substituting Eq. (3.4.16), (3.4.19) and (3.4.20) into Eq. (3.4.18) and after some algebraic manipulations, Eq. (3.4.18) becomes

$$\Pi^A(k_z, \mathbf{k}_\perp; m_1, m_2) = \frac{1}{(2\pi)^6} \sum_{n_i} \sum_{n_j} \sum_{n_k} \sum_{n_l} \int_{-\frac{\pi}{L}}^{\frac{\pi}{L}} dk_{z_i} \int_{-\frac{\pi}{L}}^{\frac{\pi}{L}} dk_{z_j} \int d^2k_{\perp_i} \int d^2k_{\perp_j}$$

$$\times \sum_{m_1',\, m_2'} V(k_{z_i} - k_{z_j}, \mathbf{k}_{\perp_i} - \mathbf{k}_{\perp_j}; m_1', m_2') < n_i, k_{z_i} \;|\; e^{i\,(m_1' K + k_{z_i} - k_{z_j})\, z} \;|\; n_j, k_{z_j} >$$

$$\times < n_k,\ k_{z_k} = k_{z_i} - k_z\ (\pm K\ )\ \mid\ e^{-i\,(m_2' + k_{z_i} - k_{z_j})\, z_1'}\ \mid\ n_l,\ k_{z_l} = k_{z_i} - k_z\ (\pm K) >$$

$$\times < n_l,\ k_{z_l} = k_{z_i} - k_z\ (\pm K)\ \mid\ e^{-i\,(m_1 + k_z)\, z}\ \mid\ n_i,\ k_{z_i} >$$

$$\times < n_j,\ k_{z_j}\ \mid\ e^{i\,(m_2 K + k_z)\, z}\ \mid\ n_k,\ k_{z_k} = k_{z_i} - k_z\ (\pm K\ ) >$$

$$\times \left[\frac{\theta(E_j - E_f)\theta(E_f - E_k)}{E_k - E_j + i\,\eta} - \frac{\theta(E_k - E_f)\theta(E_f - E_j)}{E_k - E_j - i\,\eta} \right]$$

$$\times \left[\frac{\theta(E_i - E_f)\theta(E_f - E_l)}{E_l - E_i + i\,\eta} - \frac{\theta(E_l - E_f)\theta(E_f - E_i)}{E_l - E_i - i\,\eta} \right] \qquad (3.4.21)$$

here $k_{z_i} - (\pm K)$ has been explained under Eq. (3.4.6). The step function has been defined in Eq. (3.3.17) and the zero temperature Fermi function is $f_0(x) = 1 - \theta(x)$. Substituting $f_0(x)$ into Eq. (3.4.21) and considering that at $E_i = E_f$, $\theta(E_i - E_f)$ $\theta(E_f - E_l) = 0$, the $i\eta$ in the denominator can be omitted, we can obtain the polarization function

$$\Pi^A(k_z,\ \mathbf{k}_\perp;\ m_1,\ m_2) =$$

$$\frac{1}{(2\pi)^6} \sum_{n_j} \sum_{n_k} \int d^2 k_{\perp j} \int_{-\frac{\pi}{L}}^{\frac{\pi}{L}} dk_{z_j}\ \frac{f_0(E_k = E(\ n_k,\ k_{z_k} = k_{z_i} - k_z\ (\pm K\ )\ )\ ) - f_0(E_j)}{E_k\ -\ E_j}$$

$$\times \sum_{n_i} \sum_{n_l} \int d^2 k_{\perp i} \int_{-\frac{\pi}{L}}^{\frac{\pi}{L}} dk_{z_i} \frac{f_0(E_i) - f_0(E_l = E(n_l,\ k_{z_l} = k_{z_i} - k_z\ (\pm K)\ )\ )}{E_i\ -\ E_l}$$

$$\times \sum_{m_1',\, m_2'} V(k_{z_i} - k_{z_j},\ \mathbf{k}_{\perp i} - \mathbf{k}_{\perp j};\ m_1',\ m_2') < n_i, k_{z_i}\ \mid\ e^{i\,(m_1' K + k_{z_i} - k_{z_j})\, z}\ \mid\ n_j,\ k_{z_j} >$$

$$\times < n_k,\ k_{z_k} = k_{z_i} - k_z\ (\pm K)\ \mid e^{-i\,(m_2' + k_{z_i} - k_{z_j})\,z_1'} \mid n_l,\ k_{z_l} = k_{z_i} - k_z\ (\pm K) >$$

$$\times < n_l,\ k_{z_l} = k_{z_i} - k_z\ (\pm K)\ \mid e^{-i\,(m_1 + k_z)\,z} \mid n_i,\ k_{z_i} >$$

$$\times < n_j,\ k_{z_j}\ \mid e^{i\,(m_2 K + k_z)\,z} \mid n_k,\ k_{z_k} = k_{z_i} - k_z\ (\pm K) > \qquad (3.4.22)$$

This is a rather complicated formula. Use of this formula in a computer numerical calculation will be described in the next chapter.

Section III.5 The Tight Binding Approximation for a Superlattice

From Eq. (3.4.14), (3.4.23), (3.4.6) and (3.6.16), we know that to obtain the polarization function, the exchange eigenenergy and band bending, a complete set of energies and eigenfunctions is required. Numerov's algorithm is used to obtain an energy and eigenfunction with momentum $k_z = 0$ or π / L (to be discussed in chapter IV). The other eigenenergies and eigenfunctions will be obtained based on these equations derived in the subsections that follow. In applying numerical methods to solve these equations, a large number of summation and multiplication steps may be involved. The error accumulated by these calculation steps are determined by the number of calculation steps and the relative error $(\frac{\text{error value}}{\text{exact value}})$ of the items which involved in numerical calculation[37]. For this reason, in order to obtain a proper result, each item which involves numerical calculation must be as accurate as possible. In most computers, a double precision variable provides 15 significant digits. These factors must be taken into consideration in deriving the tight binding approximation equations. For example, if $L = 75\text{Å}$ then $e^{\beta_2 \cdot L} \approx 10^{-2}$ (here $\beta_2 = \left[\frac{2m^*}{\hbar^2} (v_0 - E_2) \right]^{1/2}$, E_2 is the second sub-band eigenenergy (please refer to equations below). If a wave interacts with another wave which belongs to a potential well four wells away, the proportional part value generated by this two wave interaction is $\approx 10^{-9}$. This example shows that the equations in the following subsections may look cumbersome but are nevertheless necessary.

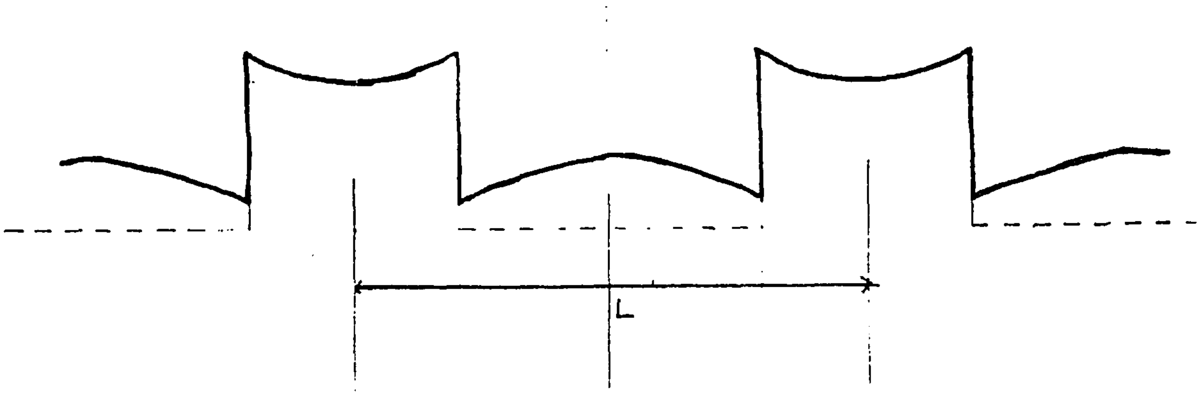
The tight binding approximation wave function takes the form of an LCAO (linear combination of atomic orbitals):

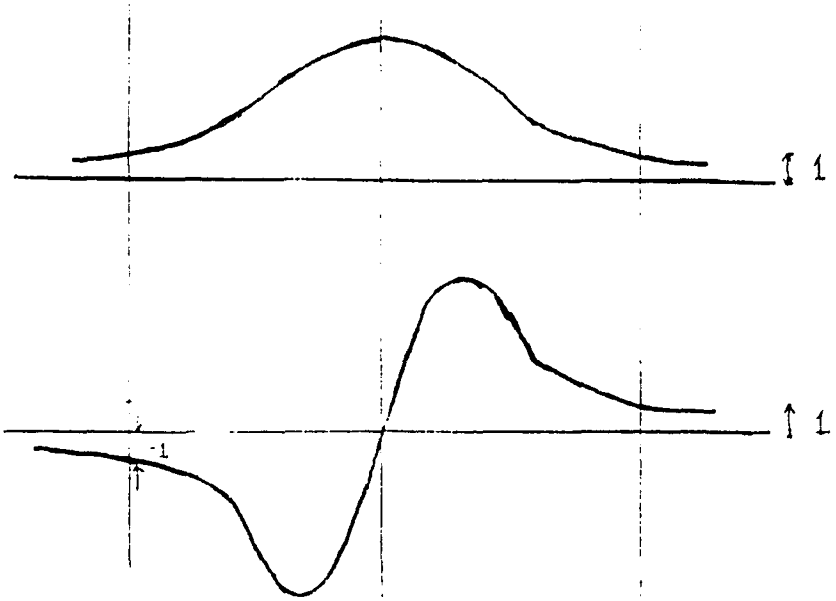
$$F_{n,k_z}(z) = \frac{1}{[N(n, k_z)]^{1/2}} \sum_m e^{i k_z m L} \phi_n(z - m L) \tag{3.5.1}$$

where $N(n, k_z)$ is the normalization factor, n is the sub-band index, ϕ_n is the single potential well wave function, and m is the potential well indicator. Separating $\sum_m$ into $\sum_{m>0}$, the contribution from the right hand side potential wells, $\sum_{m<0}$, the left hand side wells and $m = 0$, the central well. Eq. (3.5.1) becomes

$$F_{n\,k_z}(z) = \frac{1}{[N(n, k_z)]^{1/2}} \left(\phi_n(z) + \sum_{m>0} e^{i k_z m L} \phi_n(z - m L) + \sum_{m<0} e^{i k_z m L} \phi_n(z - m L) \right) \tag{3.5.2}$$

Let $\phi_n(z) = e^{\beta_n L/2 - \beta_n |z|}$ at $z \geq L/2$ and $\phi_n(z) = (-1)^{n+1} e^{\beta_n L/2 - \beta_n |z|}$ at $z \leq -L/2$ be the wave function outside the single potential regions. The $\beta_n = \left[\frac{2m^*}{\hbar^2} (v_0 - E_n) \right]^{1/2}$, v_0 is the energy difference between the conduction band of $\mathrm{Al}_x\mathrm{Ga}_{(1-x)}\mathrm{As}$, and the conduction band of GaAs, E_n is the eigenenergy of the single potential well wave function.





The equation can be rewritten as

$$F_{n,\,k_z}(z) = \frac{1}{[N(n,\,k_z)]^{1/2}}\Big(\phi_n(z) + \sum_{m>0} (-1)^{n+1} e^{\beta_n z}\, e^{-(\,|\,m\,|\,-1)\,\beta_n L}\, e^{\beta_n L/2}\, e^{i\,k_z m L}$$

$$+ \sum_{m<0} e^{-\beta_n z}\, e^{-(\,|\,m\,|\,-1)\,\beta_n L}\, e^{\beta_n L/2}\, e^{i\,k_z m L}\Big) \qquad (3.5.3)$$

Sub-Section : The Normalization Factor for Tight Binding Approximation

The tight binding approximation wave function equation then becomes

$$F_{n,\,k_z}(z) = \frac{1}{[N(n,\ k_z)]^{1/2}} \left[\phi_n(z) + e^{\beta_n z}\omega(k_z) + e^{-\beta_n z}\mu(k_z) \right] \tag{3.5.4}$$

where $\mu(k_z) = \dfrac{e^{-i k_z L - \beta_n L/2}}{1 - e^{-i k_z L - \beta_n L}}$ and $\omega(k_z) \equiv (-1)^{n+1}\,\mu^*(k_z)$. Define

$$D(1,\ k_z) \equiv \mu^*(k_z)\ \mu(k_z) = \omega^*(k_z)\ \omega(k_z) = \frac{e^{\beta_n L}}{e^{2\beta_n L} + 1 - 2\cos(k_z\ L)\ e^{\beta_n L}} \tag{3.5.5a}$$

$$D(2,\ k_z) \equiv \mu^*(k_z) + \mu(k_z) = 2\ D(1,\ k_z)\ e^{\beta_n L/2}[\cos(k_z\ L) - e^{-\beta_n L}] \tag{3.5.5b}$$

$$D(3,\ k_z) \equiv \omega(k_z)\ \mu^*(k_z) + \omega^*(k_z)\ \mu(k_z) =$$

$$(-1)^{n+1}\ 2\ e^{\beta_n L}\ [D(1,\ k_z)]^2\ [\cos(2\ k_z L) - 2\ e^{-\beta_n L}\cos(k_z\ L) + e^{-2\beta_n L}] \tag{3.5.5c}$$

As

$$\int_{-\frac{L}{2}}^{\frac{L}{2}} dz\ F_{n,\,k_z}{}^*(z) F_{n,\,k_z}(z) = 1$$

and the normalization factor

$$N(n\ k_z) = intg\,1 + intg\,2 \cdot D(1,\ k_z) + intg\,3 \cdot D(2,\ k_z) + D(3,\ k_z) \tag{3.5.6}$$

where

$$intg\,1 \equiv \int_{-\frac{L}{2}}^{\frac{L}{2}} dz\ \phi_n^*(z)\ \phi_n(z) \tag{3.5.7a}$$

$$intg\,2 \equiv \int_{-\frac{L}{2}}^{\frac{L}{2}} dz\,[e^{-\beta_n z}\phi_n(z) + (-1)^{n+1}\,e^{\beta_n z}\phi_n^*(z)] \tag{3.5.7b}$$

$$intg\,3 \equiv \int_{-\frac{L}{2}}^{\frac{L}{2}} dz\,[e^{2\beta_n z} + e^{-2\beta_n z}] \tag{3.5.7c}$$

If the potential is a periodic square potential, the analytic result for these integrations can be obtained

$$intg\,1 = \frac{1}{\beta_n}[e^{2\beta_n(b_z - a_z)} - 1\,] + \frac{e^{2\beta_n(b_z - a_z)}\left\{2\,a_z + (-1)^{n+1}\,\dfrac{\sin(2\,\alpha_n\,a_z)}{\alpha_n}\right\}}{1 + (-1)^{n+1}\cos(2\,\alpha_n\,a_z)} \tag{3.5.8a}$$

here a_z is half the width of the GaAs layer, $b_z = L/2$ is a_z plus half the width of $Al_xGa_{(1-x)}As$ layer, $\alpha_n = [\frac{2m^*}{\hbar^2}E_n\,]^{1/2}$.

$$Intg\,2 = \frac{1}{\beta_n}[e^{2\beta_n b_z} - e^{-2\beta_n b_z}] \tag{3.5.8b}$$

For the odd sub-band (n is odd)

$$Intg\,3 = e^{\beta_n b_z}[b_z - a_z] + \frac{e^{\beta_n b_z}}{2\,\beta_n}\left[e^{-2\beta_n a_z} - e^{-2\beta_n b_z}\right] + \frac{e^{\beta_n(b_z - a_z)}}{\cos(\alpha_n\,a_z)\,(\alpha_n^2 + \beta_n^2)}$$

$$\times\left\{\left[e^{-\beta_n z}(-\beta_n\cos(\alpha_n\,z) + \alpha_n\sin(\alpha_n\,z))\right]\Big|_{-a_z}^{a_z}\right\}. \tag{3.5.8c1}$$

For the even sub-band

$$Intg\,3 = -\,e^{\beta_n b_z}[b_z - a_z] + \frac{e^{\beta_n b_z}}{2\,\beta_n}\left[e^{-2\beta_n a_z} - e^{-2\beta_n b_z}\right] - \frac{e^{\beta_n(b_z - a_z)}}{\sin(\alpha_n\,a_z)\,(\alpha_n^2 + \beta_n^2)}$$

$$\times \left\{ \left[e^{-\beta_n z} (\beta_n \sin(\alpha_n z) + \alpha_n \cos(\alpha_n z) \right] \Big|_{-a_z}^{a_z} \right\}. \tag{3.5.8c2}$$

Sub-Section: The Energy Shift in the Tight Binding Approximation

From earlier in this section, we expressed the eigenenergy in terms of its direct and exchange parts:

$$E(n,\ k_z,\ \mathbf{k}_\perp) = E_{\text{dir}}(n,\ k_z,\ \mathbf{k}_\perp) + E_{\text{xc}}(n,\ k_z,\ \mathbf{k}_\perp) \tag{3.5.9}$$

and we approximated the direct part by an effective mass:

$$E_{\text{dir}}(n,\ k_z,\ \mathbf{k}_\perp) = E_{\text{dir}}(n,\ k_z,\ \mathbf{k}_\perp = 0) + \frac{\hbar^2}{2m^*}\mathbf{k}_\perp^2 \equiv E_{\text{dir}}(n,\ k_z) + \frac{\hbar^2}{2m^*}k_\perp^2 \tag{3.5.10}$$

The one-dimensional eigenenergy can be obtained using

$$E_{\text{dir}}(n,\ k_z) = \int_{-\frac{L}{2}}^{\frac{L}{2}} dz\ F^*_{n,\ k_z}(z)\left[-\frac{\hbar^2}{2m^*}\ \nabla_z^2 + V(z)\right]F_{n,\ k_z}(z) \tag{3.5.11}$$

If $F_{n,\ k_z}(z)$ is the tight binding wave function, then

$$F_{n,\ k_z}(z) = \frac{1}{[N(n,\ k_Z)]^{1/2}}\sum_m e^{ik_z \cdot m \cdot L}\phi_n(z - mL) \tag{3.5.12}$$

here $N(n,\ k_z)$ is the normalization factor and $\phi_n(z)$ is the single potential well eigenfunction. The potential

$$V(z) = \sum_m \text{v}(z - mL) \tag{3.5.13}$$

here the $\text{v}(z)$ is the single well potential. The single well potential wave equation is

$$E_n\phi_n(z - mL) = \left[-\frac{\hbar^2}{2m^*}\ \nabla_z^2 + \text{v}(z - mL)\right]\phi_n(z - mL) \tag{3.5.14}$$

Then, using the LCAO expression, Eq. (3.5.1)

$$E_{\mathrm{dir}}(n,\ k_z)F_{n,\ k_z}(z) = \left[-\frac{\hbar^2}{2m^*}\ \nabla_z{}^2 + V(z) \right] F_{n,\ k_z}(z)$$

$$= \frac{1}{[N(n,\ k_Z)]^{1/2}} \sum_i \left\{ [\ E_n + \sum_{m \neq j} \mathrm{v}(\ z - m\ L)]\ \phi_n(z - jL)\ e^{ik_z\, j\, L} \right\} \tag{3.5.15}$$

From the above we can obtain the energy shift equation

$$\Delta\, E_{\mathrm{dir}}(n,\ k_z) = E_{\mathrm{dir}}(n,\ k_z) - E_n = \frac{1}{n} \int_{-\frac{L}{2}}^{\frac{L}{2}} \sum_u \phi_n{}^*(z - u\ L)\ e^{-\,ik_z\, u\, L} dz$$

$$\times \sum_t \left\{ \sum_{s \neq t} \mathrm{v}(z - s\ L)\ \phi_n(z - t\ L)\ e^{ik_z\, t\, L} \right\} \tag{3.5.16}$$

To obtain the energy shift, we have to sum up the terms with different indices $s,\ u,\ t \neq s$. However, according to the tight binding approximation, the single well wave function ϕ_n will not deviate very much from the completed wave-function. For this reason, only the following cases are considered.

A) $u = s$ for all t except $t = s$; this means that $\phi_n{}^*$ will be interacting with the potential, $\mathrm{v}(z - s\ L)$ it belongs to, and also with ϕ_n, which belongs to another potential well at $\mathrm{v}(z - t\ L)$.

B) $t = u$ for all s except $s = t + u$. This means that $\phi_n{}^*$ and ϕ_n belong to the same potential well and both of them are interacting with other potential wells than the one to which they belong.

C) $t = s \pm m,\ u = s \mp m$; this means that the potential well to which $\phi_n{}^*$ belongs and the potential well to which ϕ_n belongs are at opposite sides of the potential well which they are interacting with and at the same distance.

D) $[u = s - 2,\ t = s - 1\ ]$, $[u = s - 1,\ t = s - 2\ ]$, $[u = s + 2,\ t = s + 1\ ]$, and $[u = s + 1,\ t = s + 2\ ]$; This means that the potential well $\Phi_n{}^*$ belongs to or the potential which ϕ_n belongs to is next and second next to the potential well they are interacting with. Also, they are on the same side of the potential.

E) $[u = s - 2,\ t = s + 1\ ]$, $[u = s - 1,\ t = s + 2\ ]$, $[u = s + 2,\ t = s - 1\ ]$, and $[u = s + 1,\ t = s - 2\ ]$. This is the same as case D) except that ϕ_n and $\phi_n{}^*$ are on different sides of the potential they are interacting with.

Equation (3.5.16) in case A) is

$$\Delta E_A(n,\ k_z) = \frac{1}{N(n,\ k_z)}$$

$$\times \sum_{u} \sum_{t \neq u} \int_{-\frac{L}{2}}^{\frac{L}{2}} \phi_n{}^*(s - u\ L) e^{-i\,u\,k_z L} v(z - u\ L) \phi_n(z - t\ L) e^{i\,t\,k_z L} dz \qquad (3.5.17)$$

Assuming that a superlattice has M layers and $M >> 1$ then

$$\Delta E_A(n,\ k_z) = \frac{1}{N(n,\ k_z)}$$

$$\times \sum_{u} \sum_{t \neq u} \int_{-\infty}^{\infty} \phi_n{}^*(s - u\ L)\ e^{-i\,u\,k_z L}\ v(z - u\ L)\ \phi_n(z - t\ L) e^{i\,t\,k_z L} dz$$

$$= \frac{1}{n(n,\ k_z)} \sum_{t > 0} e^{-\beta_n (t - 1) L - \beta_n L / 2}$$

$$\times \left[(-1)^{n+1} \, e^{i \iota k_z L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \mathrm{v}(z) \, \phi_n{*}(z) \, e^{\beta_n z} dz + e^{-i \iota k_z L} \int_{-\frac{L}{2}}^{\frac{L}{2}} \phi_n{*}(z) e^{-\beta_n z} dz \right] \tag{3.5.18}$$

Since $\mathrm{v}(z)$ is symmetrical, $\phi_n(z)$ will be symmetrical for odd sub-bands and anti-symmetrical for even sub-bands (the first sub-band is called band 1). Because

$$(-1)^{n+1} \int_{-\frac{L}{2}}^{\frac{L}{2}} \mathrm{v}(z) \, \phi_n{*}(z) \, e^{\beta_n z} dz = \int_{-\frac{L}{2}}^{\frac{L}{2}} \mathrm{v}(z) \, \phi_n{*}(z) e^{-\beta_n z} dz, \tag{3.5.19}$$

the energy shift equation becomes

$$\Delta E_A(n, \; k_z) = \sum_{m > 0} \frac{2\cos(\, m k_z L \,)}{N(n, \; k_z)} \, e^{-\beta_n (m-1)L - \beta_n L/2} \int_{-\frac{L}{2}}^{\frac{L}{2}} \phi_n{*} \, \mathrm{v}(z) \, e^{-\beta_n z} dz \tag{3.5.20}$$

If the potential is the square well potential, the energy shift equation simplifies to

$$\Delta E_A(n, \; k_z) = \sum_{m > 0} e^{-\beta_n (m-1)L - \beta_n L/2} \cos \left(\, m k_z \, L \, \right) \frac{2}{N(n, \; k_z)} \mathrm{v}_0$$

$$\times \frac{e^{\beta_n (L/2 - a_z)}}{\cos\alpha_n a_z} \, \frac{1}{\alpha_n^2 + \beta_n^2} \left\{ \left[e^{-\beta_n z} (\alpha_n \sin\alpha_n z - \beta_n \cos \left(\, \alpha_n z \right) \right]_{z = -a_z}^{z = a_z} \right\} \tag{3.5.21a}$$

for an odd sub-band, and

$$\Delta E_A(n, \; k_z) = \sum_{m > 0} e^{-\beta_n (m-1)L - \beta_n L/2} \cos \left(\, m \; k_z L \right) \frac{2}{N(n, \; k_z)} \mathrm{v}_0$$

$$\times \frac{e^{\beta_n (L/2 - a_z)}}{\sin(\alpha_n a_z)} \, \frac{1}{\alpha_n^2 + \beta_n^2} \left\{ \left[e^{-\beta_n z} (\beta_n \sin \left(\, \alpha_n z \right) + \alpha_n \cos \left(\, \alpha_n z \right)) \right]_{z = -a_z}^{z = a_z} \right\} \tag{3.5.21b}$$

for an even sub-band. Here $\alpha_n \mathrm{v}_0$ and β_n have been defined in Eq. (3.5.13) and (3.5.8a).

The equation for the energy shift contributed in case B) defined after Eq. (3.5.16) is

$$\Delta E_B(n,\ k_z) = \frac{1}{N(n,\ k_z)}\int_{-\infty}^{\infty} \phi_n{}^*(z)\ \phi_n(z)\ [V(z) - v(z)]\ dz =$$

$$\frac{1}{N(n,\ k_z)}\int_{\frac{L}{2}}^{3\frac{L}{2}} e^{2\beta_n L/2}\ e^{-2\beta_n z}\left[1 + e^{-2\beta_n L} + e^{-4\beta_n L} + \ \ldots\ldots\ldots\right] v(s - L)\ dz$$

$$= \frac{2\cdot e^{-\beta_n L}}{N(n,\ k_z)}\int_{-\frac{L}{2}}^{\frac{L}{2}} e^{-2\beta_n z} v(z)\frac{dz}{1 - e^{-2\beta_n z}} \qquad (3.5.22)$$

If the potential is the square well potential, then

$$\Delta E_B = \frac{-2}{N(n,\ k_z)}\cdot\frac{e^{-\beta_n L}}{1 - e^{-2\beta_n L}}\cdot v_0\ \frac{[e^{2\beta_n a_z} - e^{-2\beta_n a_z}]}{2\ \beta_n} \qquad (3.5.23)$$

here v_0 and a_z have been defined in Eq. (3.5.1) and (3.5.8a). The equation for the energy shift contributed by case C) is

$$\Delta E_C(n,\ k_z) = \sum_{m>0}\frac{1}{N(n,\ k_z)}\int_{-\frac{L}{2}}^{\frac{L}{2}} \phi_n{}^*(z + mL)\ \phi_n(z - mL)\ v(z)e^{i\ m\cdot k_z L}dz$$

$$= \frac{(-1)^{n+1}}{n(n,\ k_z)}\sum_{m>0} 2\cos(2k_z\ m\ L)e^{(-2m+1)\beta_n L}\int_{-\frac{L}{2}}^{\frac{L}{2}} v(z)dz. \qquad (3.5.24)$$

For the square well potential $\int_{-\frac{L}{2}}^{\frac{L}{2}} v(z)dz = -2v_0 a_z$, a_z has been defined under Eq. (3.5.8a). The energy shift equation contributed by case D) is

$$\Delta E_D(n,\ k_z) = \sum_{m>0} \frac{1}{N(n,\ k_z)} \int_{-\frac{L}{2}}^{\frac{L}{2}} dz$$

$$\times \left\{ \phi_n{}^*(z+L)\phi_n(z+2L)e^{i\,k_zL} + \phi_n{}^*(z-L)\phi_n(z-2L)e^{-i\,k_zL} + \right.$$

$$\left. \phi_n{}^*(z+2L)\phi_n(z+L)e^{-i\,k_zL} + \phi_n{}^*(z-2L)\phi_n(z-L)e^{i\,k_zL} \right\}$$

$$= \frac{4}{n(n,\ k_z)} \cos(\ k_zL) \cdot e^{-2\beta_nL} \int_{-\frac{L}{2}}^{\frac{L}{2}} v(z)\ e^{-2\beta_nz} dz \qquad (3.5.25)$$

If the potential is the square well potential, then

$$\int v(z)e^{-2\beta_nz}dz = -\frac{v_0}{2\beta_n}\left[e^{-2\beta_na_z} - e^{-\beta_nb_z}\right] \qquad (3.5.26)$$

Similarly,

$$\Delta E_E(n,\ k_z) = \sum_{m>0} \frac{4}{N(n,\ k_z)} \cos(\ k_zL)\ \ (-1)^{n+1}\ e^{-\beta_nL} \int_{-\frac{L}{2}}^{\frac{L}{2}} v(z)dz \qquad (3.5.27)$$

The total energy shift

$$\Delta E_{\text{dir}}(n,\ k_z) = \Delta E_A(n,\ k_z) + \Delta E_B(n,\ k_z) + \Delta E_C(n,\ k_z) + \Delta E_D(n,\ k_z) + \Delta E_E(n,\ k_z) \qquad (3.5.28)$$

Here, all important interacting terms have been included. This is a highly accurate tight binding approximation energy shift equation.

Next the derivation of the matrix element $<n_1,\ k_{z_1}\ |e^{i\,q_z z}\ |n_2,\ k_{z_2}>$ will be discussed. This matrix element is important in many calculations such as the exchange potential, polarization function and transport coefficients. One reason for using the tight binding approximation is that the tight binding wave function can lead to a fairly accurate evaluation of the matrix element:

$$<n_1, k_{z_1} | e^{i\, q_z\, z} | n_2, k_{z_2}> = [\, N(n_1, k_{z_1})\, N(n_2, k_{z_2})\,]^{-1/2}$$

$$\times \int_{-\frac{L}{2}}^{\frac{L}{2}} \sum_{m_1} e^{-i\, k_{z_1}\, m_1\, L} \phi_{n_1}{}^*(z - m_1\, L) \sum_{m_2} e^{i\, k_{z2}\, m_2 L} \phi_{n_2}{}^*(z - m_2\, L) e^{i\, q_z\, z} dz =$$

$$[\, N(n_1, k_{z_1})\, N(n_2, k_{z_2})\,]^{-1/2} \sum_{m_1} \left\{ e^{-i\, [\, k_{z2} - k_{z_1} + q_z]\, m_1\, L} \right\}$$

$$\times \sum_{m_2'} \left\{ \int_{-\frac{L}{2}}^{\frac{L}{2}} dz\ \phi_{n_1}{}^*(z')\, e^{i\, q_z\, z'} \phi_{n_2}(z' - m_2' L)\, e^{i\, k_{z2}\, m_2'\, L} \right\} =$$

$$[\, N(n_1, k_{z_1})\, N(n_2, k_{z_2})\,]^{-1/2}\ \delta(q_z + k_{z_2} - k_{z_1}(\pm\frac{2\pi}{L})\,)$$

$$\times \sum_{m_2'} \left\{ \int_{-\infty}^{\infty} dz'\ \phi_{n_1}{}^*(z')\, e^{i\, q_z z'} \phi_{n_2}(z' - m_2' L)\, e^{i\, k_{z2} m_2'\, L} \right\} \qquad (3.5.29)$$

Here, it has been assumed that the number of layers of a superlattice is much larger than 1, $(\pm\frac{2\pi}{L})$ has been explained under Eq. (3.4.6), $z = z' - m_1\, L$ and $m_2' = m_2 - m_1$. We can write the integration as :

$$\int_{-\infty}^{\infty} dz\ \phi_{n_1}{}^*(z')\, e^{i\, q_z\, z'} e^{i\, k_{z2}\, m_2'\, L} \phi_{n_2}(z' - m_2' L) = I_L + I_R + I_\alpha + I_\beta + I_\gamma \qquad (3.5.30)$$

here, I_L is integrated from $-\infty$ to $-L/2$ when $m_2' \geq 0$ or from $-\infty$ to $(-\,|\, m_2'\,| - 1/2\,)\, L$ when $m_2' < 0$, I_R is integrated from $L/2$ to ∞ when $m_2' \leq 0$ or from $(\, m_2' + 1/2)\, L$ to ∞ when $m_2 > 0$, I_α is integrated from $-L/2$ to $L/2$ when

$m_2' \geq 0$ or from $(-\mid m_2' \mid - 1/2)\,L$ to $(-\mid m_2' \mid + 1/2)\,L$ when $m_2' < 0$, I_β is integrated from $L/2$ to $(m_2' - 1/2)\,L$ when $m_2' > 0$ or from $(-\mid m_2' \mid + 1/2)\,L$ to $-L/2$ when $m_2' < 0$ no I_β for $m_2' = 0$ and $\mid m_2 \mid = 1$, I_γ is integrated from $(m_2' - 1/2)\,L$ to $(m_2' + 1/2)L$ when $m_2' > 0$, or from $-L/2$ to $L/2$ when $m_2' < 0$ no I_γ for $m_2' = 0$.

When $m_2' = 0$

$$I_L = (-1)^{n_1 + n_2} \frac{e^{-i\,q_z L/2}}{\beta_{n_1} + \beta_{n_2} + i\,q_z} \tag{3.5.31a}$$

$$I_R = \frac{e^{i\,q_z L/2}}{\beta_{n_1} + \beta_{n_2} - i\,q_z} \tag{3.5.31b}$$

$$I_\alpha = \int_{-\frac{L}{2}}^{\frac{L}{2}} e^{i\,q_z\,z} \phi_{n_1}{}^*(z)\phi_{n_2}(z)dz \tag{3.5.31c}$$

When $m_2' > 0$

$$I_L = (-1)^{n_1 + n_2} \frac{e^{-i\,q_z L/2}}{\beta_{n_1} + \beta_{n_2} + i\,q_z} e^{m_2'(i\,k_{z2}\,L - \beta_{n_2} L)} \tag{3.5.32a}$$

$$I_R = \frac{e^{i\,q_z L/2}}{\beta_{n_1} + \beta_{n_2} - i\,q_z} e^{m_2'(i\,q_z L + i\,k_{z2}\,L - \beta_{n_1} L)} \tag{3.5.32b}$$

$$I_\alpha = (-1)^{n_1 + 1} e^{\beta_{n_2} L/2 + m_2'(i\,k_{z2} L - \beta_{n_2}\,L)} \int_{-\frac{L}{2}}^{\frac{L}{2}} e^{i\,q_z\,z + \beta_{n_2}\,z} \phi_{n_1}{}^*(z)dz \tag{3.5.32c1}$$

$$I_\beta = (-1)^{n_2 + 1} \frac{e^{[\beta_{n2} - \beta_{n1} + i\,q_z\,](m_2' - \frac{1}{2})\,L} - e^{[\beta_{n2} - \beta_{n1} + i\,q_z\,]\,\frac{L}{2}}}{\beta_{n_2} - \beta_{n_1} + i\,q_z} e^{(\beta_{n_1} + \beta_{n_2})\,\frac{L}{2} + m_2'(i\,k_{z2} L - \beta_{n_2} L\,)}$$

(3.5.32c2)

$$I_\gamma = e^{\beta_{n_1} L/2 + m_2' (i k_{z2} + i q_z - \beta_{n_1}) L} \int_{-\frac{L}{2}}^{\frac{L}{2}} e^{i q_z z - \beta_{n_1} z} \phi_{n2}(z) \, dz \tag{3.5.32c3}$$

When $m_2' < 0$

$$I_L = (-1)^{n_1 + n_2} \frac{e^{-i q_z L/2}}{\beta_{n_1} + \beta_{n_2} + i q_z} \, e^{| m_2' | (- i q_z L - i k_{z2} L - \beta_{n_1} L)} \tag{3.5.33a}$$

$$I_R = \frac{e^{i q_z L/2}}{\beta_{n_1} + \beta_{n_2} - i q_z} \, e^{| m_2' | (- i k_{z2} L - \beta_{n2} L)} \tag{3.5.33b}$$

$$I_\alpha = (-1)^{n_1 + 1} e^{\beta_{n_1} L/2 + | m_2' | (- \beta_{n_1} - i k_{z2} - i q_z) L} \int_{-\frac{L}{2}}^{\frac{L}{2}} e^{i q_z z + \beta_{n_1} z} \phi_{n2}(z) dz \tag{3.5.33c1}$$

$$I_\beta = (-1)^{n_1 + 1} \frac{e^{-[\beta_{n_1} - \beta_{n_2} + i q_z] (| m_2' | - 1/2) L} - e^{-[\beta_{n_1} - \beta_{n_2} + i q_z] L/2}}{\beta_{n_1} - \beta_{n_2} + i q_z}$$

$$\times e^{(\beta_{n1} + \beta_{n2}) \cdot \frac{L}{2} - | m_2' | (i k_{z2} L + \beta n_1) \frac{L}{2}} \tag{3.5.33c2}$$

$$I_\gamma = e^{\beta_{n2} L/2 + | m_2' | (- i k_{z2} - \beta_{n2}) L} \int_{-\frac{L}{2}}^{\frac{L}{2}} e^{i q_z z} \phi_{n_1}{}^*(z) e^{- \beta_{n2} z} dz \tag{3.5.33c3}$$

Let us define

$$T_1 = \frac{e^{- i k_{z2} 2 L - i q_z L/2}}{\beta_{n_1} - \beta_{n2} + i q_z} \left\{ \frac{e^{- \beta_{n2} L}}{1 - e^{- i k_{z2} L - \beta_{n2} L}} - \frac{e^{- \beta_{n1} L - i q_z L}}{1 - e^{i k_{z2} L - i q_z L - \beta_{n1} L}} \right\} \tag{3.5.34}$$

$$T_2 = \frac{e^{i k_{z2} L - \beta_{n2} L_z/2}}{1 - e^{i k_{z2} L - \beta_{n2} L}} \tag{3.5.35}$$

$$T_3 = \frac{e^{i\,(k_{z2} + q_z)L - \beta_{n1} L/2}}{1 - e^{i\,(k_{z2} + q_z)L - \beta_{n1} L}} \tag{3.5.36}$$

$$T_4 = \frac{e^{i\,q_z L/2}}{\beta_{n_1} + \beta_{n2} - i\,q_z} \left\{ \frac{e^{-(i\,k_{z2} + \beta_{n2})L}}{1 - e^{-(i\,k_{z2} + \beta_{n2})L}} - \frac{e^{(\,i\,k_{z2} + i\,q_z - \beta_{n1}\,)\,L}}{1 - e^{i\,k_{z2}L + (i\,q_z - \beta_{n1}\,)\,L}} \right\} \tag{3.5.37}$$

$$I_1 = \int_{-\frac{L}{2}}^{\frac{L}{2}} e^{i\,q_z z}\,\phi_{n_1}{}^*(z)\phi_{n_2}(z)dz \tag{3.5.38}$$

$$I_2 = \int_{-\frac{L}{2}}^{\frac{L}{2}} e^{i\,q_z z}\,e^{-\beta_{n_1} z}\phi_{n2}(z)dz \tag{3.5.39}$$

$$I_3 = \int_{\frac{L}{2}}^{\frac{L}{2}} e^{i\,q_z z}\,\phi_{n_1}{}^*(z)e^{-\beta_{n2} z}dz \tag{3.5.40}$$

Then

$$<n_{1,}\,k_{z_1}\,|e^{i\,q_z z}\,|n_2,\,k_{z_2}> = I_1 + (-1)^{n1+n2}\,T_4^* + T_4 + (-1)^{n2+1}\,T_1^* + (-1)^{n1+1}\,T_1$$

$$+ T_2\,I_3 + (-1)^{n1+n2}\,I_2{}^*T_3^* + T_3\,I_2^* + (-1)^{n1+n2}T_2^*\,I_3 \tag{3.5.41}$$

here A^* is the complex conjugate of A. This is an accurate but complicated formula. Since calculations of the coefficients such as polarization function Π^A include the summation of a huge number of matrix elements, accurate matrix elements are necessary.

Section III.6 Electron Distribution And Poisson's Equation In a Superlattice

The first equation to be derived in this section is the equation for obtaining the Fermi-level of a superlattice. This is similar to the derivation of the electron distribution function as well as the state density function of the superlattice.

The eigenenergy of a superlattice is

$$E(n,\, k_z,\, \mathbf{k}_\perp) = E_{\rm dir}(n,\, k_z,\, \mathbf{k}_\perp) + E_{\rm xc}(n,\, k_z,\, \mathbf{k}_\perp) = E_{\rm dir}(n,\, k_z,\, \mathbf{k}_\perp = 0) + \frac{\hbar^2}{2m^*}k_\perp^2 + E_{\rm xc}(n,\, k_z,\, \mathbf{k}_\perp) \tag{3.6.1}$$

here m^* is the electron effective mass of the homogeneous medium. We have approximated

$$E(n,\, k_z,\, \mathbf{k}_\perp) \approx E_{\rm dir}(n,\, k_z,\, \mathbf{k}_\perp = 0) + \frac{\hbar^2}{2m^*_n}k_\perp^2 \tag{3.6.2}$$

here m^*_n can be defined as an effective mass of the n_{th} sub-band of a superlattice. This approximation will simplify some of the important calculations to be discussed in the next chapter. The eigenfunction has been defined as

$$\psi_{n,\,k_z,\,\mathbf{k}_\perp}(z) = e^{i\mathbf{k}_\perp \cdot \rho} F_{n,\,k_z}(z) \tag{3.6.3}$$

The normalization requirement is

$$\int_{-\frac{L}{2}}^{\frac{L}{2}} F^*_{n,\,k_z}(z) F_{n,\,k_z}(z)dz = 1 \tag{3.6.4}$$

Let N be the average electron carrier density, $f_0(E)$ be the electron distribution function, then

$$N \cdot \Omega = \sum_{n} \sum_{\mathbf{k}_\perp,\, k_z} 2 \int_{\Omega} d\mathbf{r} \left| \psi_{n,\, k_z,\, \mathbf{k}_\perp}(z) \right|^2 f_0(E(n,\, k_z,\, \mathbf{k}_\perp)) \qquad (3.6.5)$$

here the value 2 is for spin and $\Omega = L_x L_y L$. The L_x and L_y are crystal widths in x and y directions, L is the width of the superlattice cell.

$f_0(E)$ is the Fermi-Dirac distribution function

$$f_0(\, E(n,\, k_z,\, \mathbf{k}_\perp)) = \frac{1}{\left[1 + \exp \left[\dfrac{(E(n,\, k_z,\, \mathbf{k}_\perp) - E_f)}{kT} \right] \right]}, \qquad (3.6.6)$$

here k is Kelvin constant and T is temperature. Then

$$N = \sum_{n} \sum_{\mathbf{k}_\perp} \sum_{k_z} \cdot 2 \, \frac{1}{1 + \exp \left[\dfrac{E(n,\, k_z,\, \mathbf{k}_\perp) - E_f}{kT} \right]} \qquad (3.6.7)$$

where $\sum\limits_{\mathbf{k}_\perp} = \dfrac{1}{(2\pi)^2} \int dk_x \int dk_y$, $\sum\limits_{k_z} = \dfrac{L}{2\pi} \int_{-\frac{\pi}{L}}^{\frac{\pi}{L}} dk_z$ with $E(n,\, k_z,\, \mathbf{k}_\perp) = E(n,\, k_z,\, |\, \mathbf{k}_\perp \,|\,)$ and $E(n,\, k_z,\, \mathbf{k}_\perp) = E(n,\, -k_z,\, \mathbf{k}_\perp)$. Thus

$$N = \frac{1}{(2\pi)^2} \cdot 2 \cdot \sum_{n} \int_{0}^{\infty} \frac{d \,|\, \mathbf{k}_\perp \,|^2}{2}$$

$$\times \int_{0}^{\frac{\pi}{L}} \frac{1}{1 + \exp \left[\dfrac{\hbar^2 k_\perp^2 / 2m_n^* + E(n,\, k_z,\, \mathbf{k}_\perp = 0) - E_f}{kT} \right]} \qquad (3.6.8)$$

$$= \sum_{n} \int_{0}^{\frac{\pi}{L}} dk_z \frac{4 m_n^* kT}{\hbar^2 (2\pi)^2} \ln \left[1 + \exp \frac{E_f - E(n,\, k_z,\, \mathbf{k}_\perp = 0)}{kT} \right] \qquad (3.6.9)$$

here 2 in Eq (3.6.8) arises from spin. From this equation we can define $\dfrac{4 m_n^* kT}{\hbar^2 (2\pi)^2}$ as the state density function for a superlattice and $\ln\left[1+\exp\frac{E_f - E(n,\, k_z,\, \mathbf{k}_\perp = 0)}{kT}\right]$ as the electron distribution function of a superlattice. Also, if we know the average electron carrier density and eigenenergy $E(n,\, k_z,\, \mathbf{k}_\perp = 0)$, we can easily get the Fermi-level from this equation by applying a self-consistent computer calculation (to be discussed in the next chapter). For low temperatures, $\exp\left[\frac{E_f - E(n,\, k_z,\, \mathbf{k}_\perp = 0)}{kT}\right]$ tends to ∞. By this reason, if $E(n,\, k_z,\, \mathbf{k}_\perp = 0) < E_f$

$$\ln\left[1+\exp\frac{E_f - E(n,\, k_z,\, \mathbf{k}_\perp = 0)}{kT}\right] \approx \frac{E_f - E(n,\, k_z,\, \mathbf{k}_\perp = 0\,)}{kT} \tag{3.6.10a}$$

and if $E(n,\, k_z,\, \mathbf{k}_\perp = 0) > E_f$

$$\ln\left[1+\exp\frac{E_f - E(n,\, k_z,\, \mathbf{k}_\perp = 0)}{kT}\right] \approx 0 \tag{3.6.10b}$$

Eq. (3.6.9) becomes

$$N = \sum_n \int_0^{\frac{\pi}{L}} dk_z \frac{4m_n^*}{\hbar^2(2\pi)^2}\, \theta(E_f - E(n,\, k_z,\, \mathbf{k}_\perp = 0)) \tag{3.6.11}$$

In this paper only the zero temperature screening effect will be determined. Eq. (3.6.11) will be used to obtain the Fermi level.

The electron density function can be written as

$$\rho(z) = \sum_n \sum_{k_z,\, \mathbf{k}_\perp} \int dx \int dy \left| \phi_{n,\, k_z,\, \mathbf{k}_\perp}(z) \right|^2 f_0(E) \cdot 2 \tag{3.6.12}$$

Using the same procedure as above, the electron density function then becomes

$$\rho(z) = \sum_n \frac{4m_n^*kT}{\hbar^2(2\pi)^2} \int_0^{\frac{\pi}{L}} dk_z \ln\left[1 + \exp \frac{E_f - E(n,\, k_z,\, \mathbf{k}_\perp = 0)}{kT}\right] \left| F_{n,\, k_z}(z) \right|^2 \tag{3.6.13}$$

From the last section using Eq. (3.5.2) we obtain

$$\left| F_{n,\, k_z}(z) \right|^2 = N(n,\, k_z)^{-1} \Bigg\{ D(3,\, k_z) + \phi_n^*(z)\phi_n(z) +$$

$$\phi_n(z)[e^{-\beta_n z} + (-1)^{n+1}\, e^{\beta_n z}\,]\, D(2,\, k_z) + [e^{2\beta_n z} + e^{-2\beta_n z}]\, D(1,\, k_z) \Bigg\} \tag{3.6.14}$$

Let

$$intg\,1 \equiv \sum_n \int_0^{\frac{\pi}{L}} dk_z \frac{D(1,\, k_z)}{N(n,\, k_z)}\; \frac{4m_n^*kT}{\hbar^2(2\pi)^2} \ln\left[1 + \exp \frac{E_f - E(n,\, k_z,\, \mathbf{k}_\perp = 0)}{kT}\right] \tag{3.6.15a}$$

$$intg\,2 \equiv \sum_n \int_0^{\frac{\pi}{L}} dk_z \frac{D(2,\, k_z)}{N(n,\, k_z)}\; \frac{4m_n{*}kT}{\hbar^2(2\pi)^2} \ln\left[1 + \exp \frac{E_f - E(n,\, k_z,\, \mathbf{k}_\perp = 0)}{kT}\right] \tag{3.6.15b}$$

$$intg\,3 \equiv \sum_n \int_0^{\frac{\pi}{L}} dk_z \frac{D(3,\, k_z)}{N(n,\, k_z)}\; \frac{4m_n{*}kT}{\hbar^2(2\pi)^2} \ln\left[1 + \exp \frac{E_f - E(n,\, k_z,\, \mathbf{k}_\perp = 0)}{kT}\right] \tag{3.6.15c}$$

$$intg\,4 \equiv \sum_n \int_0^{\frac{\pi}{L}} dk_z \frac{1}{N(n,\, k_z)}\; \frac{4m_n{*}kT}{\hbar^2(2\pi)^2} \ln\left[1 + \exp \frac{E_f - E(n,\, k_z,\, \mathbf{k}_\perp = 0)}{kT}\right] \tag{3.6.15d}$$

The final electron density function is

$$\rho(z) = \phi_n^*(z)\phi_n(z)\; intg\,4 + [\, e^{2\beta_n z} + e^{-2\beta_n z}\,]\; intg\,1$$

$$+\, \phi_n(z)\, [\, e^{-\beta_n z} + (-1)^{n+1}\, e^{\beta_n z}\,]\; intg\,2 + intg\,3 \tag{3.6.16}$$

Because all the intg1, intg2, intg3, and intg4 are independent of z, the computer time required to obtain the electron density will be short.

Band bending is a very important phenomenon in a superlattice. This phenomenon is generated by the non-uniform charge distribution and this electric potential change obeys Poisson's equation. One of the important reasons for using the tight binding approximation is that we need to have an accurate electron charge density function to be used in Poisson's equation in order to obtain the electron potential change.

In a superlattice the charge distribution is uniform in the x and y directions; both the electric potential and the charge distribution are dependent on z only. The Poisson's equation can be written as

$$\nabla_z^2 \phi(z) = \frac{4\pi}{\varepsilon} [\, \rho_e(z) + \rho_d(z) \,] \tag{3.6.17}$$

here ρ_d is the charge density generated by the impurity doping and ρ_e is the charge density generated by the electron carrier, $\rho_e(z) = -\mid e \mid \rho(z)$, $\rho(z)$ is the electron density function that can be obtained by Eq. (3.5.15). The method to solve Eq. (3.6.17) will be discussed in the next chapter.

Chapter IV Numerical Methods

All the theories and equations necessary to obtain the screening effect of a superlattice have been developed in the previous chapter. There remains the problem of solving these equations by computer methods. In this chapter, I will discuss first some techniques which have been used in this program other than the technique which has been applied to solve for the polarization functions $\Pi^0(\mathbf{k}_\perp, k_z; m_1, m_2)$ and $\Pi^A(\mathbf{k}_\perp, k_z; m_1, m_2)$.

If Eq. (3.4.16) is applied directly to calculate $\Pi^A(\mathbf{k}_\perp, k_z; m_1, m_2)$ a huge C.P.U. time will be required. It is therefore necessary to use some approximation to reduce the computation time. Both the eigenenergy and the reciprocal of electric potential are approximated as a quadratic function of momentum. I will then discuss in detail how to apply these approximations and what advantages we will get from the calculation of the polarization function. Special techniques described here include how to treat a singularity in calculating the polarization function $\Pi^0(\mathbf{k}_\perp, k_z; m_1, m_2)$ and how to make the calculation of the polarization function Π^A faster using the smoothness of some functions.

Section IV.1 Numerov's Method to Solve the Eigen Equation in a Superlattice and Others

In this section I will discuss some techniques which have been used in this program but which are not related to the polarization function. These techniques include the method to obtain the eigenenergy and eigenfunction for a single well potential (Numerov's method), the method to obtain the Fermi level and the method to solve Poisson's equation.

In the lowest approximation, the potential is a square well potential. The eigenenergy of the single square potential must obey the equation

$$(\varepsilon^2 - \varepsilon'^2)^{1/2} = \varepsilon \tan \varepsilon \tag{4.1.1}$$

for even wave functions and

$$(\varepsilon^2 - \varepsilon'^2)^{1/2} = -\, \varepsilon \cot \varepsilon \tag{4.1.2}$$

for odd wave functions. Here $\varepsilon' = \left[\frac{m^* v_0\, a^2}{2\hbar^2} \right]^{1/2}$, v_0 is the height of the potential well and a is the width of the well, $\varepsilon = \left[\frac{m^* E a^2}{2\hbar^2} \right]^{1/2}$ and E is the eigenenergy of the electron. The eigenfunction is a simple cosine wave (even wave function) or sine wave (odd wave function) in the well and decays exponentially outside the potential well. When the potential is slightly changed, the eigenenergy will be shifted an amount approximately equal to the average potential change. Numerov's algorithm[4] provides an efficient calculation of the energy and eigenfunction. The formula of Numerov's algorithm can be derived as follows:

A one dimensional Schrodinger equation can be written by

$$\left\{ \frac{d^2}{dz^2} + C \left[E - V(z) \right] \right\} \psi = 0 \tag{4.1.3}$$

here $C = \frac{2m^*}{\hbar^2}$. If the energy changes to $E + \Delta E$, the wave function ψ will also be changed to $\psi + \Delta\psi$, Eq. (4.1.3) becomes

$$\left\{ \frac{d^2}{dz^2} + C \left[E + \Delta E - V(z) \right] \right\} \left\{ \psi + \Delta\psi \right\} = 0 \tag{4.1.4}$$

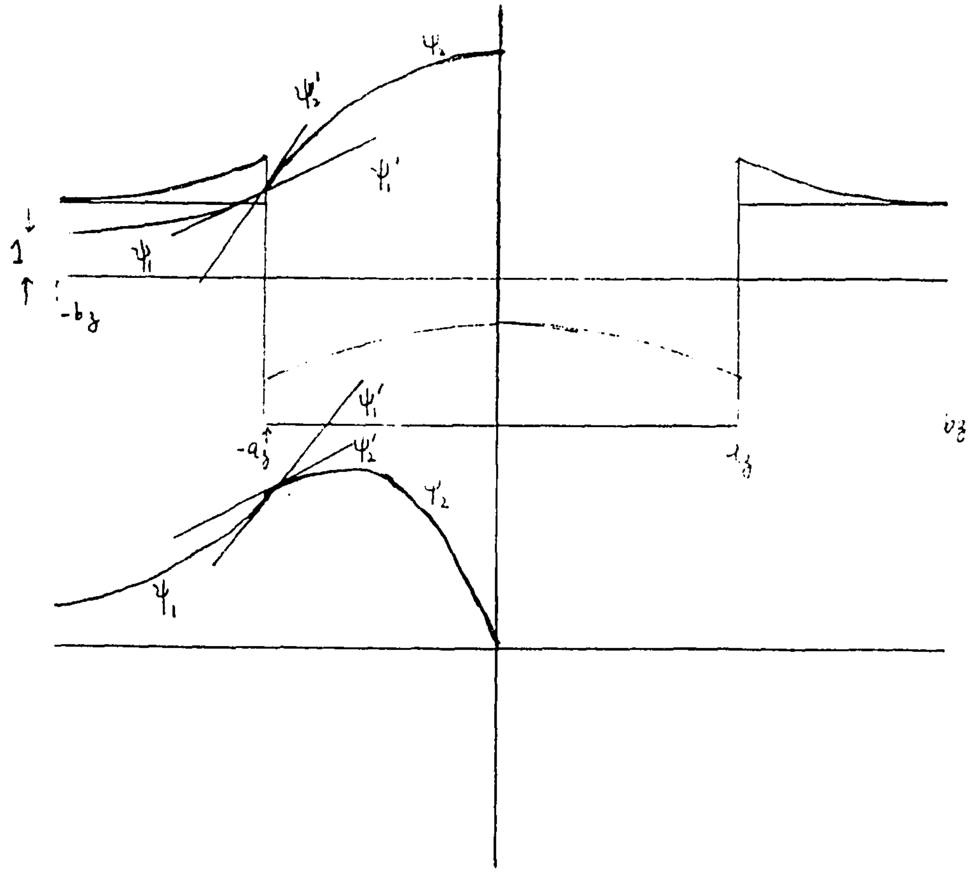
Subtracting (4.1.4) from (4.1.3) we get

$$\left\{ \frac{d^2}{dz^2} + C \left[E + \Delta E - V(z) \right] \right\} \Delta\psi = - C \, \Delta E \, \psi \tag{4.1.5}$$

After multiplying Eq. (4.1.5) by ψ (here ψ is real), and subtracting Eq. (4.1.5) multiplying to $\Delta\psi$, omitting the high order derivative terms and integrating the equation, we get an equation for the shift in energy ΔE:

$$\left[\psi \frac{d}{dz} \Delta\psi - \Delta\psi \, d\frac{\psi}{dz} \right] \Bigg|_{\alpha}^{\beta} \approx - \Delta E \, C \int_{\alpha}^{\beta} | \psi |^2 \, dz \tag{4.1.6}$$

Let ψ_1 be the wave function outside the well (refer to the figures below), ψ_1 will decay exponentially for $| z | > L/2 = b_z$ and choosing its absolute value equals 1 at $| z | = b_z$. Let ψ_2 be the wave function inside the well. It will be equal to ψ_1 at $| z | = a_z$ (a_z is the width of the well). At $z = 0$ the wave function will be zero for the odd wave function. Its derivative will be zero for the even wave function.



Since, at $z = 0$ either $\psi_2 = 0$ (even wave function) or $\psi_2' = 0$ (odd wave function) the $[\psi_2 \cdot \Delta\psi_2' - \Delta\psi_2 \cdot \psi_2']$ will be zero at $z = 0$. The Eq. (4.1.6) for ψ_2 becomes

$$\int_{-a_z}^{0} | \psi_2 |^2 \Delta E \; C \; dz = \left[\psi_2 \cdot \Delta\psi_2' - \Delta\psi_2 \cdot \psi_2' \right] \Big|_{z = -a_z} \qquad (4.1.7)$$

here ψ' is the derivative of ψ, ψ_1 is the wave function in GaAs layer and ψ_2 is the wave function in $Al_xGa_{1-x}As$. Also, ψ_1 is 1 at $z = -b_z$ we get

$$-\int_{-b_z}^{-a_z} |\ \psi_1\ |^2\, \Delta E\ C\ dz = \left[\psi_1 \cdot \Delta\psi_1' - \Delta\psi_1 \cdot \psi_1'\right]\Big|_{z=-a_z} - \psi_1 \cdot \Delta\psi_1'\Big|_{z=-b_z} \qquad (4.1.8)$$

Subtract Eq. (4.1.8) from Eq. (4.1.7) then

$$\Delta E\ C \cdot \int_{-b_z}^{0} |\ \psi\ |^2\, dz = \Delta E\ C \cdot \left[\int_{-b_z}^{-a_z} + \int_{-a_z}^{0} |\ \psi\ |^2\, dz\right] =$$

$$\left\{ \left[\psi_2 \cdot \Delta\psi_2' - \Delta\psi_2 \cdot \psi_2'\right] - \left[\psi_1 \cdot \Delta\psi_1' - \Delta\psi_1 \cdot \psi_1'\right]\Big|_{z=-a_z} + \psi_1 \cdot \Delta\psi_1'\Big|_{z=-b_z}\right\} \qquad (4.1.9)$$

The wave function and its derivative should be continuous at $z=-a_z$. We can adjust ψ_2 by multiplying a constant to make ψ_2 equal to ψ_1 at $z=-a_z$.

$$[\ \psi_2 \cdot \Delta\psi_2' - \Delta\psi_2 \cdot \psi_2'\ ] - [\ \psi_1 \cdot \Delta\psi_1' - \Delta\psi_1 \cdot \psi_1'\ ]\Big|_{z=-a_z}$$

$$= \psi_1\ [\Delta\psi_2' - \Delta\psi_1'\ ] - \left[\Delta\psi_2 \cdot \psi_2' - \Delta\psi_1 \cdot \psi_1'\ \right]\Big|_{z=-a_z} \qquad (4.1.10)$$

In order to make ψ's derivative continuous at $z=-a_z$, we need to find a ΔE to make $\Delta\psi_1' - \Delta\psi_2'$ equal to $-(\ \psi_1' - \psi_2'\ )$, then

$$[\ \psi_2 \cdot \Delta\psi_2' - \Delta\psi_2 \cdot \psi_2'\ ] - [\ \psi_1 \cdot \Delta\psi_1' - \Delta\psi_1 \cdot \psi_1'\ ]\Big|_{z=-a_z}$$

$$= \psi_1\ [\psi_1' - \psi_2'\ ] - [\ \Delta\psi_2 \cdot \psi_2' - \Delta\psi_1 \cdot \psi_1'\ ]\Big|_{z=-a_z} \qquad (4.1.11)$$

ψ_2 always requires to be adjusted to be equal to ψ_1 at $z=-a_z$, as explained under Eq. (4.1.9). This means that $\Delta\psi_2$ should be equal to $\Delta\psi_1$ at $z=-a_z$. Since the eigenenergy E change to $E+\Delta E$, may cause a change in the "constant" which is used to adjust ψ_2 to be equal to ψ_1 at $z=-a_z$. Here we have made an approximation that omitted this "constant" change. Applied $\psi_1 = \psi_2$ and $\Delta\psi_1 \approx \Delta\psi_2$ to Eq. (4.1.11) we get

$$[\,\psi_2 \cdot \Delta\psi_2' - \Delta\psi_2 \cdot \psi_2'\,] - [\,\psi_1 \cdot \Delta\psi_1' - \Delta\psi_1 \cdot \psi_1'\,] = [\psi_1' - \psi_2']\,[\psi_1 + \Delta\psi_1] \tag{4.1.12}$$

Eq. (4.1.9) becomes

$$\Delta E\; C \cdot \int_{-b_z}^{0} |\,\psi\,|^2\, dz = \left\{ [\psi_1' - \psi_2']\,[\psi_1 + \Delta\psi_1]\Big|_{z=-a_z} + \psi_1 \cdot \Delta\psi_1'\Big|_{z=-b_z} \right\} \tag{4.1.13}$$

As the $\Delta\psi$ is not easy to apply to computer numerical calculation, we need some modification as following. The ψ decays exponentially at $b \le -b_z$. We have set the boundary condition that $|\,\psi\,| = 1$ at $b \le -b_z$. The wave function at $b \le -b_z$ can be written by $e^{\beta_n z\;\beta_n b_z}$. By this reason $\psi_1' = \beta_n e^{\beta_n b_z} e^{\beta_n z}$ with $\Delta\psi \approx \dfrac{\partial\psi}{\partial E}\,\Delta E$, and $\dfrac{\partial}{\partial E} = \dfrac{\partial}{\partial\beta_n}\,\dfrac{\partial\beta_n}{\partial E}$, at $z \le -b_z$.

$$\psi_1\;\Delta\psi_1'\Big|_{z=-b_z} = -\beta_n \frac{\Delta E}{2\,(\,V - E\,)} \tag{4.1.14}$$

At $-a_z \ge z >= -b_z$ $V(z) \approx 0$, the wave function is approximately equal to $\beta_n e^{\beta_n b_z} e^{\beta_n z}$ then

$$\Delta\psi_1\Big|_{z=-a_z} \approx -\,\Delta E\;\psi_1\;\beta_n\,\frac{(b_z - a_z\,)}{2(\,V - E\,)} \tag{4.1.15}$$

Substituting Eq. (4.1.14) and (4.1.15) into Eq. (4.1.13) we get

$$\Delta E = \frac{\psi_1 \cdot (\psi_1' - \psi_2'\,)\Big|_{z=-a_z}}{C \int_{-b_z}^{0} |\,\psi\,|^2 dz \;+\; \dfrac{\beta_n}{2\,(\,V - E)} \left[1 + \psi_1\,(\,\psi_1' - \psi_2')\,(\,b_z - a_z\,) \right] \Big|_{z=-a_z}} \tag{4.1.16}$$

We can apply this equation to obtain the shift in eigenenergy and eigenfunction of the single well potential quickly by the following steps.

First, an energy E is chosen (as close to the exact eigenenergy as possible, such as adding the average of potential shifting). Using numerical method (by imposing proper boundary condition) we can find the wave functions ψ_1 and ψ_2. Second, after numerical evaluation of $\int_{-b_z}^{0} | \psi |^2 dz$, $\psi_1(-a_z)$, $\psi_1'(-b_z)$ and $\psi_2'(-b_z)$ and inserting into Eq. (4.1.16) ΔE can be obtained. After readjusting the value of E, the same procedure is repeated. The value of E should converge rapidly to the single potential well eigenenergy. The eigenfunction can also be obtained at the same time.

Obviously, Eq. (3.6.11) is easy to apply such that given a value of the Fermi level E_f, the corresponding average electron carrier density N can be easily computed. On the other hand, if the process is reversed with N given in order to find the E_f , the following is a method to be used. First, two values of E_{f1} and E_{f2} are chosen and substituted into Eq. (3.6.11). Two corresponding $N1$ and $N2$ are obtained. If neither $N1$ nor $N2$ equals the expected N, then E_{f2} is changed to

$$E_{f2} = E_{f1} + \frac{(N - N1) * (E_{f1} - E_{f2})}{N2 - N1} \tag{4.1.17}$$

and E_{f1} replaces the old E_{f2}. Repeating the procedure with Eq. (3.6.11) and (4.1.17), E_{f1} and E_{f2}, after each iteration, will be closer to the Fermi level and $N1$ and $N2$ will be nearer to the value of N.

Because the FFT (fast Fourier transformation subroutine, supported by Bell Laboratory's Port Library) is very efficient, we apply it to solve Poisson's equation. From Eq. (3.6.16) we can obtain the Fourier's component Poisson equation.

$$\phi(k_z) = -\frac{4\pi}{\varepsilon\, k_z^2}[\,\rho_e(k_z) + \rho_d(k_z)] \qquad (4.1.18)$$

To solve Poisson's equation, the Fourier's components of $[\rho_e(z) + \rho_d(z)]$ is obtained first, each Fourier component is then multiplied by $\frac{-4\pi}{\varepsilon\, k_z^2}$ Fourier component and finally Fourier transformation is applied back to real space to obtain $\phi(z)$.

Section IV.2 Quadratic Approximation

In this section I will discuss why both the reciprocal of electron-electron interacting potential and the energy of a superlattice wave function can be approximated by a quadratic equation of its momentum. I will also discuss how the approximation is made.

The reciprocal of the Thomas-Fermi screened electron-electron interacting potential is

$$\frac{1}{V(\mathbf{k})} = k^2 + \lambda^2 = k^2 + C \ . \tag{4.2.1}$$

Here $4\pi e^2$ has been set equal to one and the Thomas-Fermi screening length λ is independent of k. An equation for the reciprocal screened electron-electron interacting potential (of a homogeneous medium) which includes exchange and correlation effects can be expressed as

$$\frac{1}{V(\mathbf{k})} = A'k^2 + C'(k) \tag{4.2.2}$$

here C' is dependent on k and A' is nearly equal to 1. In a calculation involving this kind of potential Eq. (4.2.2) can be approximated by

$$\frac{1}{V(\mathbf{k})} \approx Ak^2 + C \tag{4.2.3}$$

when k is in a suitable region. Eq. (4.2.3) is similar to Eq. (4.2.1). For a superlattice the electron-electron interacting potential can be expressed as (this potential has been discussed in section III.2)

$$\frac{1}{V(k_z,\, \mathbf{k}_\perp;\, m_1,\, m_2)} \approx A'(k_z,\, \mathbf{k}_\perp;\, m_1,\, m_2) \cdot (k_\perp^2 + (m_2\, K + k_z)^2) + C'(k_z,\, \mathbf{k}_\perp;\, m_1,\, m_2) \tag{4.2.4}$$

where $K = \frac{2\pi}{L}$ and can be approximated by

$$\frac{1}{V(k_z, \mathbf{k}_\perp; m_1, m_2)} \approx \text{CoefA}'(k_z, \mathbf{k}_\perp; m_1, m_2, k_\perp^2) + \text{CoefB}'(k_z, \mathbf{k}_\perp; m_1, m_2, k_\perp^2)\, k_\perp^2 \tag{4.2.5}$$

$$\approx \text{CoefA}(m_1, m_2) + \text{CoefB}(m_1, m_2)\, k_\perp^2 \tag{4.2.6}$$

The method to obtain the coefficients is similar to using a quadratic equation $y = Ax^2 + B$ to fit a set of points (x_i, y_i). In order to minimize the deviation, the coefficient must obey the equation

$$< y_i > - A < x_i^2 > - B = 0 \tag{4.2.7}$$

and

$$< y_i x_i^2 > - A < x_i^4 > - B < x_i^2 > = 0 \tag{4.2.8}$$

here $< x_i > = \sum_i^N \frac{x_i}{N}$

If we know the values of $\Pi^0(k_z, \mathbf{k}_\perp; m_1, m_2)$ and $\Pi^A(k_z, \mathbf{k}_\perp; m_1, m_2)$, for different values of k_z, $\mathbf{k}_\perp$, m_1 and m_2, we can use Eq. (3.3.5) to obtain $\eta(\mathbf{k}_\perp, k_z + mk; \mathbf{k}_\perp, k_z + m' k)$. Also from the relationship $\overleftrightarrow{X}(\mathbf{k}_\perp, k_z) = [\overleftrightarrow{\Lambda}(k_\perp, k_z)]^{-1}$ and $V(\mathbf{k}_\perp, k_z + mK; \mathbf{k}_\perp, k_z + m'K) = \frac{4\pi e^2}{k_\perp^2 + (k_z + m'k)^2} \times X(\mathbf{k}_\perp, k_z + mK; \mathbf{k}_\perp, k_z + m'K)$, we can obtain $V(\mathbf{k}_\perp, k_z + mK; \mathbf{k}_\perp, k_z + m'K)$ for different values of k_z, $\mathbf{k}_\perp$, m and m' and ($\eta(\mathbf{k}_\perp, k_z + mk; \mathbf{k}_\perp, k_z + m' k)$ is the element of matrix Λ). Applying Eq. (4.2.7) and (4.2.8), we can obtain CoefA$'(k_z, \mathbf{k}_\perp; m_1, m_2)$ and CoefB$'(k_z, \mathbf{k}_\perp; m_1, m_2)$. After further apply the slower vary approximation method (please refer to section IV) to those two coefficients. The CoefA$'(k_z, \mathbf{k}_\perp; m_1, m_2)$ and CoefB$'(k_z, \mathbf{k}_\perp; m_1, m_2)$ become

CoefA(m_1, m_2) and CoefB(m_1, m_2). This approximation enables much faster computer calculation of the polarization functions $\Pi^0(k_z, \mathbf{k}_\perp; m_1, m_2)$ and $\Pi^A(k_z, \mathbf{k}_\perp; m_1, m_2)$. Further discussion will follow in section IV.4.

It has been mentioned in section III.4 that the eigenenergy of the superlattice wave function can be approximated by a quadratic function of its momentum. The eigenenergy $E(n, k_z, \mathbf{k}_\perp)$ includes the direct energy $E_{\mathrm{dir}}(n, k_z, \mathbf{k}_\perp = 0)$ and $\hbar^2 k_\perp^2/2m^*$ and the exchange correlation energy $E_{\mathrm{xc}}(n, k_z, \mathbf{k}_\perp)$. The direct energy can be obtained from Numerov's algorithm calculation and the tight binding approximation theory, while the exchange correlation energy can be obtained from Eq. (3.4.6). Once we know $E(n, k_z, \mathbf{k}_\perp)$, we can use the same method as in the reciprocal electron-electron interacting potential to obtain a quadratic expression of the eigenenergy

$$E(n, k_z, \mathbf{k}_\perp) = E(n, k_z, \mathbf{k}_\perp = 0) + \frac{\hbar^2}{2m_n^*} k_\perp^2 \tag{4.2.9}$$

here, m_n* is the electron effect mass at n^{th} sub-band in a superlattice, which has considered the effect of the exchange and correlation interaction.

The equation for $\Pi^0(k_z, \mathbf{k}_\perp; m_1, m_2)$ is

$$\Pi^0(k_z, \mathbf{k}_\perp; m_1, m_2) = \frac{2}{(2\pi)^3} \sum_{n_i, n_j} \int d\mathbf{k}_{\perp_i} \int_{-\frac{\pi}{L}}^{\frac{\pi}{L}} dk_{z_i}$$

$$\times \frac{n(E_i) - n(\, E(n_j, k_{z_j} = k_{z_i} - q_z \ (\pm K), \mathbf{k}_{\perp_j} = \mathbf{k}_{\perp_i} - \mathbf{q}_\perp)\,)}{E_i \quad - \quad E_j}$$

$$\times < n_i, k_{z_i} \mid e^{i(m_2 K + q_z) z} \mid n_j, k_{z_i} - q_z \ (\pm K) >< n_j, k_{z_i} - q_z \ (\pm K) \mid e^{-i(m_1 K + q_z) z} \mid n_i, k_{z_i} > \tag{4.2.10}$$

Here ($\pm K$) has been explained under Eq. (3.4.6). Substituting Eq. (4.2.9) into Eq. (4.2.10), the perpendicular momentum integration becomes

$$\int d\theta_i \int k_{\perp_i} dk_{\perp_i} \frac{1}{A_1 + B_1 \cos\theta_i} \tag{4.2.11}$$

here

$$A_1 = E(n_i,\, K_{z_i},\, \mathbf{k}_{\perp_i} = 0) - E(n_j,\, k_{z_j} = k_{z_i} - q_z\ (\pm K),\, \mathbf{k}_{\perp_j} = 0) + \frac{\hbar^2}{2m_j{}^*} k_{\perp_i}^2 - \frac{\hbar^2}{2m_j{}^*}[\, k_{\perp_i}^2 + q_\perp^2\,]$$

and $B_1 = 2\, \frac{\hbar_2}{2m_j{}^*}\, k_{\perp_i}\, q_\perp$. Determining the integration region is a difficult task. This will be discussed in detail in the next section. Note that the definite integral

$$\int_0^{2\pi} \frac{d\theta}{A + B\cos\theta} = \frac{2\pi}{(A^2 - B^2)^{1/2}} \qquad \text{if } |\, A\, | > |\, B\, | \tag{4.2.12}$$

and the indefinite integral is given by :

$$\int \frac{d\theta}{A + B\cos\theta} = \frac{2}{(A^2 + B^2)^{1/2}} \tan^{-1} \frac{(A^2 - B^2)^{1/2} \tan\frac{\theta}{2}}{A + B}$$

$$\text{for } |\, A\, | \geq |\, B\, | \text{ and } \theta \neq \pm\pi \tag{4.2.13}$$

$$\int \frac{d\theta}{A + B\cos\theta} = \frac{2}{(A^2 + B^2)^{1/2}} \log \left[\frac{(A^2 - B^2)^{1/2} \tan\frac{\theta}{2} + A + B}{(A^2 - B^2)^{1/2} \tan\frac{\theta}{2} - A - B} \right]$$

$$\text{for } |\, A\, | \leq |\, B\, | \text{ and } |\, \theta\, | < \pi \tag{4.2.14}$$

Applying the eigenenergy approximation in Eq. (4.2.9) to Eq. (4.2.10), the integration in $\Pi^0(k_z,\, \mathbf{k}_\perp;\, m_1,\, m_2)$ can be reduced by one dimension and the computer time is only one tenth of the original one. For the $\Pi^{\Lambda}(k_z, \mathbf{k}_\perp; m_1, m_2)$ calculation, it is necessary that the eigenenergy approximation be applied to the $\Pi^0(k_z, \mathbf{k}_\perp; m_1, m_2)$ calculation first. The reciprocal potential approximation can then also be applied to reduce computation time.

Section IV.3 Domain of Integration

In this section I will discuss in detail the integration region and how to treat the singularities of the calculation for the polarization function $\Pi^0(k_z, \mathbf{k}_\perp; m_1, m_2)$.

The major term in determining the integration region is

$$\frac{N(E_i) - N(E_j)}{E_i - E_j} \tag{4.3.1}$$

here $E_i = E(n_i, k_{z_i}, \mathbf{k}_{\perp i})$, $E_j = E(n_j, k_{z_j}, \mathbf{k}_{\perp j})$ and k_{z_j} must be equal to $k_{z_i} - q_z$ ($\pm K$). Also $\mathbf{k}_{\perp_j}$ must be equal to $\mathbf{k}_{\perp_i} - \mathbf{q}_\perp$. The electron distribution function is

$$N(E) = f_0(E) = \begin{cases} 1 & \text{when } E \le E_f \\ 0 & \text{when } E > E_f \end{cases} \tag{4.3.2}$$

in the degenerate limit. For the i^{th} electron

$$N(E_i) = \begin{cases} 1 & \text{when } |\, \mathbf{k}_{\perp_i} \,| \le \left[\dfrac{\hbar^2}{2m_i{*}} \left(E_f - E(n_i, k_{z_i}, k_{\perp_i} = 0)\right) \right]^{\frac{1}{2}} \\ 0 & \text{when } |\, \mathbf{k}_{\perp_i} \,| > \left[\dfrac{\hbar^2}{2m_i{*}} \left(E_f - E(n_i, k_{z_i}, k_{\perp_i} = 0)\right) \right]^{\frac{1}{2}} \\ & \qquad \text{or } \quad E(n_i, k_{z_i}, k_{\perp_i} = 0) > E_f \end{cases} \tag{4.3.3}$$

For the j^{th} electron

$$N(E_j) = \begin{cases} 1 & \text{when } |\, \mathbf{k}_{\perp_i} - q_\perp \,| \le \left[\dfrac{\hbar^2}{2m_j{*}} \left(E_f - E(n_j, k_{z_i} - q_z(\pm K), k_{\perp_j} = 0) \right) \right]^{\frac{1}{2}} \\ 0 & \text{when } |\, \mathbf{k}_{\perp_i} - q_\perp \,| > \left[\dfrac{\hbar^2}{2m_i{*}} \left(E_f - E(n_j, k_{z_i} - q_z(\pm K), k_{\perp_j} = 0) \right) \right]^{\frac{1}{2}} \\ & \qquad \text{or } \quad E(n_j, k_{z_i} - q_z(\pm K), k_{\perp_j} = 0) > E_f \end{cases}$$

(4.3.4)

Eq. (4.3.1) is non-zero only in condition that $N(E_i) = 1$ and $N(E_j) = 0$ or $N(E_i) = 0$ and $N(E_j) = 1$. In order to make coding easier for program calculation, we will use six cases to represent different situations about the perpendicular momentum integration region (refer to Fig. 4-3 through Fig. 4-8 where the shadow region is the integration region).

case 1: $E(n_j,\, k_{z_j},\, k_{\perp j} = 0) > E_f$ the integration region is $|\, \mathbf{k}_{\perp i} \,| \leq k_{\perp i,\, \max}$

case 2: $E(n_i,\, k_{z_i},\, k_{\perp i} = 0) > E_f$ the integration region is $|\, k_{\perp i} - \mathbf{q}_\perp \,| \leq k_{\perp i,\, \max}$

From case 3 to case 6 both $E(n_j,\, k_{z_j},\, k_{\perp j} = 0)$ and $E(n_i,\, k_{z_i},\, k_{\perp i} = 0)$ are $> E_f$

case 3: $q_\perp + k_{\perp j,\, \max} \leq k_{\perp i,\, \max}$

case 4: $-k_{\perp i,\, \max} > -k_{\perp j,\, \max} - q_\perp$

case 5: $k_{\perp i,\, \max} < -k_{\perp j,\, \max} + q_\perp$

case 6: the momentum spheres intersect each other

here we define $k_{\perp j,\, \max} = \left[\dfrac{\hbar^2}{2m_j^*} \left(E_f - E(n_j,\, k_{z_i} - q_z(\pm K),\, k_{\perp j} = 0)\right) \right]^{1/2}$ and $k_{\perp i,\, \max} = \left[\dfrac{\hbar^2}{2m_j{*}} \left(E_f - E(n_i,\, k_{z_i},\, k_{\perp i} = 0)\right) \right]^{1/2}$

In case 6, the intersection points of the two momentum spheres are singularity points, which means that $E(n_i,\, k_{z_i},\, \mathbf{k}_{\perp i})$ will be equal to $E(n_j,\, k_{z_j},\, \mathbf{k}_{\perp j})$. At these points Eq. (4.3.1) will satisfy the condition

$$\frac{N(E_i) - N(E_j)}{E_i - E_j} \approx \left.\frac{\partial f_0}{\partial E}\right|_{E = E_i = E_j = E_f} = \delta(E_i - E_j) \qquad (4.3.5)$$

The perpendicular momentum part of integration of the polarization function in Eq. (4.2.10) at these points will be (refer to Fig 4.9)

$$\int\int_{\text{in small range}} \frac{dk_{\perp i}\, k_{\perp i} d\theta_i \,[\, n(E_i) - n(E_j)\,]}{E_i - E_j} = \int\int dk_{\perp i}\, k_{\perp i} d\theta_i \delta(E_i - E_j)$$

$$\approx \int\int dk_{\perp i}\, k_{\perp i}\, d\theta_i \frac{-\delta(\theta_i - \theta_0)}{\partial(E_i - E_j)/\partial\theta_i} =$$

$$\int\int k_{\perp i}\, dk_{\perp i}\, d\theta_i \frac{-\,\delta(\theta_i - \theta_0)}{-\left|\, 2k_{\perp i} q_\perp \sin\theta_i \dfrac{\hbar^2}{2m_j{}^*} \right|} = \frac{-\left|\, k_{\perp i1} - k_{\perp i2} \,\right|}{\left|\, \dfrac{\hbar^2}{2m_j{}^*}\, q_\perp \sin\theta_0 \right|} \tag{4.3.6}$$

Here θ_0 is the position of θ coordinate where the singularity point is located. The region belonging to this singularity treatment in $k_\perp$ direction is from $k_{\perp i2}$ to $k_{\perp i2}$.

Case 1:

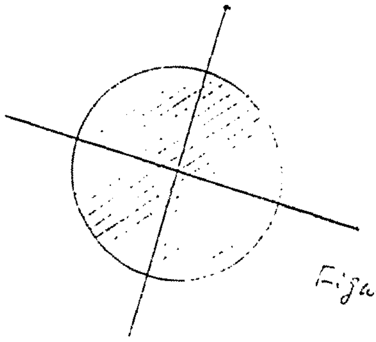


Figure 4-3

Case 2:

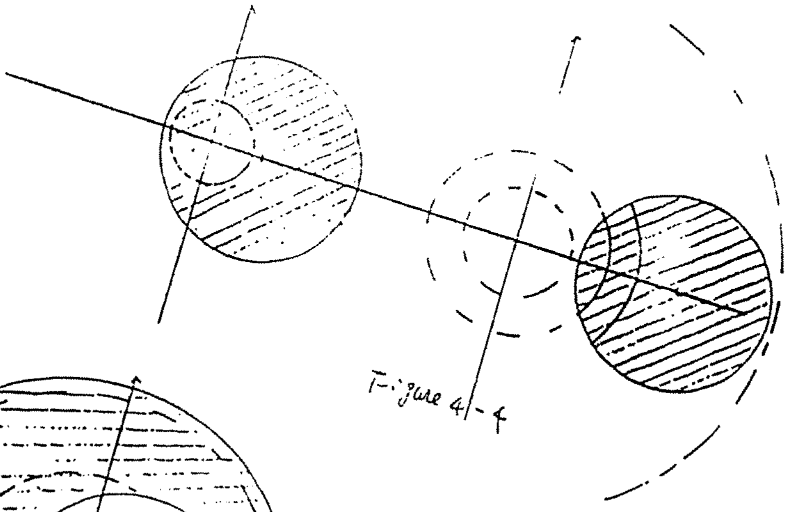


Figure 4-4

Case 3:

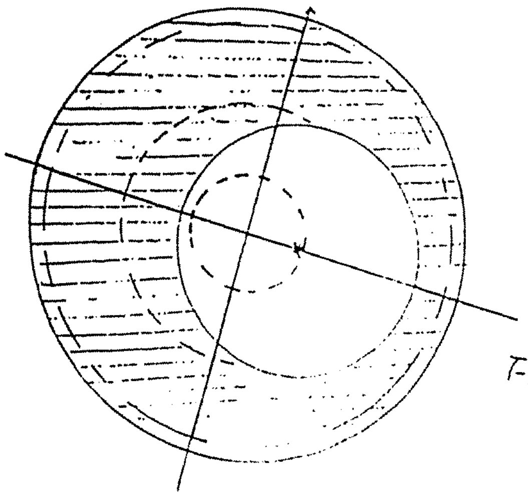


Figure 4-5

Case 4:

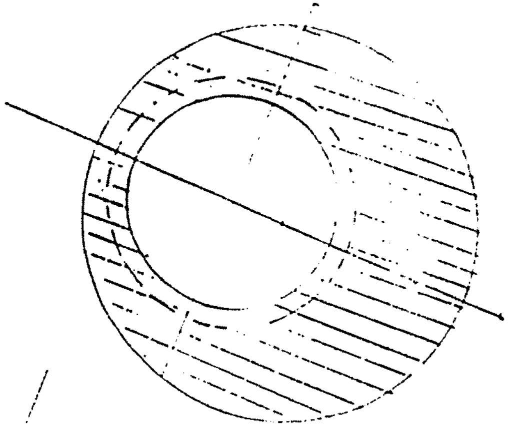


Figure 4-6

Case 5:

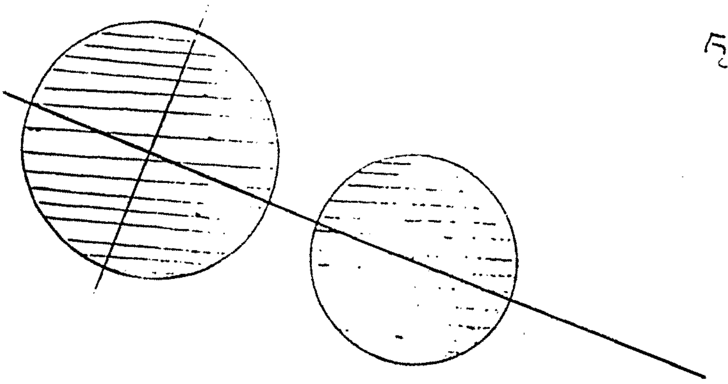


Figure 4-7

Case 6:

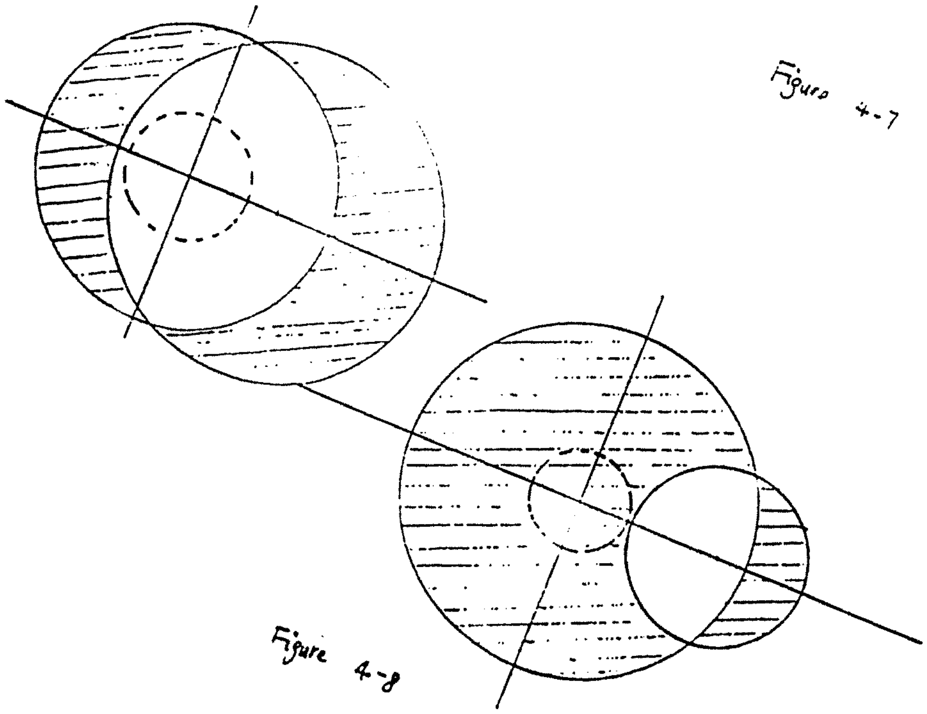


Figure 4-8

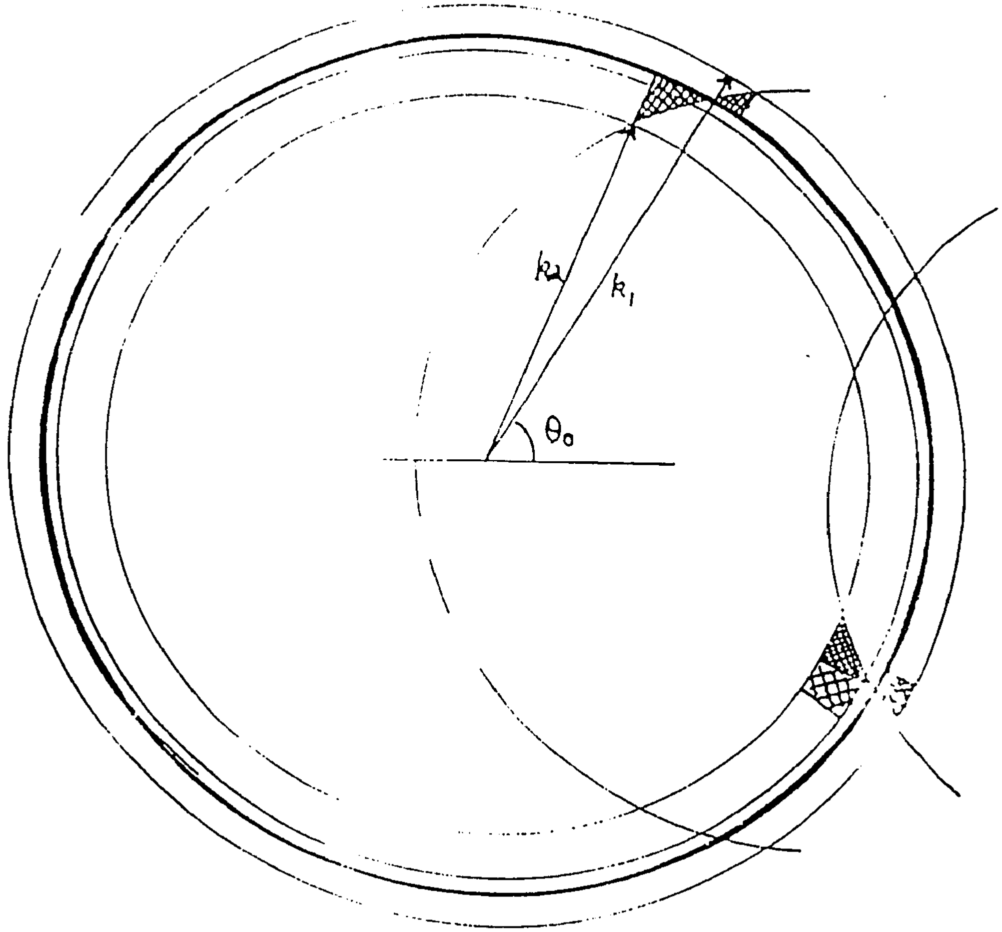


Fig 5-9

Section IV.4 Evaluation of the Polarization Function

$\Pi^A(k_z, \mathbf{k}_\perp; m_1, m_2)$

In Eq. (3.4.23) the portion of the integration which includes the variables of the momentum angular θ_i and θ_j can be expressed as

$$\int d\theta_i \int d\theta_j \frac{1}{A1 + B1 \cos \theta_i} \cdot \frac{1}{A2 + B2 \cos \theta_j} \cdot \frac{1}{A3 + B3 \cos (\theta_i - \theta_j)} \tag{4.4.1}$$

here

$$A1 = E(n_i,\, k_{z_i},\, \mathbf{k}_{\perp_i} = 0) + \frac{\hbar^2}{2m_i{}^*} k_{\perp i}^2 - E(n_l,\, k_{z_l} = k_{z_i} - q_z(\pm K),\, \mathbf{k}_{\perp_l} = 0) - \frac{\hbar^2}{2m_l{}^*}\,(\, k_{\perp_i}^2 + q_\perp^2)$$

$$B1 = -\,2\, \frac{\hbar_2}{2m_l{}^*}\, k_{\perp_i}\, q_\perp \tag{4.4.1a}$$

$$A2 = E(n_j,\, k_{z_j},\, \mathbf{k}_{\perp_j} = 0) + \frac{\hbar_2}{2m_j{}^*} k_{\perp i}^2 - E(n_k,\, k_{z_k} = k_{z_j} - q_z(\pm K),\, \mathbf{k}_{\perp_k} = 0) - \frac{\hbar_2}{2m_k{}^*}\,(\, k_{\perp k}^2 + q_\perp^2)$$

$$B2 = -\,2\, \frac{\hbar_2}{2m_l{}^*}\, k_{\perp_j}\, q_\perp \tag{4.4.1b}$$

$$A3 = \text{CoefA}\,(k_{z_i} - k_{z_j}(\pm K\,);\, m_1{}',\, m_2{}') + \text{CoefB}\,(m_1{}',\, m_2{}'')\,(k_{\perp_i}^2 + k_{\perp_j}^2)$$

and

$$B3 = \text{CoefB}(m_1{}',\, m_2{}') \cdot 2\, k_{\perp_i} \cdot k_{\perp_j} \tag{4.4.1c}$$

Also define $R3(\theta_i, \theta_j) = \dfrac{1}{A3 + B3 \cos (\theta_i - \theta_j)}$, $R2(\theta_j) = \dfrac{1}{A2 + B2 \cos \theta_j}$, and $R1(\theta_i) = \dfrac{1}{A1 + B1 \cos \theta_i}$. Here CoefA, CoefB have been defined in Eq. (4.2.6).

CoefA ($k_{z_i} - k_{z_j}(\pm K)$; $m_{1'}$, m_2') is comparable to or larger than CoefB (m_1', m_2'') ($k_{\perp_i}^2 + k_{\perp_j}^2$). Also $k_{\perp_i}^2 + k_{\perp_j}^2 \geq 2\, k_{\perp_i}\, k_{\perp_j}$. Therefore $R3(\theta_i, \theta_j)$ can be treated as a slowly varying function and defined by $S(\theta_i, \theta_j)$. When $E(n_i, k_{z_i}, \mathbf{k}_{\perp_i})$ is equal to $E(n_l, k_{z_l}, \mathbf{k}_{\perp_l})$, $R1(\theta_i)$ will be a delta function. Similarly, if $E(n_j, k_{z_j}, \mathbf{k}_{\perp_j})$ is equal to $E(n_k, k_{z_k}, \mathbf{k}_{\perp_k})$. $R2(\theta_j)$ will be a delta function. For this reason, the $R1(\theta_i)$ and $R2(\theta_j)$ can be treated as rapidly varying functions. Since $\cos(\alpha) = \cos(-\alpha)$, $R1(\theta_i) = R1(-\theta_i)$, $R2(\theta_j) = R2(-\theta_j)$ and $S(\theta_i, \theta_j) = S(-\theta_i, -\theta_j)$; letting $R1(\theta) = R11(\theta) + R12(\theta)$ and

$$R11(\theta) = \begin{cases} R1(\theta) & \text{when } \theta \geq 0 \\ 0 & \text{when } \theta < 0 \end{cases} \tag{4.4.2}$$

$$R12(\theta) = \begin{cases} 0 & \text{when } \theta \geq 0 \\ R1(\theta) & \text{when } \theta < 0 \end{cases} \tag{4.4.3}$$

Similarly, let $R2(\theta) = R21(\theta) + R22(\theta)$, Eq. (4.4.1) becomes

$$\int \int [\, R11(\theta_1)R21(\theta_2) + R12(\theta_1)R21(\theta_2) + R11(\theta_1)R22(\theta_2) + R12(\theta_1)R22(\theta_2)\,]$$

$$\times S(\theta_1, \theta_2)\, d\theta_1 d\theta_2 \tag{4.4.4}$$

Eq. (4.4.4) can be rewritten as

$$\int_{\theta_1 \geq 0} \int_{\theta_1 \geq 0} d\theta_1 d\theta_2\, [\, R11(\theta_1)R21(\theta_2)S(\theta_1, \theta_2) + R12(-\theta_1)R21(\theta_2)S(-\theta_1, \theta_2) +$$

$$R11(\theta_1)R22(\theta_2)S(\theta_1, -\theta_2) + R12(-\theta_1)R22(-\theta_2)S(-\theta_1, -\theta_2)\,] \tag{4.4.5}$$

With the symmetrical characteristic of $R1(\theta_1)$, $R2(\theta_2)$ and $S(\theta_1, \theta_2)$, Eq. (4.4.5) becomes

$$2 \cdot \int\limits_{\theta_1 \geq 0} \int\limits_{\theta_1 \geq 0} d\theta_1 d\theta_2 [\, R1(\theta_1) R2(\theta_2)\,]\,[\, S(\theta_1, \theta_2) + S(\theta_1, -\theta_2)\,] \tag{4.4.6}$$

$S(\theta_1, \theta_2)$ is a slowly varying function

$$S(\theta_1, \theta_2) \approx S(\bar{\theta}_1, \theta_2) + (\theta_1 - \bar{\theta}_1) \left[\frac{\partial S(\theta_1, \theta_2)}{\partial \theta_1} \right] \Bigg|_{\theta_1 = \bar{\theta}_1} \tag{4.4.7}$$

also

$$\approx S(\theta_1, \bar{\theta}_2) + (\theta_2 - \bar{\theta}_2) \left[\frac{\partial S(\theta_1, \theta_2)}{\partial \theta_2} \right] \Bigg|_{\theta_2 = \bar{\theta}_2} \tag{4.4.8}$$

The mean value approximation consists in taking $\bar{\theta}_1 = \dfrac{\int_{\theta_1 > 0} d\theta_1 \; \theta_1 R1(\theta_1)}{\int_{\theta_1 > 0} d\theta_1 \; R1(\theta_1)}$ and $\bar{\theta}_2 = \dfrac{\int_{\theta_2 > 0} d\theta_2 \; \theta_2 R2(\theta_2)}{\int_{\theta_2 > 0} d\theta_2 \; R2(\theta_2)}$. Then

$$\int\limits_{\theta_1 \geq 0} \int\limits_{\theta_2 \geq 0} R1(\theta_1) R2(\theta_2)\; S(\theta_1, \theta_2) \approx$$

$$\int\limits_{\theta_1 > 0} R1(\theta_1)\, d\theta_1 \left[\int\limits_{\theta_2 > 0} d\theta_2 S(\bar{\theta}_1, \theta_2) R2(\theta_2) \right] \approx S(\bar{\theta}_1, \bar{\theta}_2) \int\limits_{\theta_1 > 0} R1(\theta_1) d\theta_1 \int\limits_{\theta_2 > 0} R2(\theta_2) d\theta_2 \tag{4.4.9}$$

Substituting Eq. (4.4.9) into Eq. (3.4.23) and changing the order of summation, the polarization function becomes

$$\Pi^A(q_z, \mathbf{q}_\perp; m_1, m_2) \approx \frac{2}{(2\pi)^6} \sum_{n_i,\, n_l} \sum_{n_j,\, n_k} \int dk_{\perp i}\; k_{\perp i} \sum_{k_{zi}} \int dk_{\perp j}\; k_{\perp j} \sum_{k_{zj}}$$

$$\sum_{m_1', m_2'} \left\{ \frac{1}{A3(m_1', m_2', k_{z_i}, k_{z_j}, k_{\perp i}, k_{\perp j}) + B3(m_1', m_2', k_{\perp i}, k_{\perp j}) \cos(\bar{\theta}_i - \bar{\theta}_j)} + \right.$$

$$\left. \frac{1}{A3(m_1', m_2', k_{z_i}, k_{z_j}, k_{\perp i}, k_{\perp j}) + B3(m_1', m_2', k_{\perp i}, k_{\perp j}) \cos(\bar{\theta}_i + \bar{\theta}_j)} \right\}$$

$$\times \frac{1}{2} \cdot \int d\theta_i R1(n_i, n_l, k_{z_i}, q_z, k_{\perp i}, q_\perp; \theta_i) \int d\theta_j R2(n_j, n_k, k_{z_j}, q_z, k_{\perp j}, q_\perp; \theta_j)$$

× A term with four matrices multiplied together $(m_1, m_2, m_1', m_2', n_i, n_j, n_k, n_l, k_{z_i}, k_{z_j}, q_z)$

(4.4.10)

Since $B3$ is independent of k_{z_i}, k_{z_j} and $A3$ changes slowly as k_{z_i}, k_{z_j} change (please refer to Eq. (4.2.4), (4.2.6) and (4.4.1c)), the above approximation can be a step further by taking $\bar{\bar{\theta}}_i = \dfrac{\sum_{k_{z_i}} \int_{\theta_i > 0} d\theta_i \, \theta_i R1(k_{z_i}, \theta_i)}{\sum_{k_{z_i}} \int_{\theta_i > 0} d\theta_i \, R1(k_{z_i}, \theta_i)}$ and $\bar{\bar{\theta}}_j = \dfrac{\sum_{k_{z_j}} \int_{\theta_j > 0} d\theta_j \, \theta_j R2(k_{z_j}, \theta_j)}{\sum_{k_{z_j}} \int_{\theta_j > 0} d\theta_j \, R2(k_{z_j}, \theta_j)}$.

Then

$$\sum_{k_{z_i}} \sum_{k_{z_j}} \int_{\theta_i \geq 0} \int_{\theta_j \geq 0} R1(k_{z_i}, \theta_i) \, R2(k_{z_j}, \theta_j) \frac{1}{A3 + B3\cos(\theta_i, \theta_j)} \approx$$

$$\left[\sum_{k_{z_j}} \int_{\theta_j > 0} d\theta_j \frac{1}{A3 + B3\cos(\bar{\bar{\theta}}_i, \theta_j)} R2(k_{z_j}, \theta_j) \right] \sum_{k_{z_i}} \int_{\theta_i > 0} R1(k_{z_i}, \theta_i) \, d\theta_i \approx$$

$$\frac{1}{A3 + B3\cos(\bar{\bar{\theta}}_i, \bar{\bar{\theta}}_j)} \sum_{k_{z_i}} \int_{\theta_i > 0} R1(k_{z_i}, \theta_i) d\theta_i \sum_{k_{z_j}} \int_{\theta_j > 0} R2(k_{z_j}, \theta_j) d\theta_j \qquad (4.4.11)$$

Eq. (4.4.10) then becomes

$$\Pi^{A}(q_z,\, \mathbf{q}_\perp : m_1,\, m_2) \approx \frac{2}{(2\pi)^6} \sum_{n_i,\, n_l} \sum_{n_j,\, n_k} \int dk_{\perp_i}\, k_{\perp_i} \int dk_{\perp_j}\, k_{\perp_j}$$

$$\sum_{m_1',\, m_2'} \left\{ \frac{1}{A3(m_1',\, m_2',\, k_{z_i},\, k_{z_j},\, k_{\perp_i},\, k_{\perp_j}) + B3(m_1',\, m_2',\, k_{\perp_i},\, k_{\perp_j}) \cos(\bar{\bar{\theta}}_i - \bar{\bar{\theta}}_j)} + \right.$$

$$\left. \frac{1}{A3(m_1',\, m_2',\, k_{z_i},\, k_{z_j},\, k_{\perp_i},\, k_{\perp_j}) + B3(m_1',\, m_2',\, k_{\perp_i},\, k_{\perp_j}) \cos(\bar{\bar{\theta}}_i + \bar{\bar{\theta}}_j)} \right\}$$

$$\times \frac{1}{2} \cdot \left\{ \sum_{k_{z_i}} \int d\theta_i R1(n_i,\, n_l,\, k_{z_i},\, q_z,\, k_{\perp_i},\, q_\perp;\, \theta_i) \right\} \left\{ \sum_{k_{z_j}} \int d\theta_j R2(n_j,\, n_k,\, k_{z_j},\, q_z,\, k_{\perp_j},\, q_\perp;\, \theta_j) \right\}$$

$$\times \text{ A term with four matrices multiplied together } (m_1,\, m_2,\, m_1',\, m_2',\, n_i,\, n_j,\, n_k,\, n_l,\, k_{z_i},\, k_{z_j},\, q_z) \tag{4.4.12}$$

The integration value of $\sum_{k_z} \int d\theta R(n1,\, n2,\, k_z,\, q_z,\, q_\perp;\, \theta)$ can be obtained from the calculation of $\Pi^0(q_z,\, \mathbf{q}_\perp,\, m_1,\, m_2)$ and matrices are independent of $k_{\perp_i}$ etc. The computation time of the integration of $\Pi^A(q_z,\, \mathbf{q}_\perp,\, m_1,\, m_2)$ is much shorter when (4.4.12) is used instead of (3.4.23), proving that this method is a practical choice.

Chapter V Conclusion and Homogeneous Result

The purpose of this thesis is to derive a method for solving the screening problem in a superlattice. This method starts by using the Numerov method to solve for the Hartree-Fock wave functions in a single potential well including band bending effects. These wave functions determine the eigenfunction at the bottom of a superlattice sub-band. The tight binding approximation is then used (with the single potential wave functions) to obtain the eigenenergies and eigenfunctions for different k_z. These eigenfunctions are then used to obtain the (screening) polarization functions in a superlattice. These eigenfunctions are self-consistent in the conduction band bending and the exchange potential Hartree-Fock equation should be adjusted by the polarization functions (please refer to chapter 1 for a detailed discussion). As we can see from the previous chapters, this method involves many numerical techniques and complicated equations. One might question whether it is necessary to incur all such troubles in using the tight binding approximation wave function instead of another simple wave function, whether the result has periodic characteristics and whether the result involves the exchange and correlation interaction.

Every equation in this thesis has been developed using a periodic basis. There is no doubt that the results derived by this method possess the appropriate periodicity. In section I, the wave function of the superlattice will be discussed. Some of the results of the one particle wave function calculation will be shown first, giving a first insight into the tight binding approximation. Those included conduction band bending, electron distribution and wave function in a superlattice. In the same section, comparison will also be made between E(k) curves for the tight binding approximation and the Kronig-Penny equation in a non-doped superlattice (The Kronig-Penny[3] equation only applies to a periodic square well potential). This is to establish that the tight binding works well in a superlattice. The sub-band energy level and its shift are also shown. This is one of the major arguments that a simple wave function can not be applied to a superlattice. Some of the matrix $< i \mid e^{ikz} \mid j >$ values are also listed in this section. This produces another proof that the simple wave function is not a good application for a superlattice study and shows the periodicity characteristic of the proposed method. Two calculated results, obtained by applying the proposed method to a homogeneous medium, will be shown in section II. This provides proof that the proposed method in this thesis has considered the exchange and correlation effect and that this method is an adequate one.

Section V.1 Tight binding Approximation Method

Using a simple wave function to study the screening problem makes the whole process easier. Yet the chosen function should include the characteristics of a superlattice. Until now, only a few investigators have used this kind of wave function to study the superlattice. X. L. Lei and his colleagues have published several papers on superlattice transport properties [38–48]. Most of these papers use the sine/cosine wave function and assume the electron only occupies the lowest sub-band of the superlattice. S. L. Chuang and K Hess[49] use the sine/cosine wave to study the electron distribution under an electric field and M. H. Degani and O. Hipolito[50] similarly use this wave to study the polaron in a superlattice. The sine/cosine wave is not adequate for a superlattice study. This will be discussed later in this section. Two of Lei's papers[40,43] used the Fang-Howard-Stern variational wave function, a very successful wave function in the inversion layer study, which considered the screening effect and the wave penetration through the potential barrier. The inversion layer's potential is different from the superlattice's potential. Moreover, the inversion layer wave function is not always adequate to be applied to a superlattice especially when the $Al_xGa_{1-x}As$ layer is thin. The Kronig-Penny wave function has been used by J. F. Palmier and his colleagues[51] and I. Dharssi and P. N. Butcher[52] to study superlattice properties. The Kronig-Penny wave function is only adequate for a low doping superlattice and some of the equations in these two papers were still derived using the sine/cosine wave function. D. Aitelhabti and P. Vasilopoulos[53,54] have used the transfer matrix method to study superlattices. The transfer matrix method is an innovative method. But these two papers did not consider band bending or screening and only the first sub-band was considered.

Figures 5-1a, 5-1b and 5-1c show the wave functions of the first, second and third sub-bands in a superlattice. The width in both the GaAs and $Al_xGa_{1-x}As$ layer is 100 Å and the doping is uniform in both layers with concentration 10^{18}. Each figure contains the tight binding waves with $k_z = 0$ and $k_z = \pi/L$ (L has been defined in chapter I), the single potential well wave function and the sine/cosine wave function. Figures 5-2a, 5-2b and 5-2c are similar to the figure 5-1 series except that the width of $Al_xGa_{1-x}As$ layer is 50 Å and the width of $Al_xGa_{1-x}As$ layers in figure 5-3a, 5-3b and 5-3c is 150 Å.

From the figure 5-1 series and 5-2 series, we know that the tight binding approximation wave is not quite like that of the single potential waves or the sine/cosine waves. The major reason is due to one of the superlattice characteristics: the wave will penetrate to adjacent potential wells. The penetration can be omitted only when the $Al_xGa_{1-x}As$ layer is very thick (please refer to figure 5-3 series). Not only the wave function will penetrate but also the top sub-band wave function is changed due to the doping concentration change (please refer to figures 5-4 series, same like 5-1 series except the doping concentration is 5×10^{18}). The wave function is a basic element of our study of the properties of a superlattice. Accurate calculation results call for an accurate wave function.

Figure 5-5 series, 5-6 series and 5-7 series present the electron distribution in a superlattice. Those graphs show how the shape of the electron distribution function varies, depends on the thickness of the layers and the doping concentration. Some of the superlattice characteristics depend on these shapes[55]. Figure 5-8 series and figure 5-9 series show the conduction band bending in a superlattice. This conduction band bending is not linearly proportional to the doping concentration. The banding bending effect can be ignored for the low doping, but not for the high doping.

One of the major reasons for choosing an accurate wave function is that the simple wave function does not offer an accurate sub-band eigenenergy. Not only is the eigenenergy different but also the band width of the sub-band obtained by tight binding approximation is not zero. The band width will determine some superlattice characteristics[56]. The electron transport properties are determined by electron scattering. One of the major factors in determining electron scattering is the electron distribution function (please refer to Eq. (5.5) and (5.7)). The electron distribution function is determined by the sub-band eigenenergy sensitively (please refer to Eq (3.6.9)). A slight deviation in sub-band energy level will cause a vast difference in transport coefficients. From the discussion above, we know that the transportation coefficients will be vastly different when different wave functions are used, especially at low temperatures (please refer to Eq (3.6.9)).

Some investigators may think that the shift of the sub-band eigenenergy level will approximate to the average of the conduction band change (band bending) namely

$$\frac{1}{L}\left[\int_{-1/L}^{1/L} v(z)\, dz - 2\, v_0\, a_z\right] \tag{5.1}$$

here $v(z)$ is the potential of the bent band and v_0 and a_z are defined under Eq. (3.5.1) and (3.5.6). Those investigators suggest that band bending does not effect the calculated result. The numerical values of the last paragraph show that the shift of the sub-band eigenenergy are different for different sub-bands and these differences are not negligible. This shift is strong for the high doped superlattice (for example, the Fig 5-4's superlattice, the average of conduction band change is 0.05491ev. The eigenenergies shifting of the low and the top of the first sub-band are 0.09479 and 0.09475ev. The eigenenergies after shifting are 0.12935ev and 0.12940ev. For the second sub-band and the third sub-band the shifting are 0.07856ev; 0.07851ev and 0.04871ev; 0.06805ev respectively. The eigenenergies after shifting are 0.21294ev; 0.21241ev and 0.31758ev; 0.34848ev.) The eigenenergy of the sub-bands is very important for studying superlattices. The eigenenergy values are dependent on which of the wave function approximation is used. In order to obtain accurate results, a good wave function will have to be chosen for superlattice studies.

The previous paragraphs show that choosing a good wave function is very important for superlattice studies. Can the tight binding approximation wave function meet this requirement? Figure 5-10 shows the tight binding approximation wave function and the exact wave function (solved by Kramer's method[57]) in a superlattice. These curves, which show the two different types wave functions, are very similar. The Kronig-Penny[3] equation is an E(k) function for a periodic square well potential with no approximation applied. Figures 5-11, 5-12, 5-13 show that except for the top sub-band which has a slight discrepancy, the E(k) curve for those two methods are exactly matched. But, at low temperature, the top band is only occupied by very few electrons. For this reason, the use of the tight binding approximation in studying the characteristics of a superlattice can yield good results. Table 5-2 contains some values of $< i \mid e^{ikz} \mid j >$ which present the periodic characteristics of tight binding approximation wave function. These values can not be obtained by some simple wave function. From chapter III we know that the tight binding approximation wave function can be applied to most superlattice studies, if computer numerical methods are used. This is the reason why the tight binding approximation is chosen in this thesis.

Section V.2 Polarization Function Π

From the discussion in chapter II, we know that the screening effect is very important in a superlattice study. Lax, Cai and his colleagues have published a series of significant papers on superlattice studies [58–69]. Some later papers[64–68] use an equation derived by the transfer matrix which is more concerned with screening. These papers have better matched experimental results. In recent years a few papers related to screening in a superlattice have been published. Only a few of these papers have been completed taking into consideration the superlattice characteristics: periodicity, multi-subband, conduction band bending, wave function penetration to adjacent wells with consideration of exchange and correction. Some of these important works are described below. Most of X. L. Lei and his colleague's work have derived screening theory in a superlattice. Those theories are based on applying the sine/cosine wave function to R.P.A. screening theory with P. J. Price's[70] $G(\mathrm{q})$ (please refer to Eq. (2.1.14)). M. Aniya and M. Kobayashi[71] and A. M. Belyantser and A. V. Okomrl'kov [72] have used electromagnetic theory with a very simple charge distribution function and the background dielectric constant change between layers to solve for the screening in a superlattice. This charge distribution function did not possess the superlattice characteristics nor did it consider band bending. L. Wendler and R. Pechstedt[73] use many-body theory to study the two dimension electron gas problems. That paper considered exchange and other high order perturbation terms. If a suitable superlattice's eigenfunction and eigenenergy are applied to the formulas in that paper, a significant calculation result would be obtained. N. J. K. Horing, G. Fiorenza and H. L. Cui[74] has derived the screening in multi (periodic) two dimension electron gas. R.D. King-Smith and J.C. Inkson[75] have used tight binding approximation without considering the wave function overlap between wells to study the dielectric properties of a non-doped superlattice. G. Gumbs[76] has used sine/cosine wave function and P. Hawerylak, J.W. Wu and J.J. Quinn[77] take the assumption $E_{nkl}=E_n + \hbar^2 k^2 / 2m$ (here n is sub-band index and l is potential well index) to derive lowest order polarization function.

We concluded in the last section that the eigenfunction, eigenenergy and conduction band bending can not be oversimplified and that the tight binding approximation wave function meets the requirements for a study on a superlattice. There remains the question of whether applying the tight binding approximation wave function to the method suggested in this thesis can yield a solution to the screening problem in a superlattice.

The screening theory in a homogeneous medium has been studied for several decades. The screening theory for a superlattice can be tested by applying it to a homogeneous medium and comparing the results with previous homogeneous medium screening theories. The method to test the non-homogeneous medium's polarization function Π^0 is described in Appendix B. My numerical calculation result of Π^0 passed this test.

The exchange and correlation polarization function is an important term in the study of a superlattice. Fig. 5-14 illustrates the Π^A curve obtained by Geldart and Taylor[56] (Π^A is the major change term and the most contribution beyond the zero perturbation term, as discussed in Chapter III) and the Π^A curve in a homogeneous medium obtained by the first iterated numerical result of my suggested method. These two curves produce similar values, although the curve derived from my suggested method is not as smooth, owing to big integration steps. This result can be proved by the discussion in Section III.3, the Π^A obtained by the Hartree-Fock wave function is the same as the Π^A obtained by Hartree wave function plus high order perturbation terms.

Since the dielectric function $\varepsilon(\mathbf{q})$ and the two particle distribution function $G(\mathbf{q})$ correlate with each other (refer to Chapter II) and the real space two particle distribution function $g(\mathbf{r})$ has very defined limits, ($g(\mathbf{r})$ must be positive, $g(0) = 0$, and $g(\infty)=1$), many investigators[20,21,23–28,6,31] use $G(\mathbf{q})$ to determine whether the screening theory has considered the exchange and correlation effects. I have added the $G(\mathbf{q})$ curve using my suggested method as applied to a homogeneous medium to the graph shown in reference 24 in Fig. 5-15. (That graph has a few $G(\mathbf{q})$ curves obtained by different workers). My curve lies between "Hubbard" and "Toigo and Woodruff". The result leads me to conclude that my method is a valid one, especially as the exchange and correlation effects have been taken into account.

Screening has a major effect on superlattice properties. It must be studied. A heavily doped superlattice's mean separation between carriers, the Bohr radius and the screening length are all the same order. It should be treated like a metal, including exchange and correlation effects. The potential is periodic with strong variations. A simple wave function can not be used to study this kind of medium. Finding an appropriate method to solve for the screening effect in a superlattice which incorporates all the above characteristics requires sophisticated procedures. While the method suggested in this thesis may seem complicated, the resultant calculation, unlike those which can only be applied to a certain type of screening, can be applied to a superlattice in general.

Section V.3 Electron Transport

A common way to study the electronic transport is to start from the Boltzmann equation.

$$\left.\frac{\partial f}{\partial t}\right|_{\text{drift}} = \left.\frac{\partial f}{\partial t}\right|_{\text{coll.}} \tag{5.2}$$

means the electron distribution function changes caused by the drift process is equal to the changes caused by the collision processes. The collision part can be expressed by

$$\left.\frac{\partial f}{\partial t}\right|_{\text{coll.}} = \left.\frac{\partial f}{\partial t}\right|_{\text{e-e}} + \left.\frac{\partial f}{\partial t}\right|_{\text{e-i}} + \left.\frac{\partial f}{\partial t}\right|_{\text{e-LO}} + \left.\frac{\partial f}{\partial t}\right|_{\text{e-AL}} + \left.\frac{\partial f}{\partial t}\right|_{\text{e-AT}} + \cdots\cdots\cdots\cdots \tag{5.3}$$

The label e–e indicates the contribution of the electron distribution changes caused by electron electron collision. Similarly, the label of e–i, e–LO, e–AL and e–AT indicate the electron impurity, electron longitudinal optical phonon, electron longitudinal acoustic phonon and electron transverse acoustic phonon[62]. In a simple case the drift part can also be expressed by

$$\left.\frac{\partial f}{\partial t}\right|_{\text{drift}} = -\frac{\mathbf{F}}{\hbar}\cdot\nabla_{\mathbf{k}} f - \frac{1}{\hbar}\nabla_{\mathbf{k}}E\cdot\nabla_{\mathbf{r}} f \tag{5.4}$$

This equation can only be applied to a homogeneous medium with low external fields and in a spatial uniform case the second term can be omitted. In a superlattice the electron energy is not equal to $A + B \cdot k^2$. The first term is not adequate in general superlattice cases. Because the electron is not uniformly distributed in the $\hat{z}$ direction, in microscopic view the second term can not be omitted even in equilibrium cases. Eq. (5.4) can not be straightly applied to a superlattice. A new transport equation is required. For example, Cai used the Liouville equation to derive a Boltzmann like equation[58,62] to study quantum well properties. Also, Cai[62] changed the right hand side of Eq. (5.4) to $\partial M\mathbf{V}_e/\partial t$ (M is the total electron mass and $\mathbf{V}_e$ is the average electron velocity). This change makes the equation exhibit more physical meaning.

This thesis proposes using the high order Tight Binding Approximation wave function and considering multi-subband and screening effect to study superlattice property. Many investigators have already done significant studies for superlattice. If the proposed wave function, electron distribution function and/or the screening equation were applied to some of these studies, a better result should be obtained or some of these studies become suitable for general superlattice cases. For example, Cai[58] has derived an equation for electron longitudinal optical phonon scattering (Eq. (2.16) in reference 20). If we want to apply those proposals, this equation should be modified as follows:

$\mathbf{k}$ should be changed to $\mathbf{k}_\perp + (MK + k_z)\,\hat{e}_z$, here k_z is in the first superlattice Brillouin zone and $|\ k_z\ | < 1/2K$, $K = \pi/L$ and L has been defined in chapter I. The electron distribution function and electron energy should be changed to $f_{n,\mathbf{k}_\perp,k_z}$ and $E(n,\ \mathbf{k}_\perp,\ k_z)$. These two functions have been discussed in detail in chapter III. $\delta_{\mathbf{k}',\ \mathbf{k}+\mathbf{q}}$ should be changed to $\delta_{\mathbf{k}_\perp',\ \mathbf{k}_\perp+\mathbf{q}_\perp} \cdot \delta_{k_z',\ k_z+q_z\pm K}$, the ± has been explained under Eq. (3.4.6). Cai's equation then becomes

$$\left[\frac{\partial f_{n,\ k_\perp,\ k_z}(t)}{\partial t}\right]_{\text{e-LO}} = \frac{2\alpha^2}{\hbar A}2\pi \sum_{n',\ k_\perp',\ k_z'} \sum_{\mathbf{q}_\perp,\ M,\ q_z} \left|G_{n,\ n'}(\mathbf{q}_\perp,\ M,\ q_z)\right|^2$$

$$\times\,(\ \{\ f_{n',\ k_\perp',\ k_z'}(t)[1 - f_{n,\ k_\perp,\ k_z}(t)]\ \delta_{\mathbf{k}_\perp',\ \mathbf{k}_\perp+\mathbf{q}_\perp}\ \delta_{k_z',\ k_z+q_z\pm K}\ \delta(E_{n',\ k_\perp',\ k_z'} - E_{n,\ k_\perp,\ k_z} - \hbar\omega_L)$$

$$-f_{n,\,k_\perp,\,k_z}(t)[1-f_{n',\,k_\perp',\,k_z'}(t)]\,\delta_{\mathbf{k}_\perp',\,\mathbf{k}_\perp-\mathbf{q}_\perp}\,\delta_{k_z',\,k_z-q_z\pm K}\,\delta(E_{n,\,k_\perp,\,k_z}-E_{n',\,k_\perp',\,k_z'}-\hbar\omega_L)\ \}$$

$$\times[1+N_{\omega_L}]$$

$$+\{\ f_{n',\,k_\perp',\,k_z'}(t)[1-f_{n,\,k_\perp,\,k_z}(t)]\,\delta_{\mathbf{k}_\perp',\,\mathbf{k}_\perp-\mathbf{q}_\perp}\,\delta_{k_z',\,k_z-q_z\pm K}\,\delta(E_{n',\,k_\perp',\,k_z'}-E_{n,\,k_\perp,\,k_z}-\hbar\omega_L)$$

$$-f_{n,\,k_\perp,\,k_z}(t)[1-f_{n',\,k_\perp',\,k_z'}(t)]\,\delta_{\mathbf{k}_\perp',\,\mathbf{k}_\perp+\mathbf{q}_\perp}\,\delta_{k_z',\,k_z+q_z\pm K}\,\delta(E_{n,\,k_\perp,\,k_z}-E_{n',\,k_\perp',\,k_z'}-\hbar\omega_L)\ \}$$

$$\times N_{\omega_L}) \tag{5.5}$$

here N_{ω_L} is phonon distribution function and is equal to $[e^{\hbar\omega_L/K_BT}-1]^{-1}$, α is Frohlich electron-LO-phonon coupling constant and A is the superlattice layer area. The equation for $G_{n,\,n'}(\mathbf{q}_\perp,\,M,\,q_z)$ is determined by the electron phonon interaction. The phonon can be treated as external potential. From Eq. (3.2.13) we know that an external potential not only generates a screened potential with the same momentum, but also the screened potentials with momentum having MK difference. With Eq. (3.3.5) the $G_{n,\,n'}(\mathbf{q}_\perp,\,M,\,q_z)$ should be changed to

$$\frac{1}{Q\,L}\sum_{M_1}\int\frac{dk_z}{2\pi}\int\frac{dk_z'}{2\pi}\int\frac{\psi^*_{n,\,k_z}(z)\,e^{i\cdot(q_z+M_1K)}\psi_{n',\,k_z'}(z)}{\varepsilon(\mathbf{q}_\perp,\,q_z;\,M_1,\,M)}dz \tag{5.6}$$

here Q is the scalar length of vector $(\mathbf{q}_\perp,\,q_z+MK)$, $\psi^*_{n,\,k_z}(z)$ as $F^*_{n,\,k_z}(z)$ has been defined in Eq. (3.5.2) and $\varepsilon(\mathbf{q}_\perp,\,q_z;M_1,\,M_2)=\ 1-\Pi^*(\mathbf{q}_\perp,\,q_z;M_1,\,M_2)\ \dfrac{4\pi e^2}{Q^2}$ and $\Pi^*(\mathbf{q}_\perp,\,q_z;M_1,\,M_2)=\ \Pi^0(\mathbf{q}_\perp,\,q_z;M_1,\,M_2)+\Pi^A(\mathbf{q}_\perp,\,q_z;M_1,\,M_2)$, $\Pi^0(\mathbf{q}_\perp,\,q_z;M_1,\,M_2)$ has been defined in Eq. (3.4.14) and $\Pi^A(\mathbf{q}_\perp,\,q_z;M_1,\,M_2)$ has been defined in Eq. (3.4.23). The tight binding approximation matrix element $\int\psi^*_{n,\,k_z}(z)\,e^{i\cdot(q_z+M_1K)}\psi_{n',\,k_z'}(z)$ has been given in Eq. (3.5.39).

Referring to reference 24, the equation of electron impurity scattering in a superlattice should be

$$\frac{4\pi}{\hbar A}\sum_{\mathbf{q}_\perp}\sum_{M,\, q_z}\sum_{n',\, k_\perp',\, k_z'} \delta_{\mathbf{k}_\perp',\, \mathbf{k}_\perp - \mathbf{q}_\perp}\, \delta_{k_z',\, k_z - q_z \pm K}\, \delta(E_{n,\, k_\perp,\, k_z} - E_{n',\, k_\perp',\, k_z'})$$

$$\times f_{n,\, k_\perp,\, k_z}(t)[1 - f_{n',\, k_\perp',\, k_z'}(t)]\ |M_{n,\, n'}(\mathbf{q}_\perp,\, M,\, q_z)\ |^2 \tag{5.7}$$

Here $M_{n,\, n'}(\mathbf{q}_\perp,\, M,\, q_z)$ is the scattering matrix. The equation of the potential which is generated by a single electron and single impurity interaction is negative of Eq. (3.2.15). With

$$\int \frac{dx\ dy}{(\ 2\pi\ )^2} e^{i(\mathbf{k}_\perp' + \mathbf{q}_\perp - \mathbf{k}_\perp)\cdot(\mathbf{x}+\mathbf{y})} = \delta_{\mathbf{k}_\perp',\, \mathbf{k}_\perp - \mathbf{q}_\perp} \tag{5.8}$$

the scattering matrix becomes

$$\sum_M \frac{-\, 4\pi e^2}{q_\perp^2 + (q_z + MK)^2}\ \frac{1}{\varepsilon(\mathbf{q}_\perp,\, q_z;\, M_1,\, M)}$$

$$\times\ \int dz' \rho_i(z') \exp\left[\, -\, i\ (q_z + MK)\ z'\ \right] \int dz\ \psi^*_{n,\, k_z}(z) \exp[\ i\ (q_z + M_1 K)\ z\ ]\ \psi_{n',\, k_z'}(z) \tag{5.9}$$

Here $\rho_i(z')$ is the impurity distribution and $\varepsilon(\mathbf{q}_\perp,\, q_z;\, M_1,\, M) = 1/X(\mathbf{k}_\perp,\, k_z + mK;\, \mathbf{k}_\perp,\, k_z + m'K)$. One of the major factors which causes a high mobility in modulatd doping superlattice is that the electron impurity scattering is weak. The electron spatial distribution function is one of the major elements in determining the electron impurity scattering and the electric potential has to be adjusted for screening. As the discussion in the previous section shows, an accurate spatial electron distribution function and screening theory can be obtained by the method proposed in this thesis. By using this method to study electron impurity scattering, a better result should be obtained.

From the discussion in the previous sections we know that the screening theory obtained by the proposed method can be applied to general superlattice case. Not only for electron impurity scattering, the screening theory and the high order tight binding approximation wave function can also yield a better result for many electron transport studies. As the devices for molecular beam epitaxy crystal growth begin to develop, my suggested method can be modified and applied to these devices. It is hoped that the method suggested in this thesis will have broad application with respect to these kinds of devices. I have found my study a meaningful piece of research.

	first sub-band	second sub-band	third sub-band
sine/cosine wave	0.056967ev	0.22787ev	0.5127ev not exist
single isolated potential wave (non-doped superlattice)	0.034605ev	0.13404ev	0.27363ev
single isolated potential wave Fig 5-1's (doped superlattice)	0.065286ev	0.15891ev	0.27073ev
tight binding app. wave Fig 5-1's superlattice $K = 0$	0.06528ev	0.15897ev	0.29111ev
tight binding app. wave Fig 5-1's superlattice $K = \pi/L$	0.06529ev	0.15885ev	0.29620ev
single isolated potential wave Fig 5-2's (doped superlattice)	0.04667ev	0.14275ev	0.29159ev
tight binding app. wave Fig 5-2's superlattice $K = 0$	0.04657ev	0.14331ev	0.280040ev
tight binding app. wave Fig 5-2's superlattice $K = \pi/L$	0.04678ev	0.122219ev	0.29048ev

Table 5 - 1

The Fig 5-1's superlattice is the superlattice which width in both the GaAs and $Al_xGa_{1-x}As$ layer is 100 Å and the doping is uniform in both layers with concentration 10^{18}. The Fig. 5-2's superlattice is similar to Fig. 5-1's superlattice except that the $Al_xGa_{1-x}As$ layer width is 50 Å. The eigenenergies for sine/cosine wave and non-doped single isolated potential wave are dependent on the GaAs layer only.

$q_z=0$ $M=0$	$n_1=1$			$n_1=2$			$n_1=3$		
	real pt	imag pt	mtr valu	real pt	imag pt	mtr valu	real pt	imag pt	mtr valu
$k_{z2}=0$ $n_2=1$	1.00000	0.00000	1.00000	0.00000	0.00000	0.00000	0.00270	0.00000	0.00270
$k_{z2}=0$ $n_2=2$	0.00000	0.00000	0.00000	1.00000	0.00000	1.00000	0.00000	0.00000	0.00000
$k_{z2}=0$ $n_2=3$	0.00268	0.00000	0.00268	0.00000	0.00000	0.00000	1.00000	0.00000	1.00000
$k_{z2}=\pi/8L$ $n_2=1$	1.00000	0.00000	1.00000	0.00000	0.00000	0.00000	0.00267	0.00000	0.00267
$k_{z2}=\pi/8L$ $n_2=2$	0.00000	0.00000	0.00000	1.00000	0.00000	1.00000	0.00000	-0.00011	0.00011
$k_{z2}=\pi/8L$ $n_2=3$	0.00265	0.00000	0.00265	0.00000	-0.00011	0.00011	1.00000	-0.00001	1.00000
$k_{z2}=\pi/4L$ $n_2=1$	1.00000	0.00000	1.00000	0.00000	0.00000	0.00000	0.00258	-0.00001	0.00258
$k_{z2}=\pi/4L$ $n_2=2$	0.00000	0.00000	0.00000	1.00000	0.00000	1.00000	0.00000	-0.00021	0.00021
$k_{z2}=\pi/4L$ $n_2=3$	0.00257	-0.00001	0.00257	0.00000	-0.00021	0.00021	1.00000	-0.00003	1.00000
$k_{z2}=3\pi/8L$ $n_2=1$	1.00000	0.00000	1.00000	0.00000	0.00000	0.00000	0.00245	-0.00001	0.00245
$k_{z2}=3\pi/8L$ $n_2=2$	0.00000	0.00000	0.00000	1.00000	0.00000	1.00000	0.00000	-0.00027	0.00027
$k_{z2}=3\pi/8L$ $n_2=3$	0.00245	-0.00001	0.00245	0.00000	-0.00027	0.00027	1.00000	-0.00001	1.00000
$k_{z2}=\pi/2L$ $n_2=1$	1.00000	0.00000	1.00000	0.00000	0.00000	0.00000	0.00230	-0.00001	0.00230
$k_{z2}=\pi/2L$ $n_2=2$	0.00000	0.00000	0.00000	1.00000	0.00000	1.00000	0.00000	-0.00029	0.00029
$k_{z2}=\pi/2L$ $n_2=3$	0.00230	-0.00001	0.00230	0.00000	-0.00029	0.00029	1.00000	-0.00004	1.00000

Table 5 - 2a

$q_z=\pi/8L$ $M=0$	$n_1=1$			$n_1=2$			$n_1=3$		
	real pt	imag pt	mtr valu	real pt	imag pt	mtr valu	real pt	imag pt	mtr valu
$k_{z2}=0$ $n_2=1$	0.99721	-0.04142	0.99807	-0.00339	-0.03375	0.03392	-0.00067	-0.00471	0.00476
$k_{z2}=0$ $n_2=2$	-0.00339	-0.03375	0.03392	0.99381	-0.04432	0.99480	-0.00902	-0.04240	0.04335
$k_{z2}=0$ $n_2=3$	-0.00069	-0.00470	0.00475	-0.00902	-0.04239	0.04334	0.98191	-0.09491	0.98649
$k_{z2}=\pi/8L$ $n_2=1$	0.99721	-0.04142	0.99807	-0.00339	-0.03375	0.03392	-0.00070	-0.00471	0.00476
$k_{z2}=\pi/8L$ $n_2=2$	-0.00339	-0.03375	0.03392	0.99381	-0.04432	0.99480	-0.00902	-0.04252	0.04347
$k_{z2}=\pi/8L$ $n_2=3$	-0.00072	-0.00471	0.00476	-0.00902	-0.04252	0.04346	0.98207	-0.09495	0.98665
$k_{z2}=\pi/4L$ $n_2=1$	0.99721	-0.04142	0.99807	-0.00339	-0.03375	0.03392	-0.00079	-0.00472	0.00478
$k_{z2}=\pi/4L$ $n_2=2$	-0.00339	-0.03375	0.03392	0.99381	-0.04432	0.99480	-0.00901	-0.04263	0.04357
$k_{z2}=\pi/4L$ $n_2=3$	-0.00081	-0.00471	0.00478	-0.00903	-0.04263	0.04357	0.98218	-0.09503	0.98677
$k_{z2}=3\pi/8L$ $n_2=1$	0.99721	-0.04142	0.99807	-0.00339	-0.03375	0.03392	-0.00092	-0.00472	0.00480
$k_{z2}=3\pi/8L$ $n_2=2$	-0.00339	-0.03375	0.03392	0.99381	-0.04432	0.99480	-0.00901	-0.04270	0.04364
$k_{z2}=3\pi/8L$ $n_2=3$	-0.00094	-0.00471	0.00481	-0.00903	-0.04271	0.04366	0.98224	-0.09512	0.98683
$k_{z2}=\pi/2L$ $n_2=1$	0.99721	-0.04142	0.99807	-0.00339	-0.03375	0.03392	-0.00107	-0.00471	0.00484
$k_{z2}=\pi/2L$ $n_2=2$	-0.00339	-0.03375	0.03392	0.99381	-0.04432	0.99480	-0.00902	-0.04274	0.04368
$k_{z2}=\pi/2L$ $n_2=3$	-0.00108	-0.00471	0.00484	-0.00903	-0.04274	0.04369	0.98186	-0.09517	0.98646

Table 5 - 2b

$q_t=\pi/4L$ $M=0$	$n_1=1$			$n_1=2$			$n_1=3$		
	real pt	imag pt	mtr valu	real pt	imag pt	mtr valu	real pt	imag pt	mtr valu
$k_2=0$ $n_2=1$	0.98909	-0.08148	0.99244	-0.01303	-0.06511	0.06640	-0.01003	-0.00604	0.01171
$k_2=0$ $n_2=2$	-0.01303	-0.06511	0.06640	0.97634	-0.08374	0.97992	-0.03435	-0.07707	0.08438
$k_2=0$ $n_2=3$	-0.01002	-0.00602	0.01169	-0.03436	-0.07707	0.08438	0.93066	-0.17565	0.94709
$k_2=\pi/8L$ $n_2=1$	0.98909	-0.08148	0.99244	-0.01303	-0.06511	0.06640	-0.01003	-0.00604	0.01171
$k_2=\pi/8L$ $n_2=2$	-0.01303	-0.06511	0.06640	0 97634	-0.08374	0.97992	-0.03434	-0.07720	0.08449
$k_2=\pi/8L$ $n_2=3$	-0.01005	-0.00603	0.01172	-0.03437	-0.07721	0.08452	0.93091	-0.17574	0.94736
$k_2=\pi/4L$ $n_2=1$	0.98909	-0.08148	0.99244	-0 01303	-0.06511	0.06640	-0.01011	-0.00604	0.01178
$k_2=\pi/4L$ $n_2=2$	-0.01303	-0.06511	0.06640	0.97634	-0.08374	0.97992	-0.03434	-0.07731	0.08459
$k_2=\pi/4L$ $n_2=3$	-0.01015	-0.00603	0.01181	-0.03439	-0.07734	0.08464	0.93108	-0.17588	0.94754
$k_2=3\pi/8L$ $n_2=1$	0.98909	-0.08148	0.99244	-0.01303	-0.06511	0.06640	-0.01025	-0.00604	0.01189
$k_2=3\pi/8L$ $n_2=2$	-0.01303	-0.06511	0.06640	0.97634	-0.08374	0.97992	-0.03435	-0.07740	0.08468
$k_2=3\pi/8L$ $n_2=3$	-0.01028	-0.00604	0.01192	-0.03439	-0.07742	0.08471	0.93076	-0.17597	0.94725
$k_2=\pi/2L$ $n_2=1$	0.98909	-0.08148	0.99244	-0.01303	-0.06511	0.06640	-0.01040	-0.00604	0.01203
$k_2=\pi/2L$ $n_2=2$	-0.01303	-0.06511	0.06640	0.97634	-0.08374	0.97992	-0.03436	-0.07745	0.08473
$k_2=\pi/2L$ $n_2=3$	-0.01042	-0.00603	0.01204	-0.03437	-0.07742	0.08471	0.93002	-0.17601	0.94653

Table 5 - 2c

$q_t=0$ $M=\pi/L$	$n_1=1$			$n_1=2$			$n_1=3$		
	real pt	imag pt	mtr valu	real pt	imag pt	mtr valu	real pt	imag pt	mtr valu
$k_2=0$ $n_2=1$	0.88165	-0.25918	0.91895	-0.09801	-0.15697	0.18505	-0.03387	0.11279	0.11776
$k_2=0$ $n_2=2$	-0.09801	-0.15697	0.18505	0.85285	-0.12749	0.86232	-0.18082	0.02083	0.18201
$k_2=0$ $n_2=3$	-0.03388	0.11282	0.11780	-0.18082	0.02089	0.18202	0.54819	-0.06406	0.55192
$q_t=\pi/8L$ $M=\pi/L$	$n_1=1$			$n_1=2$			$n_1=3$		
$k_2=0$ $n_2=1$	0.86148	-0.28114	0.90620	-0.10287	-0.16586	0.19517	-0.01181	0.13642	0 13693
$k_2=0$ $n_2=2$	-0.10287	-0.16586	0.19517	0.85809	-0.12418	0.86703	-0.15677	0.05384	0.16576
$k_2=0$ $n_2=3$	-0.01182	0.13646	0.13697	-0.15678	0.05390	0.16579	0.56387	0.00032	0.56387
$q_t=\pi/4L$ $M=\pi/L$	$n_1=1$			$n_1=2$			$n_1=3$		
$k_2=0$ $n_2=1$	0.84077	-0.30279	0.89363	-0.10565	-0.17779	0.20681	0.01661	0.15279	0.15369
$k_2=0$ $n_2=2$	-0.10565	-0.17779	0.20681	0.86944	-0.12855	0.87889	-0.12012	0.07401	0.14109
$k_2=0$ $n_2=3$	0.01661	0.15287	0.15377	-0.12016	0.07409	0.14116	0.60394	0.04691	0.60576
$q_t=3\pi/8L$ $M=\pi/L$	$n_1=1$			$n_1=2$			$n_1=3$		
$k_2=0$ $n_2=1$	0.81874	-0.32440	0.88067	-0.10830	-0.19366	0.22188	0.04816	0.16012	0.16721
$k_2=0$ $n_2=2$	-0.10830	-0.19366	0.22188	0.88265	-0.14271	0.89411	-0.07746	0.07740	0.10951
$k_2=0$ $n_2=3$	0.04818	0.16026	0.16735	-0.07751	0.07752	0.10962	0.65818	0.06759	0.66164

Table 5 - 2d

$q_z=\pi/4L$ $M=2\pi/L$	$n_1 = 1$			$n_1 = 2$			$n_1 = 3$		
	real pt	imag pt	mtr valu	real pt	imag pt	mtr valu	real pt	imag pt	mtr valu
$k_{z2}=\pi/4L$ $n_2=1$	0.62957	-0.41994	0.75677	-0.20860	-0.31405	0.37702	0.14718	0.08402	0.16948
$k_{z2}=\pi/4L$ $n_2=2$	-0.20860	-0.31405	0.37702	0.80694	-0.32161	0.86867	-0.02214	-0.11124	0.11342
$k_{z2}=\pi/4L$ $n_2=3$	0.14719	0.08410	0.16952	-0.02219	-0.11115	0.11334	0.69883	-0.19480	0.72547
$q_z=\pi/4L$ $M=3\pi/L$	$n_1 = 1$			$n_1 = 2$			$n_1 = 3$		
$k_{z2}=\pi/4L$ $n_2=1$	0.38690	-0.33734	0.51331	-0.36218	-0.28711	0.46217	0.22586	0.06836	0.23597
$k_{z2}=\pi/4L$ $n_2=2$	-0.36218	-0.28711	0.46217	0.66352	-0.26945	0.71615	-0.04310	-0.02302	0.04886
$k_{z2}=\pi/4L$ $n_2=3$	0.22590	0.06842	0.23604	-0.04316	-0.02291	0.04886	0.46733	0.04769	0.46976
$q_z=\pi/4L$ $M=4\pi/L$	$n_1 = 1$			$n_1 = 2$			$n_1 = 3$		
$k_{z2}=\pi/4L$ $n_2=1$	0.24820	-0.17241	0.30221	-0.50173	-0.26757	0.56862	0.21341	-0.12370	0.24667
$k_{z2}=\pi/4L$ $n_2=2$	-0.50173	-0.26757	0.56862	0.50465	-0.33054	0.60326	-0.07507	-0.21243	0.22530
$k_{z2}=\pi/4L$ $n_2=3$	0.21346	-0.12371	0.24672	-0.07514	-0.21235	0.22525	0.42369	-0.04586	0.42617

Table 5 - 2e

The matrix value of the superlattice which width of GaAs layer is 100 Å and the widths of $Al_xGa_{1-x}As$ layers is 200 Å. Doping is uniform in two layers and concentration is 3×10^{17}.

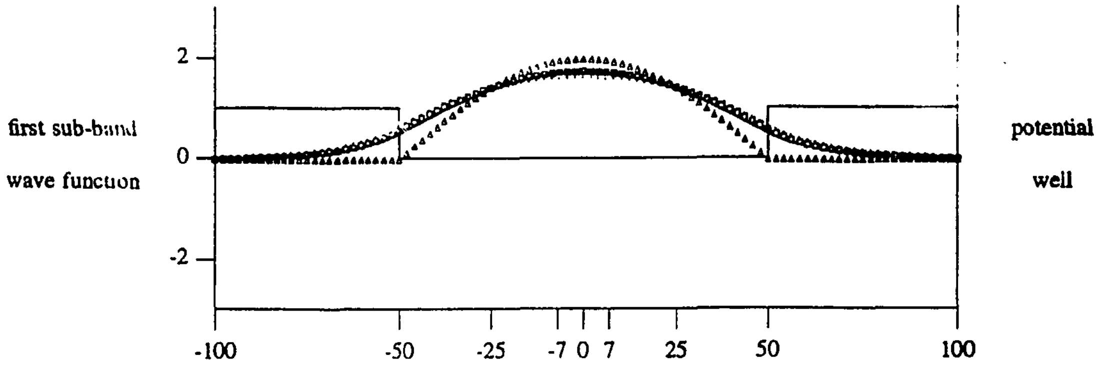


Fig. 5.1a. $\hat{z}$, unit is A°.

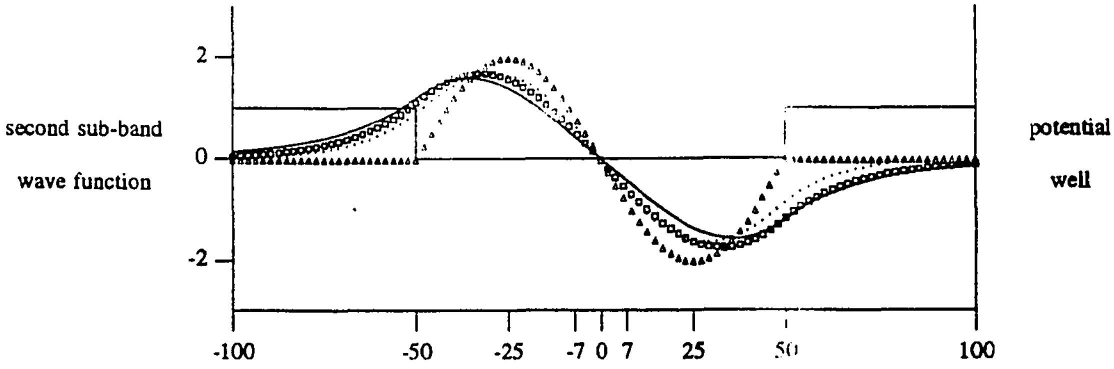


Fig. 5.1b. $\hat{z}$, unit is A°.

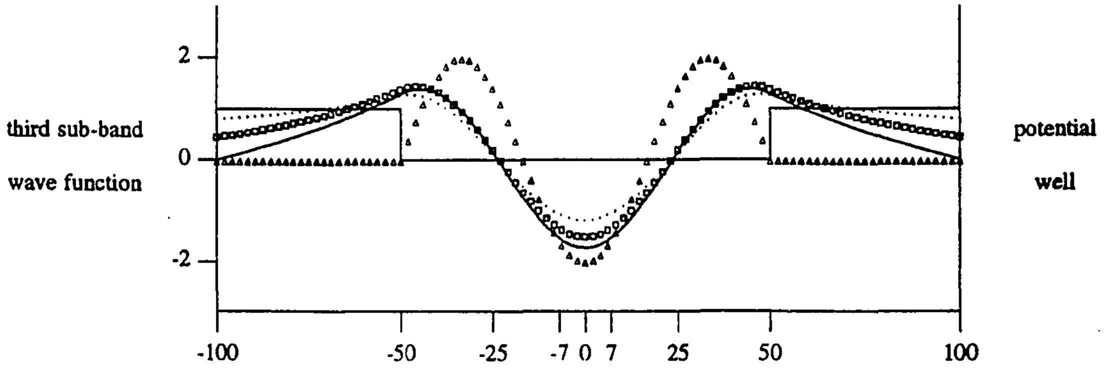


Fig. 5.1c. $\hat{z}$, unit is A°.

The widths of both GaAs and $Al_xGa_{1-x}As$ layers are 100 Å.

Doping is uniform in two layers and concentration is 10^{18}.

Dotted line is tight binding wave with $k_z = 0$, solid line is tight binding wave with $k_z = \pi/L$, square line is sine/cosine wave and delta line is single potential well wave.

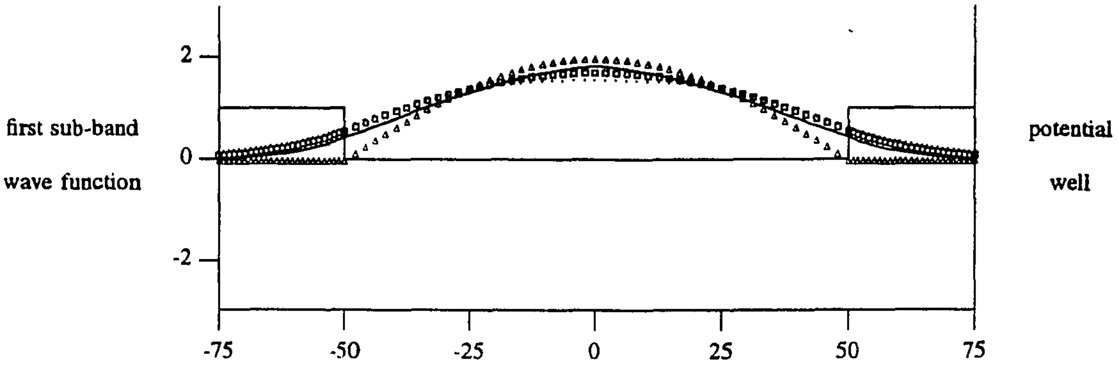


Fig. 5.2a, $\hat{z}$, unit is A°.

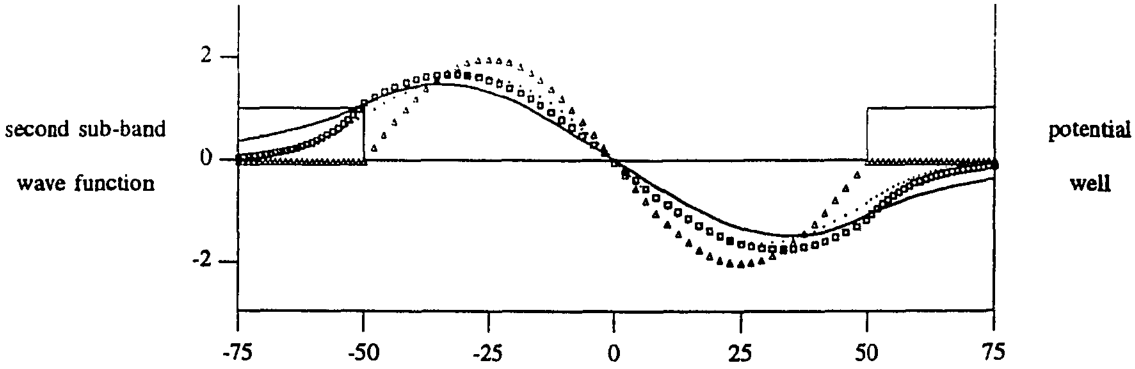


Fig. 5.2b, $\hat{z}$, unit is A°.

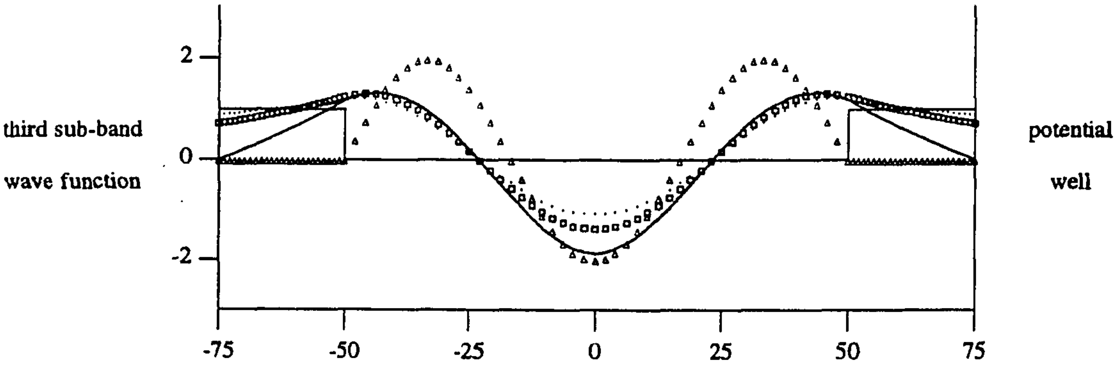


Fig. 5.2c, $\hat{z}$, unit is A°.

The width of GaAs layer is 50 Å and the widths of $Al_xGa_{1-x}As$ layers is 100 Å.

Doping is uniform in two layers and concentration is 10^{18}.

Dotted line is tight binding wave with $k_z = 0$, solid line is tight binding wave with $k_z = \pi/L$,

square line is sine/cosine wave and delta line is single potential well wave.

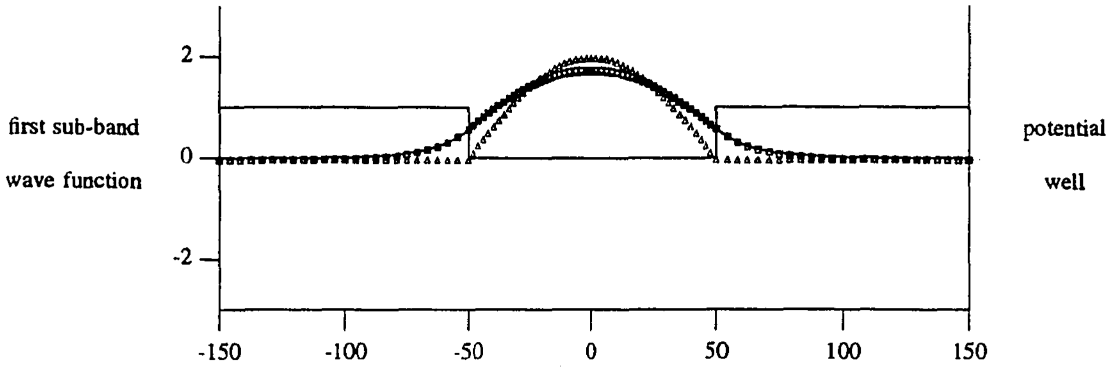


Fig. 5.3a, $\hat{z}$, unit is A°.

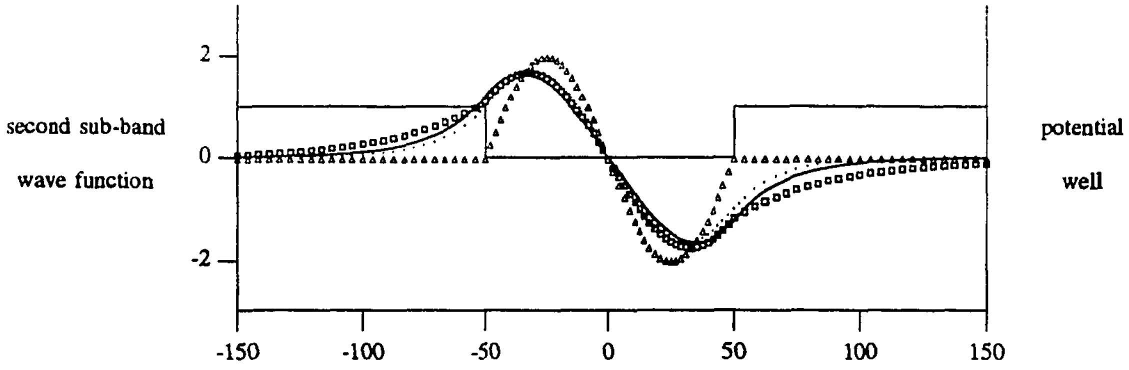


Fig. 5.3b, $\hat{z}$, unit is A°.

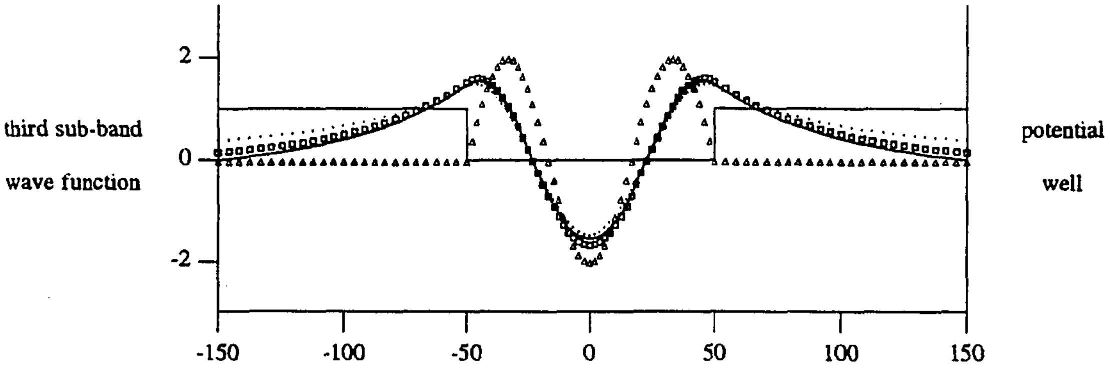


Fig. 5.3c, $\hat{z}$, unit is A°.

The width of GaAs is 100 Å and the width of $Al_xGa_{1-x}As$ layer is 200 Å.

Doping is uniform in two layers and concentration is 10^{17}.

Dotted line is tight binding wave with $k_z = 0$, solid line is tight binding wave with $k_z = \pi/L$, square line is sine/cosine wave and delta line is single potential well wave.

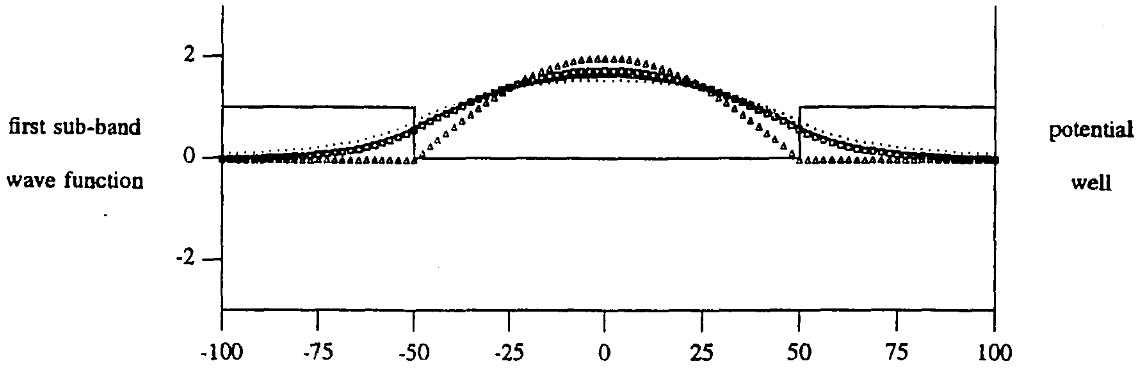


Fig. 5.4a, $\hat{z}$, unit is A°.

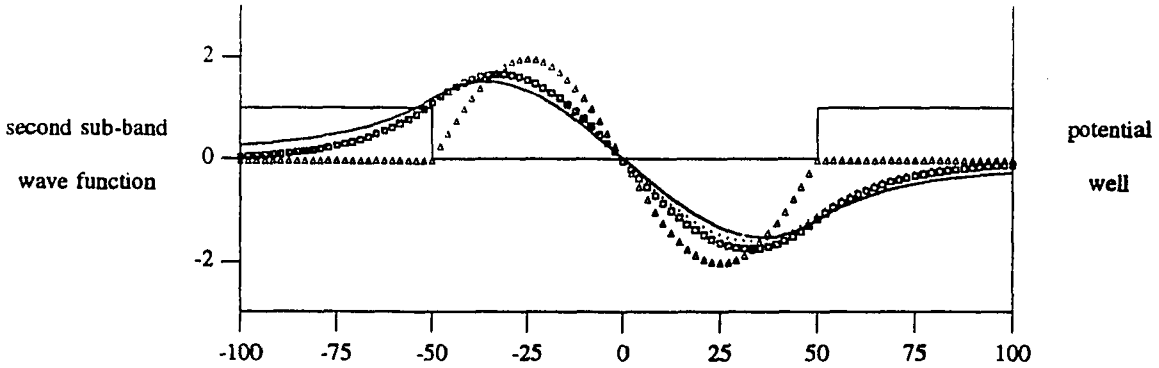


Fig. 5.4b, $\hat{z}$, unit is A°.

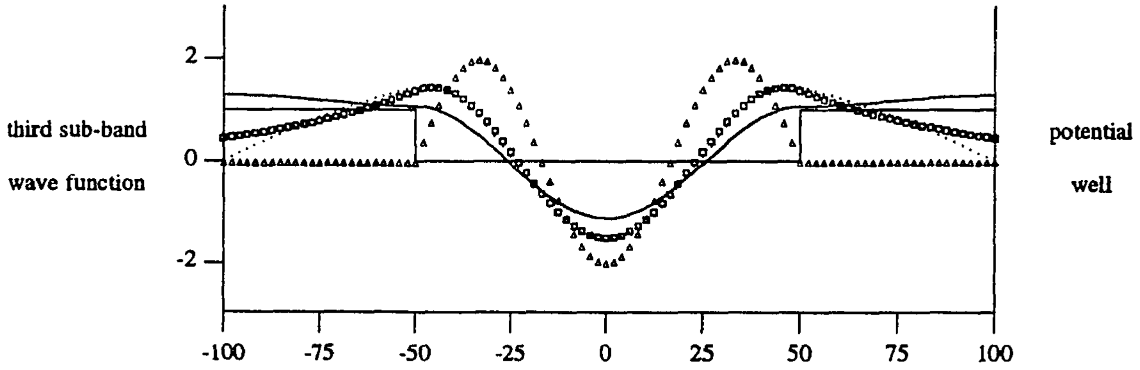


Fig. 5.4c, $\hat{z}$, unit is A°.

The widths of both GaAs and $Al_xGa_{1-x}As$ layers are 100 Å.

Doping is uniform in two layers and concentration is 5×10^{18}.

Dotted line is tight binding wave with $k_z = 0$, solid line is tight binding wave with $k_z = \pi/L$, square line is sine/cosine wave and delta line is single potential well wave.

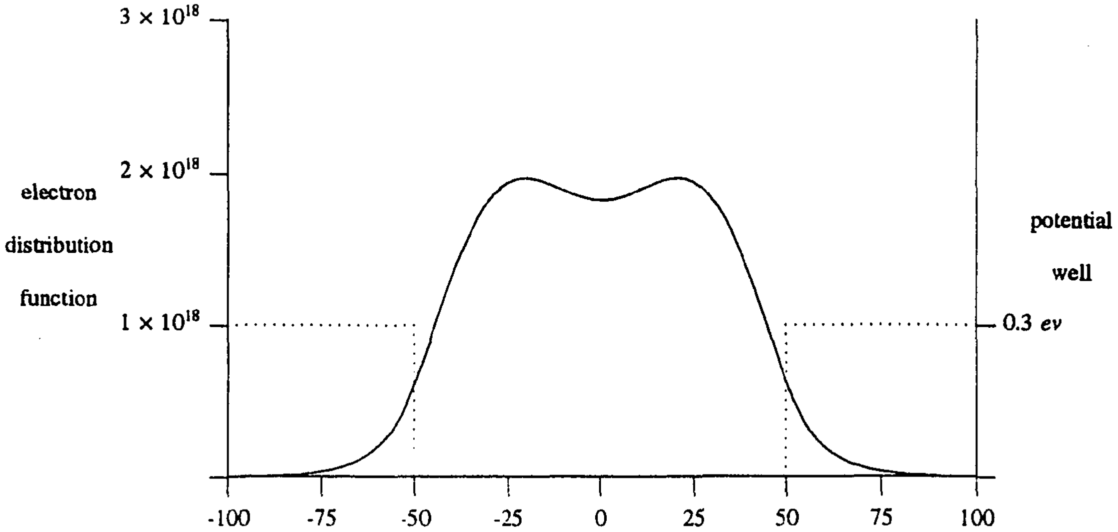


Fig. 5.5, in $\hat{z}$ direction unit is Å

Width of both GaAs and $Al_xGa_{1-x}As$ layers are 100 Å

Doping is uniform in the two layers and the concentration is 10^{18}

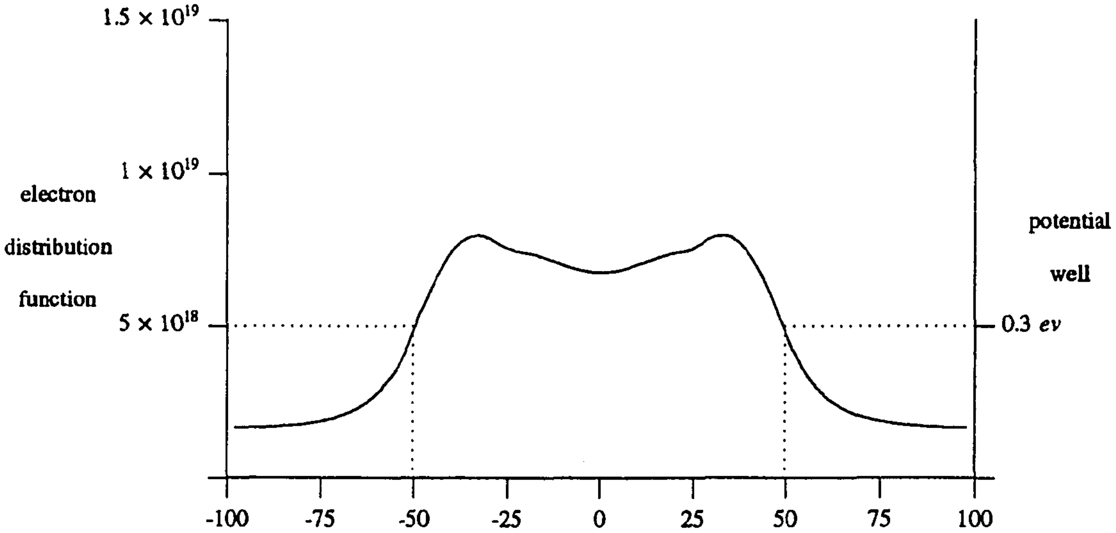


Fig. 5.6, in $\hat{z}$ direction unit is Å

Width of both GaAs and $Al_xGa_{1-x}As$ layers are 100 Å

Doping is uniform in two layers and the concentration is 5 × 10^{18}

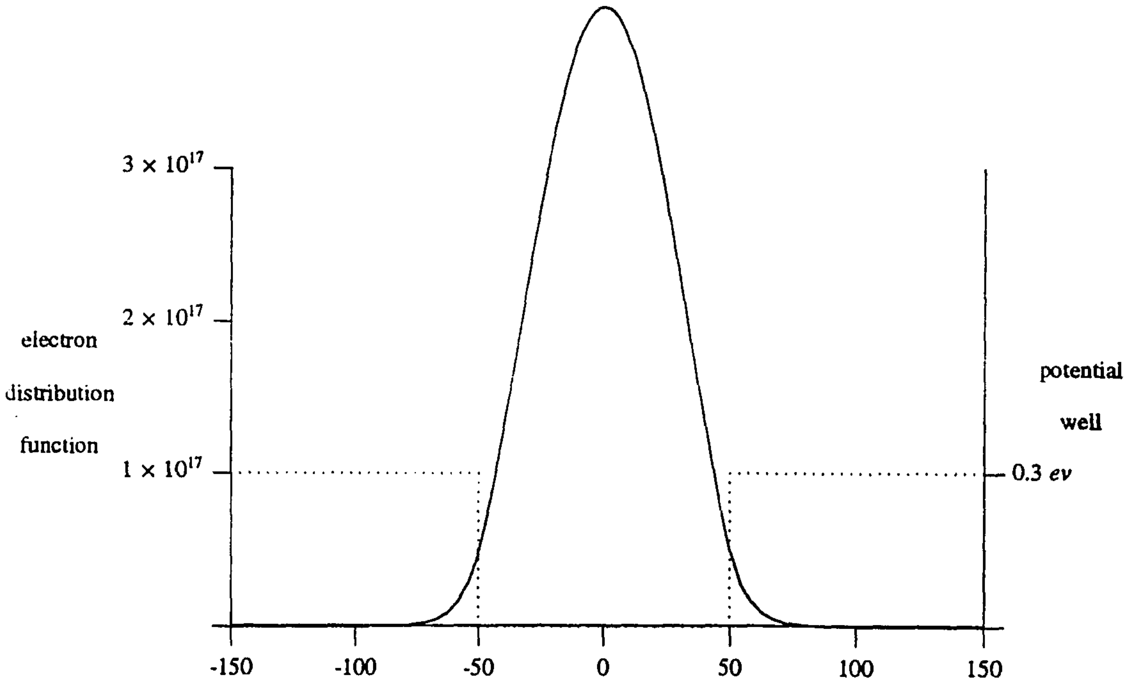


Fig. 5.7, in $\hat{z}$ direction unit is A°

Width of GaAs layer is 100 Å " Width of $Al_xGa_{1-x}As$ layers is 200 Å "

Doping is uniformly in two lays and the concentration is 10^{17}

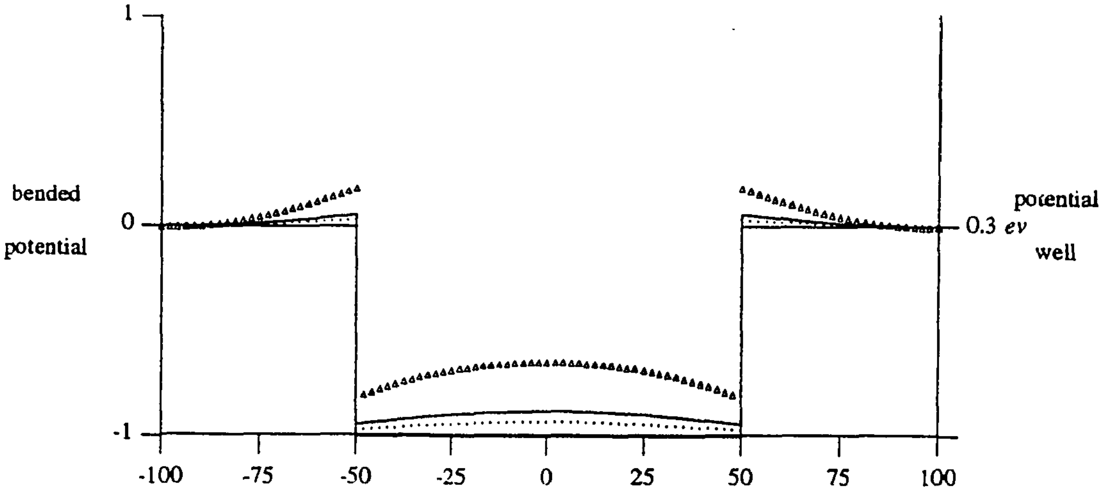


Fig. 5.8. in $\hat{z}$ direction unit is A°

The width of both $Al_xGa_{1-x}As$ layer and GaAs layers are 100 A°. Doping is uniform in two layers

Dotted line for doping concentration 5×10^{17}

Solid line for doping concentration 10^{18}

Delta point for doping concentration 5×10^{18}

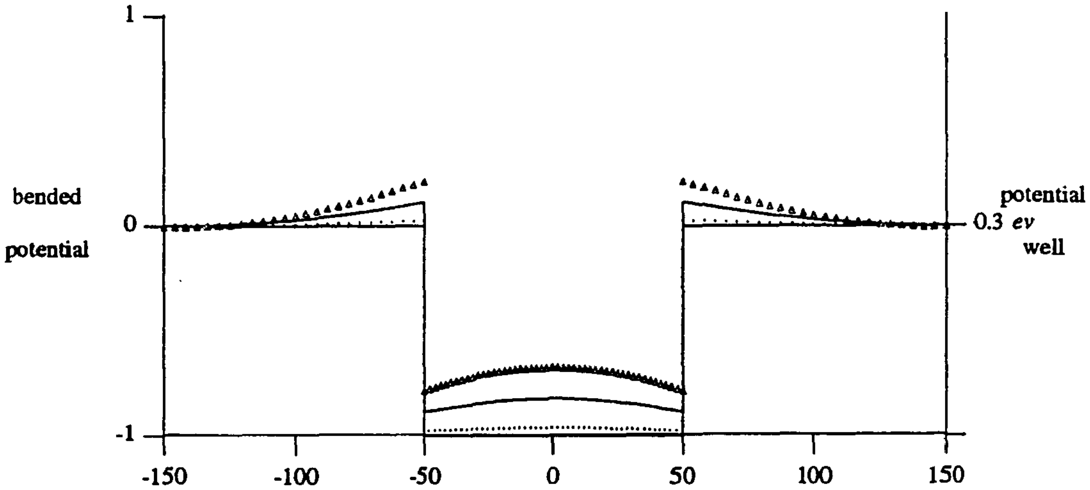


Fig. 5.9, in $\hat{z}$ direction unit is A°

The width of $Al_xGa_{1-x}As$ layer is 200 A° and the GaAs layer is 100 A°. Doping is uniform in two layers.

Dotted line for doping concentration 10^{17}. Solid line for doping concentration 5×10^{17}

Delta point for doping concentration 10^{18}

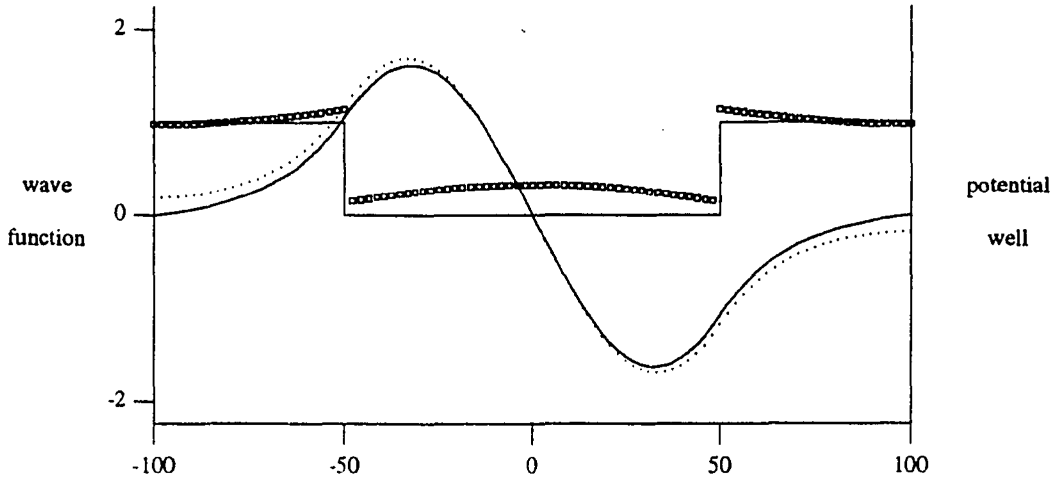


Fig. 5.10a, in $\hat{z}$ direction unit is $A\mathring{A}$

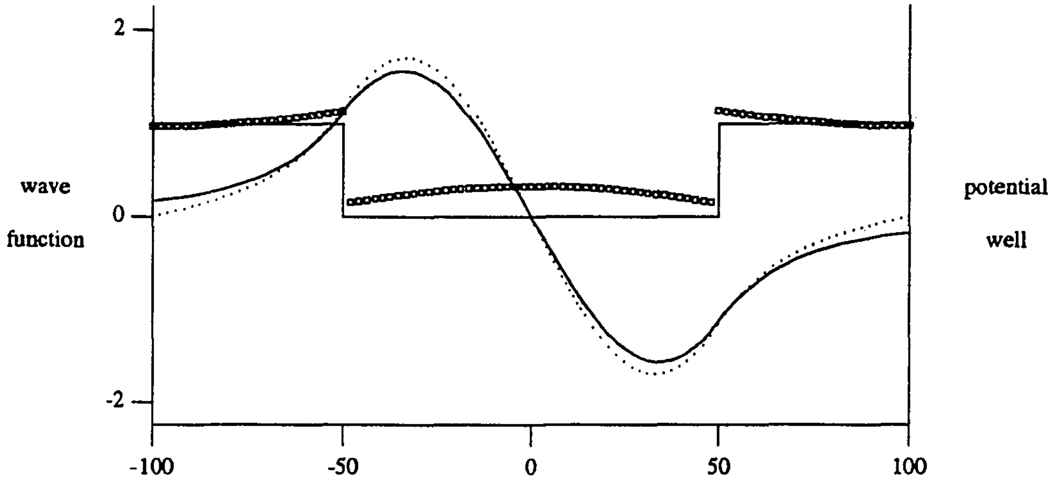


Fig. 5.10b, in $\hat{z}$ direction unit is $A\mathring{A}$

Wave function of second sub-band in superlattice, in Fig 5.10a its $k_z = 0$ and Fig. 5.10b its $k_z = \pi/L$ Solid line is Tight Binding Approximation wave and Dotted line is exactly wave obtained by Kramer's method.

Width of both GaAs and $Al_xGa_{1-x}As$ layers are 100 Å

Doping is uniformly in two lays and the concentration is 2×10^{18}

Square line is bent conduction band

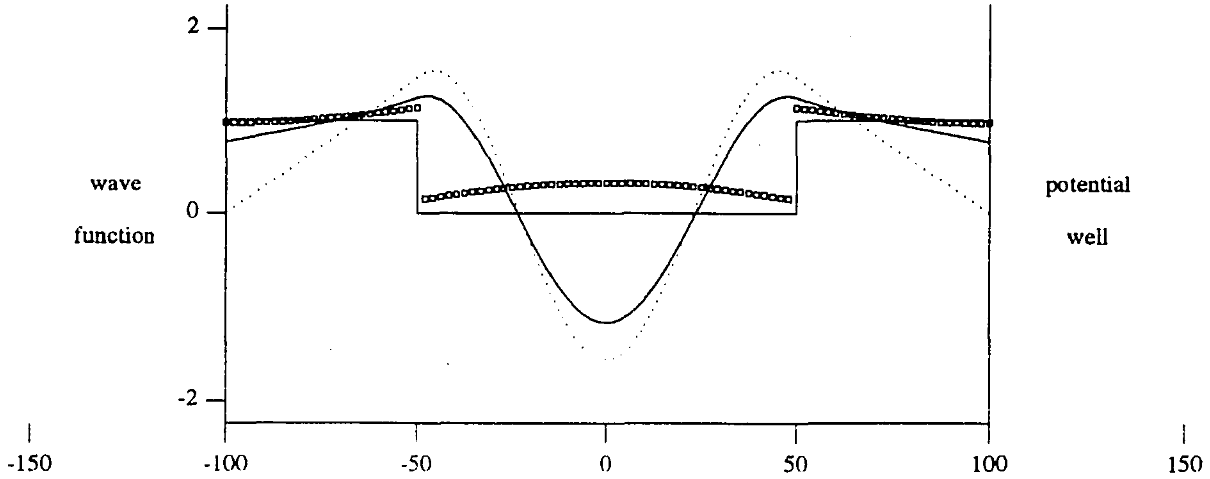


Fig. 5.10c, in $\hat{z}$ direction unit is AÅ

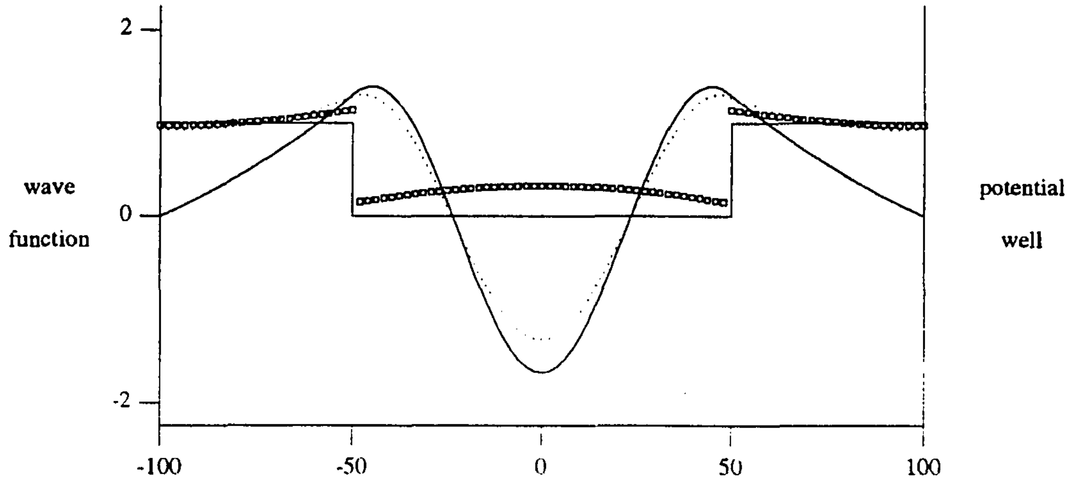


Fig. 5.10d, in $\hat{z}$ direction unit is AÅ

Wave function of third sub-band in superlattice, in Fig 5.10c its $k_z = 0$ and Fig. 5.10d its $k_z = \pi/L$ Solid line is Tight Binding Approximation wave and Dotted line is exactly wave obtained by Kramer's method.

Width of both GaAs and $Al_xGa_{1-x}As$ layers are 100 Å

Doping is uniformly in two lays and the concentration is 2×10^{18}

Square line is bent conduction band

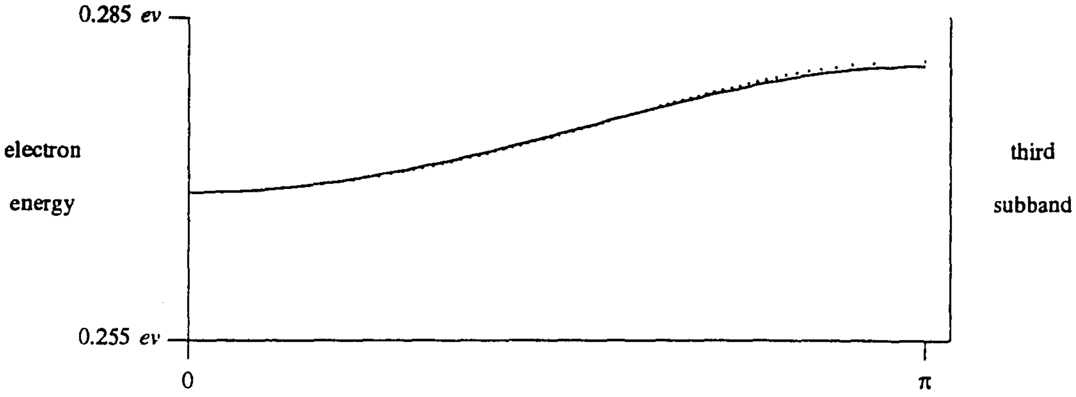


Fig. 5.11a, Momentum

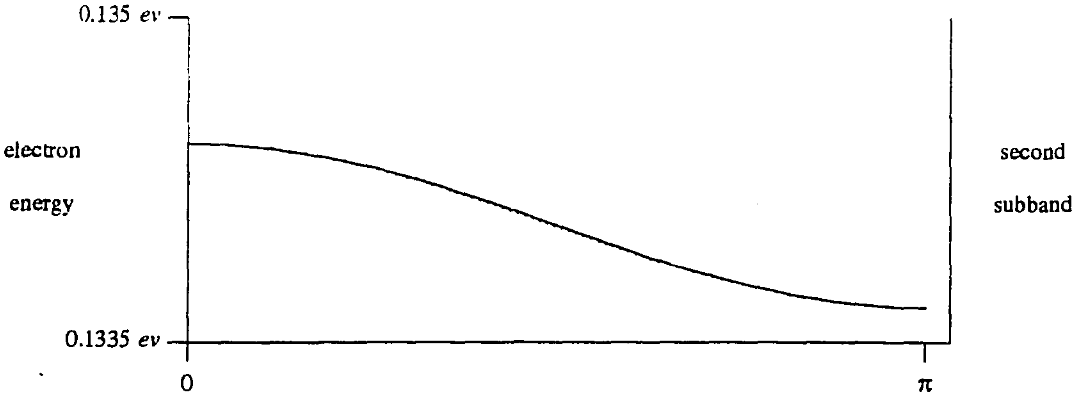


Fig. 5.11b, Momentum

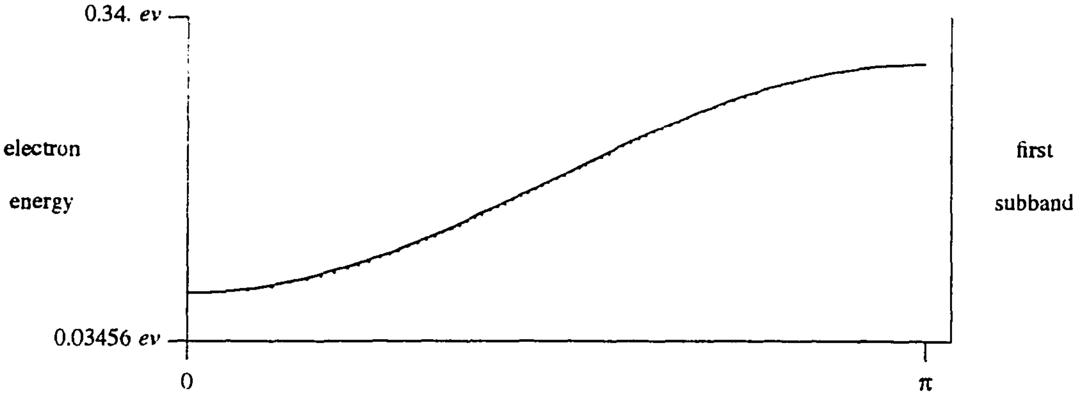


Fig. 5.11c, Momentum

The widths of both GaAs and $Al_xGa_{1-x}As$ layers are 100 Å. Dot point obtain from Kronig-Penny equation. Solid line obtain from tight binding approximation wave function.

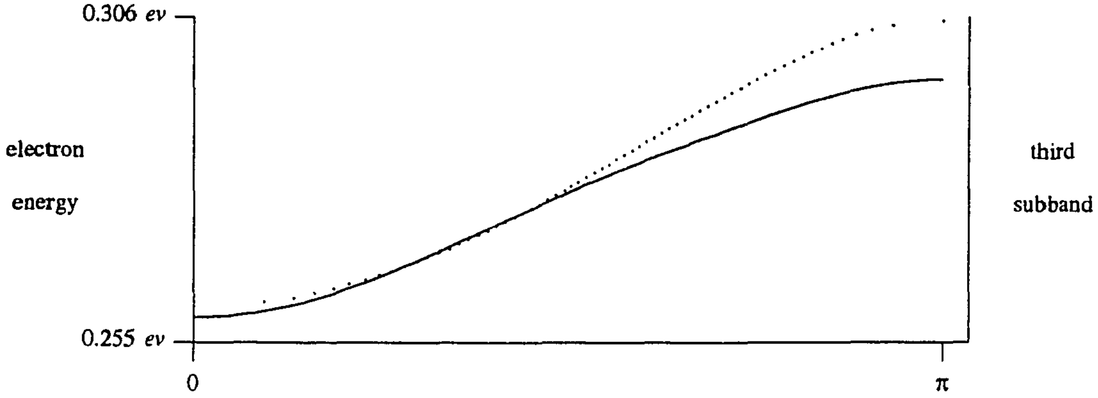


Fig. 5.12a, Momentum

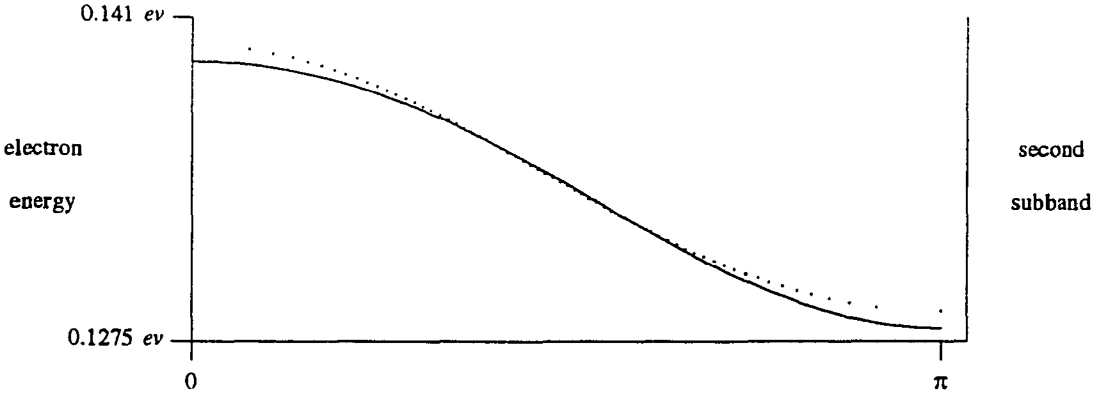


Fig. 5.12b, Momentum

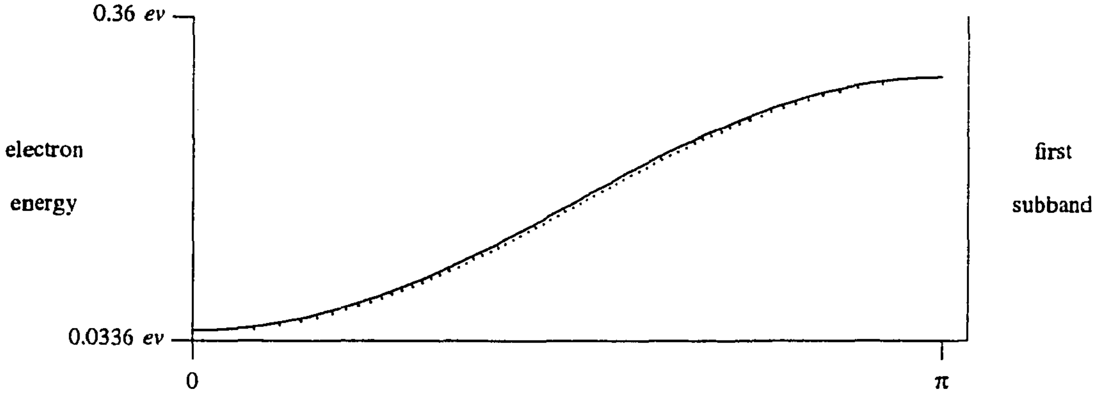


Fig. 5.12c, Momentum

The width of GaAs layer is 100 Å. The width of $Al_xGa_{1-x}As$ layer is 50 Å. Dot point obtain from Kronig-Penny equation. Solid line obtain from tight binding approximation wave function.

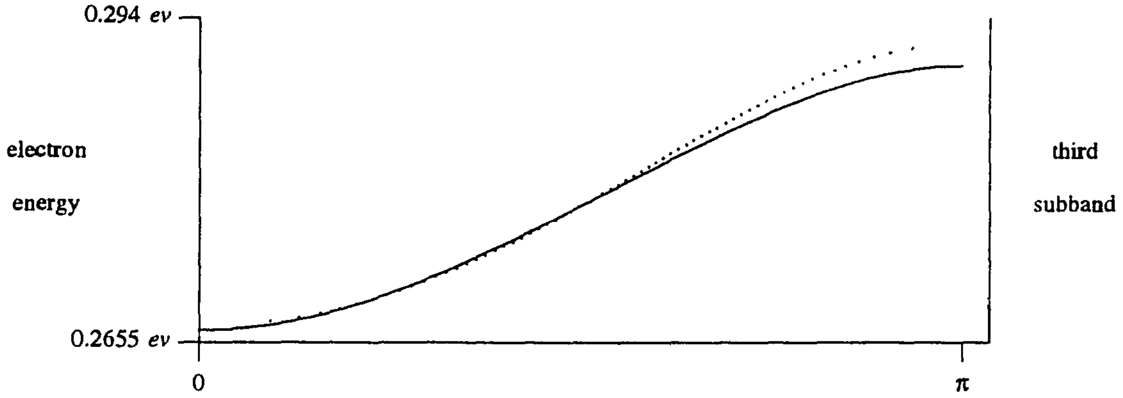


Fig. 5.13a, Momentum

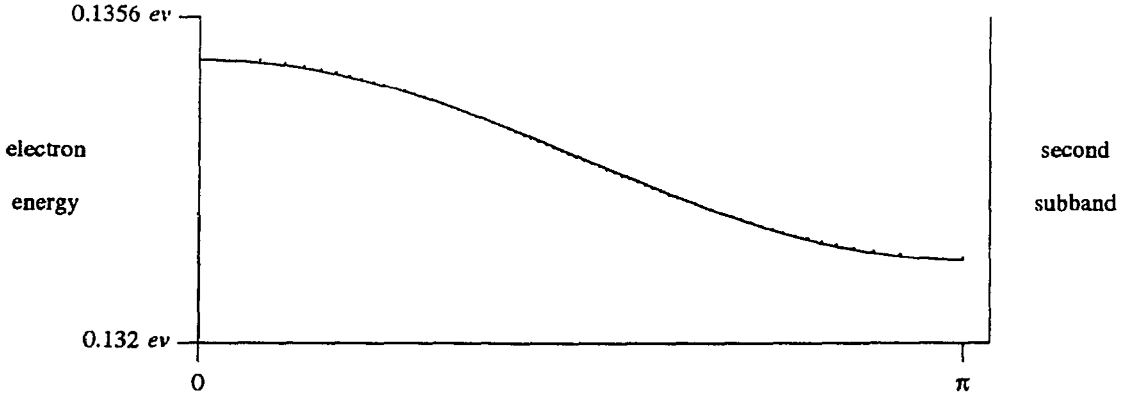


Fig. 5.13b, Momentum

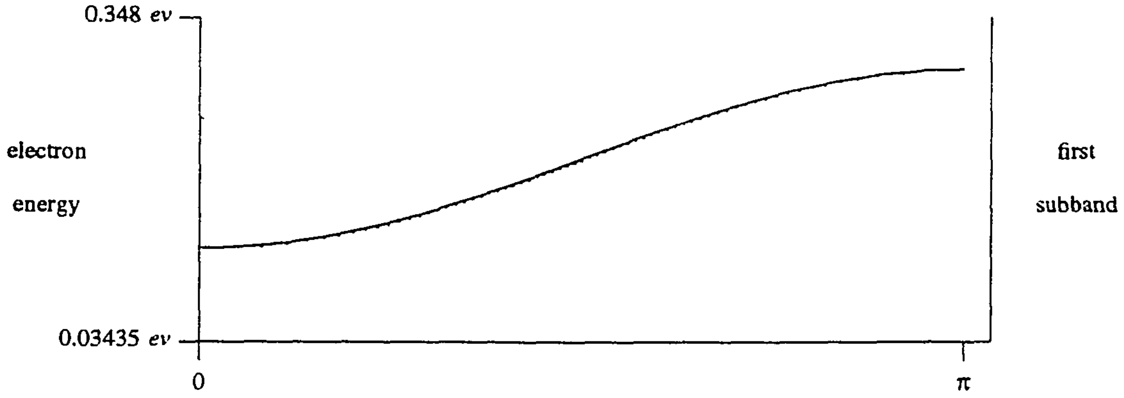


Fig. 5.13c, Momentum

The width of GaAs layer is 100 Å. The width of $Al_xGa_{1-x}As$ layer is 80 Å. Dot point obtain from Kronig-Penny equation. Solid line obtain from tight binding approximation wave function.

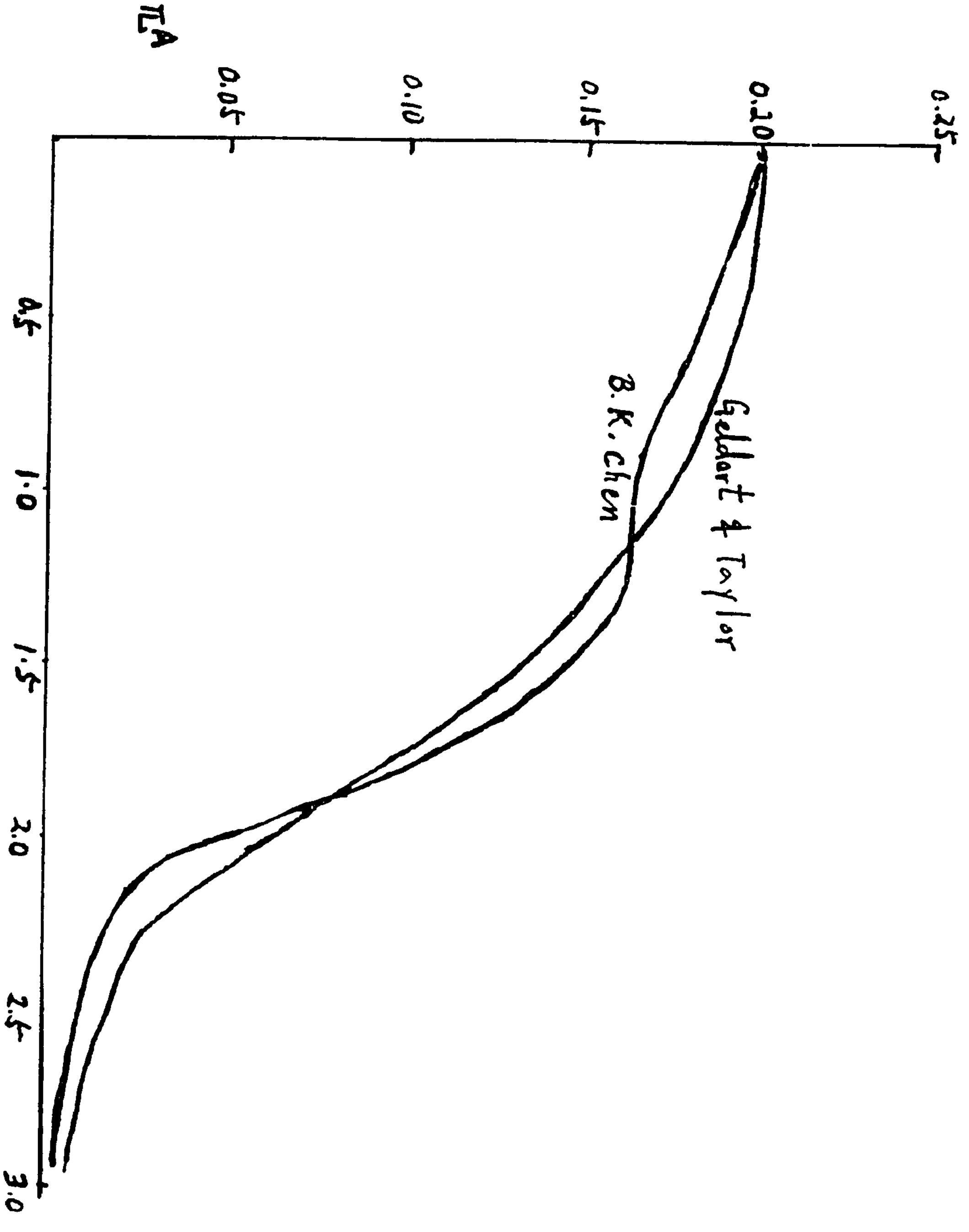

ε_A
0.05
0.10
0.15
0.20
0.25
0.5
1.0
1.5
2.0
2.5
3.0
g/g_f
Geldart & Taylor
B.K. Chen

Figure 5-14

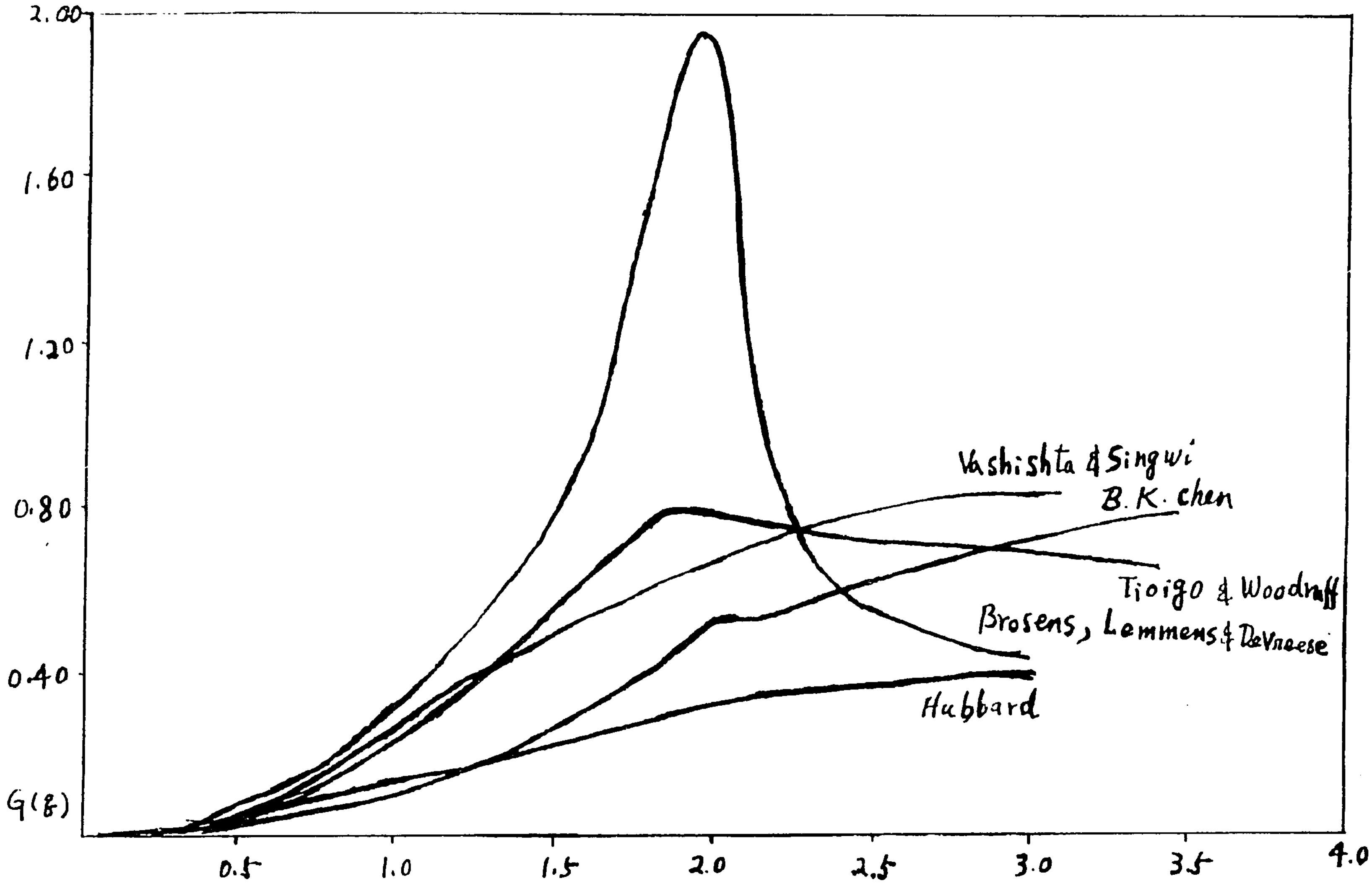

2.00
1.60
1.20
0.80
0.40
G(q)
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
q/q_f
Vashishta & Singwi
B.K. Chen
Tioigo & Woodruff
Brosens, Lemmens & Devreese
Hubbard

Figure 5-15

APPENDIX A

For convenience, I would like to change some of the notation for describing how Hubbard derived his correlation function. Let $C(\mathbf{q})$ instead of $G(\mathbf{q})$ be the correlation function used in chapter III and let $G^0(\mathbf{q})$ be the ground state Green's function. The zeroth order polarization function[12, 19] is

$$\Pi^0(k) = (-1)\ 2 \int i\ G^0(q)\ i\ G^0(q+k) d^4q \qquad \text{(Appendix.A.1)}$$

Its Feynman diagram is shown in Fig. Appendix.A.1. Here we assume $i\,\hbar = i$; q and k is a four dimensional vector; $(-) = (-1)^{n-1}$ means that the particle has gone through n completed cycles (in Feynman diagram); 2 indicates that $i\ G^0(q)$ has two different spins; and $i\ G^0(q+k)$ must have the same spins as $iG^0(q)$. The equation for the first order exchange polarization function (Fig Appendix.A.1) is[18]

$$\Pi^1_{\mathrm{xc}}(k) = \int d\mathbf{k}' V(\mathbf{k}')\ \delta(\mathbf{q}' - \mathbf{q} + \mathbf{k}') \times$$

$$(-1)\ 2 \int d^4q\ d^4q'\ i\ G^0(q)\ i\ G^0(q+k)\ i\ G^0(q')\ i\ G^0(q'+k) \qquad \text{(Appendix.A.2)}$$

Hubbard has made an approximation that the major contribution for the integration of k' is at the k' equal to $k + q_f$ (where q_f is Fermi momentum of electron) and Eq. (Appendix.A.2) becomes

$$\Pi^1_{\mathrm{xc,\,HU}}(k) \approx (-1)\ 2 \int d^4q\ d^4q'\ i\ G^0(q)\ i\ G^0(q+k)\ i\ G^0(q')\ i\ G^0(q'+k)\ V(\mathbf{k} + \mathbf{q}_f)$$

$$= -\frac{1}{2}\Pi^0(k)\; V(\,\mathbf{k} + \mathbf{q}_f)\Pi^0(k) \tag{Appendix.A.3}$$

This is the same equation as in Fig. (Appendix.A.2) except that $V(k)$ is changed to $V(k + q_f)$. Similarly, the second order exchange polarization function (Fig. Appendix.3) can be expressed by[18]

$$\Pi^2_{\mathrm{xc,\,HU}}(k) \approx \frac{1}{4}\;\Pi^0(k)\; V(k + q_f)\Pi^0(k)\; V(k + q_f)\Pi^0(k) =$$

$$\Pi^0(k)\;(\,-\frac{1}{2}\; V(\,\mathbf{k} + \mathbf{q}_f)\;\Pi^0(k)\;)^2 \tag{Appendix.A.4}$$

Hubbard's polarization function has summed up this kind of exchange polarization function, and obtains

$$\Pi_{\mathrm{HU}}(k) = \Pi^0(k)\;\sum_{n=0}^{\infty}\,[-\frac{1}{2}\;V(\,\mathbf{k} + \mathbf{q}_f)\;\Pi^0(k)\;]^n =$$

$$\frac{\Pi^0(k)}{1 + \frac{1}{2}V(k + q_f)\;\Pi^0(k)} = \frac{\Pi^0(k)}{1 + \frac{1}{2}\;\frac{k^2}{k^2 + q_f^2}\;\Phi(\mathbf{k})\;\Pi^0(k)} \tag{Appendix.A.5}$$

where $\Phi(\mathbf{k}) = \frac{4\pi e^2}{k^2}$. This is where Hubbard's correlation function $C(k) = \frac{1}{2}\;\frac{k^2}{k^2 + q_f^2}$ comes from. From discussions in chapter III we know that in a periodic medium the momentum of the interaction potential is not necessarily equal to the difference of the momentum in the two Green's functions. It can possibly be equal to that difference plus a vector of the reciprocal of lattice. In other words, the momentum relation can be applied to Fig. (Appendix.A.1), where the delta function $\delta(\mathbf{q} - \mathbf{q}' + \mathbf{k})$ in Eq. (Appendix.A.2) has to be changed to $\sum_{K}\delta(\mathbf{q} - \mathbf{q}' + \mathbf{k} + \mathbf{K})$ ($\mathbf{K}$ is the reciprocal lattice vectors). As it is very difficult to express the Feynman diagram in periodic medium like that expressed in Fig. (Appendix.A.2), it follows that Hubbard's relationship is also difficult to derive in a periodic medium.

APPENDIX B

Debugging a large scale complicated computer program is no easy task. The programs of the screening problem have an additional difficulty in that we do not know the expected result, that is, the program can create errors and not be detected by its result. We therefore divide the program into a few sub-programs such that the error of some of these sub-programs can be detected by their expected results, as described below.

A) To test the subroutine related to Numerov's method, we assume that the electron potential is a square well potential. First, a value different from the eigenenergy is assigned to its energy variable. The subroutine is then run, with the value of energy variable being changed in each iteration. If the value of the energy variable converges to the eigenenergy (refer to Eq. (Appendix.B.1) when $k_z = 0$), then the subroutine is possibly a correct one.

B) To test the subroutines related to the tight binding approximation theory such as energy shift and normalization factor, we assume that the potential is a square well potential. If the result of the function $E(n, k_z)$ is the same as the Kronig-Penney equation

$$\cos(k_z\, a) = \frac{\beta^2 - \alpha^2}{2\,\alpha\,\beta}\sinh(\beta b)\,\sin(\alpha(a-b)\,) + \cosh(\beta b)\cos(\alpha(a-b)\,) \quad \text{(Appendix.B.1)}$$

here a is the width of the G_aA_s layer, b is the width of the $Al_xG_{a\,(1-x)}A_s$ layer,

$$\alpha = \left[\frac{2m^*}{\hbar^2} E(k_z) \right]^2 ,$$

$\beta = \left[\frac{2m^*}{\hbar^2} (V - E(k_z)) \right]^2$ and V is the potential difference between $Al_xGa_{(1-x)}As$ layer and $GaAs$ layer, then the subroutine is a correct one. The normalization factor is combined with the energy shift equation. We can not get the correct energy shift without a correct normalization factor.

C) To test the subroutines which are to obtain the Fermi-level and the electron carrier density distribution function $\rho_e(z)$, we require the distribution function to obey

$$\int_{\frac{-L}{2}}^{\frac{L}{2}} \rho_z(z)\, dz = N\, L \qquad \text{(Appendix.B.2)}$$

here N is the average of the doping concentration.

D) Refering to the subroutines related to the polarization function $\Pi^0(q_z, q_\perp, m_1, m_2)$, if we set the eigenenergy $E(n, k_z, k_\perp)$ equal to eigenenergy for the electron in the homogeneous medium $\frac{\hbar^2}{2m^*} [k_\perp^2 + ((n-1) \cdot K + k_z)^2]$ and let $m_1 = m_2$, $n_iK + k_{z_i} = n_jK + k_{z_j} + m_1 + q_z$ and $\langle n_i, k_{z_i} | e^{i(m_1 + q_z) \cdot z} | n_j, k_{z_j} \rangle = 1$, the result should be equal to the random phase approximation polarization function.

$$\Pi^0(\mathbf{q}) = \frac{k_f}{\pi^2\, \hbar^2 / m^*} L(q/2K_f) \qquad \text{(Appendix.B.3)}$$

$$L(u) = \frac{1}{2} - \frac{1}{4}\, \frac{1-u^2}{u} \ln \left| \frac{1+u}{1-u} \right| \qquad \text{(Appendix.B.4)}$$

here $\mathbf{q} = (q_z + m_1K)\, \hat{z} + \mathbf{q}_\perp$

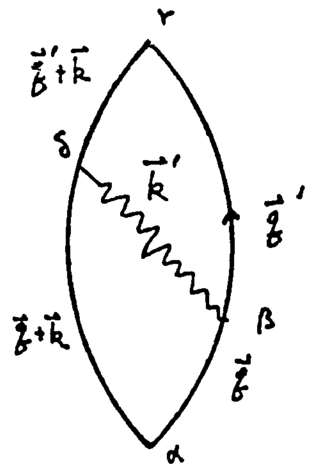


Figure App-A. 1

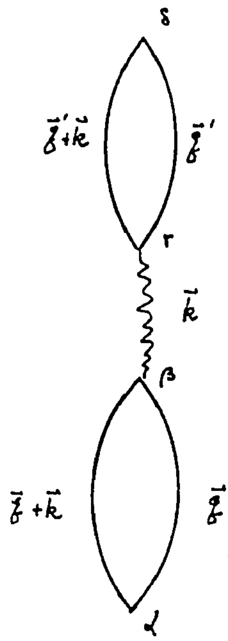


Figure App-A. 2

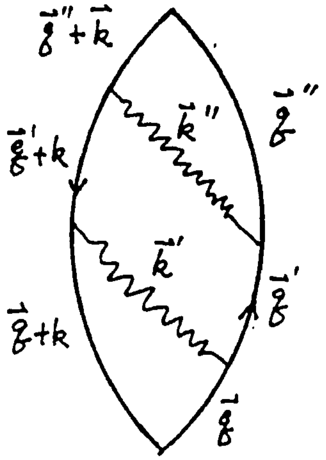


Figure App-A. 3

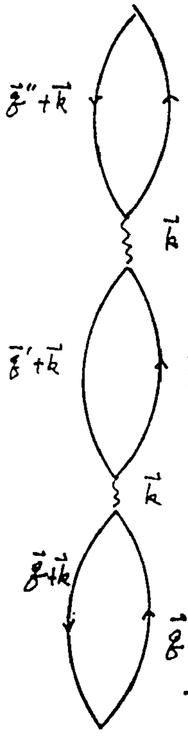


Figure App-A. 4

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