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QED EFFECTS IN HIGH-Z ATOMS; THREE-BODY POTENTIALS

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QED EFFECTS IN HIGH-Z ATOMS: THREE-BODY POTENTIALS

by

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To my Parents, and

To Judith

Introduction

QED is considered to be a pinnacle of modern physical theory, predicting measurable quantities correctly to the order of more than one part per million. Despite the great success of QED, the theory has a limitation from a practical point of view. Most calculations are done using perturbation theory, the fine structure constant being the perturbation parameter. As one proceeds to go further out in the perturbation series the number of Feynman diagrams grows geometrically. In Muonium for example, over nine hundred diagrams[1] must be evaluated in order to calculate the theoretical fine structure within the same margin of error afforded by experimental measurements available today. Although there has been some progress for helium[2], the perturbational approach seems to be exceedingly complex when one is interested in incorporating QED, into atomic structure calculations for heavy atoms. It would be very convenient if such a system obeyed some sort of Schrodinger like wave equation, all QED effects being manifest as configuration space potentials, the advent of ultrafast computing machines providing, perhaps, some numerical solutions of such an equation. This is of course a naive hope, since the concept of a potential is a throwback to the pre-Maxwellian days of action-at-a-distance, QED containing an infinite number of

degrees of freedom in the field can never be cast in this form. However it is reasonable to assume that the gross structure of a heavy atom is determined by some complicated interelectronic potential, the residual QED effects being a small perturbation on the configuration space wave function of such an equation. This is the philosophy that we shall take in this thesis. It must be pointed out that the celebrated Bethe - Salpeter equation[3] is such a configuration space equation for the case of two interacting fermions, the interparticle potential arising from the sum of all ladder diagrams of photon exchange between the fermions. However, the B - S algorithm for constructing configuration space equations does not seem amenable to generalization to a many fermion system[4]. Furthermore, an eigenvalue equation would almost be intractable since in the B-S formalism each particle has it's own time coordinate. We shall take a different viewpoint first advocated by Brown and Ravenhall[5], and generalized by M.H. Mittleman[62]. These authors obtained <u>one-time</u> configuration space equations for a multi-electron atom, compatible with QED. Although the one - time Hamiltonian formulations are not strictly covariant in contrast to the Bethe - Salpeter equation, the presence of a heavy nucleus essentially fixes the reference frame for the entire atom.

Even in the classical description, the price one must pay by recasting the Maxwell theory (a <u>field</u> theory)

into an approximate action-at-a-distance theory, is the introduction of many-body potentials. Primakoff and Holstein[7] were the first to derive the classical three-particle potential from the Maxwell theory. They showed that for an essentially nonrelativistic system, the energy contribution from this potential is quite small, on the order of $(v/c)^4$ in the particle velocities. However, in a high Z atoms the inner shell electrons travel at a significent fraction of the speed of light, and this energy might be nonnegligible. In a many-body system the three-body potential contributes to the total energy, in proportion to the cube of the number of interacting particles[6], while the contribution coming from the two particle potentials goes as the square. At a certain value of N, the number of particles, we might expect that the total three-particle energy becomes comparable to the two-body energy of the system. The above statement must be qualified by noting that the three-particle potential is only significent for triplets of particles, two of which are highly relativistic; therefore we would expect that only the inner shell electrons have an appreciable contribution to this energy.

Recent multiconfigurational Dirac-Hartree-Fock solutions[8] of one-time configuration space equations that include the the most sophisticated form for the interelectronic two body potentials, seem to consistantly give a discrepancy on the order eight electron volts for

the binding energy of heavy atoms (Z=80), when compared to experimental values. Mittleman [6] has shown through an order of magnitude calculation that such an energy might be due to the effects of three body potentials which have never been incorporated in atomic structure calculations. It is the major goal of this thesis to determine whether three-body potentials are important in the structure of heavy atoms, and contribute to the binding energy, values on the order of magnitude quoted above.

This thesis is divided into two parts. In part I we deal with the basic formalism, in part II we concentrate on the computational aspects to the thesis. In chapter one we review the semiclassical derivation of configuration space potentials obtained by Breit[9], and Primakoff and Holstein[7]. Brown and Ravenhall[5] pointed out that the Breit equation does not contain physical solutions. They stressed the point, that an acceptable multifermion configuration space equation must be compatible with pair theory. In the second section of this chapter we review the Brown - Ravenhall analysis. In chapter two, a comprehensive review of the papers by Mittleman[6], that deal with the construction of two, and three-body potentials, is given. In chapter three we deal with some ambiguities associated with the photon decoupling transformation discussed in the previous chapter. Some of these ambiguities are a result of the gauge degree of freedom. Ambiguities associated with boundary conditions

(retarded, advanced, etc. solutions), are resolved. In the second section of this chapter a curious property of the QED three particle potentials, (they seem to violate the Pauli exclusion principle) is investigated. In the last section we rederive the Primakoff-Holstein three body potential from QED by a certain limiting procedure.

Finally, in chapter four, of part II we shall evaluate the three-body contribution to the ionization potential of the lithium sequence for ions with $(Z\alpha) \approx 1$. This calculation will give us a good hint for determining the answer to the question posed in the previous paragraph i.e. are three-body potentials important in the atomic structure of heavy atoms? We shall see that the answer to the above question is in the negative. That is, estimates of the contribution of the three-body potentials to the total energy of such ions give results less than an electron volt for $Z \approx 137$, and a few hundreth's of an electron volt for $Z \approx 80$, so that the discrepancy noted above does not arise from this source.

Chapter 1

In section 1.1, we give a brief review of approximate action at a distance theories, for a set of N classical particles, interacting via an electromagnetic field. In particular, the Darwin Hamiltonian and the Primakoff Holstein three-body potential are derived.

The Breit equation based on semiclassical arguments is not compatible with pair(hole) theory. This was first pointed out by Brown and Ravenhall. Furthermore it follows that the Breit equation does not contain physical solutions for systems such as the helium atom. These points are further elucidated in section 1.2.

The transition from Fock to configuration space is made for a system containing a static two-body interaction Hamiltonian, in section 1.3. The reduction for nonrelativistic, and relativistic systems are compared. The correct reduction for the relativistic case was first done by Brown and Ravenhall, the resulting wave equation compatible with pair theory is presented, and contrasted with the Breit equation.

Section 1.1 The Classical Theory

Let us consider the Lagrangian for a set of N charged particles interacting with an electromagnetic field,

$$L = \sum_{i=1}^{N} m_i v_i^2/2 + e_i/c\ \bar{v}_i \cdot \bar{A}(r_i,t) - e_i \varphi(r_i,t) \tag{1.1.1}$$

where the subscript i refers to the coordinates of the i'th particle , and e_i is the charge of the i'th particle. The field equations for the scalar, and vector potential in the transverse gauge ($\bar{\nabla}\cdot\bar{A} = 0$), are given by,

$$\nabla^2 \varphi(r,t) = -4\pi\rho(x,t)$$

$$\nabla^2 A(r,t) - 1/c^2 \frac{\partial^2 A(r,t)}{\partial t^2} = -4\pi/c\ \bar{J}_\perp(r,t) \tag{1.1.2}$$

where $\rho(r,t)$, $\bar{J}_\perp(r,t)$ are the charge and transverse current densities,

$$\rho(r,t) = \sum_i e_i \delta(r - r_i(t))$$

$$\bar{J}_{\perp}(r,t) = 1/4\pi \; \bar{\nabla} \times \bar{\nabla} \times \sum_{i}^{N} \int dr' e_i v_i(t) \frac{\delta(r'-r_i(t))}{|r-r'|}$$

(1.1.3)

We can derive an approximate action at a distance Lagrangian, by expressing the field potentials at the i'th particle in terms of the coordinates of the other (N-1) particles. Solving the field equations (1.1.2) we get,

$$\varphi(r_i,t) = \int dr' \sum_{j \neq i}^{N} e_j / |r_i - r_j(t)|$$

$$\bar{A}(r_i,t) = 1/c \int dr' \int dt' \; G_R(r_i - r', t-t') \; \bar{J}_{\perp}(r',t')$$

$$\approx 1/c \int dr' \sum_{j \neq i}^{N} \bar{J}_{\perp}(r',t) / |r_i - r_j(t)|$$

(1.1.4)

where we have approximated the retarded Greens function[9], $G_R(r_i - r', t-t') \approx 1/|r_i - r'|$, i.e. we have neglected retardation effects, thus,

$$\bar{A}(r_i,t) \approx \sum \frac{1}{2c} \frac{e_j}{|r_i - r_j|} \left\{ \bar{v}_j(t) + \hat{r}_j(t) \left(\bar{v}_j(t) \cdot \hat{r}_j(t) \right) \right\}.$$

(1.1.5)

Inserting the above field potentials into (1.1.1) for each particle one gets,

$$L_{eff} = \sum_i m_i v_i^2/2 - \sum_{i<j} e_i e_j/|r_{ij}| +$$

$$\sum_{i<j} e_i e_j/2c^2 \left\{(\bar{v}_i \cdot \bar{v}_j + \bar{v}_i \cdot \hat{r}_{ij}\, \bar{v}_j \cdot \hat{r}_{ij})/|r_{ij}|\right\}$$

where $|r_{ij}| = |r_i - r_j|$.

(1.1.6)

This reduction which is correct to order $(v/c)^2$ in the particle velocities, was first carried out by Darwin[10]. The quantum mechanical generalization of the above reduction was done by G.Breit. Heuristically, replacing the velocities $\bar{v}_i/c$ by the Dirac matrices $\bar{\alpha}_i$ in the corresponding Hamiltonian function of L_{eff}, one gets the Breit equation[9] (N=2), for a pair of electrons with charge e,

$$\left[h(1)+h(2)+e^2/r_{12}\;\; 1 - 1/2(\,\bar{\alpha}_1 \cdot \bar{\alpha}_2 + \bar{\alpha}_1 \cdot \hat{r}_{12}\, \bar{\alpha}_1 \cdot \hat{r}_{12}\,)\right]\psi = E\psi$$

(1.1.7)

where h(i) are appropriate single-particle Dirac Hamiltonians in a central field. In the literature it has been stated[11] that the Breit operator,

$$B(1,2) = -e^2/2r_{12}\,(\,\bar{\alpha}_1 \cdot \bar{\alpha}_2 + \bar{\alpha}_1 \cdot \hat{r}_{12}\, \bar{\alpha}_2 \cdot \hat{r}_{12}\,)$$

(1.1.8)

can be expressed as a sum of two physically distinct terms, the magnetic current-current term,

$$G(1,2) = -e^2 \alpha_1 \cdot \alpha_2 / r_{12} \qquad (1.1.9)$$

called the Gaunt[12] operator, and a term due to the retardation of the Coulomb potential,

$$V_R(1,2) = -e^2/2r_{12}\,(\bar{\alpha}_1 \cdot \bar{\alpha}_2 + \bar{\alpha}_1 \cdot \hat{r}_{12}\, \bar{\alpha}_2 \cdot \hat{r}_{12}). \qquad (1.1.10)$$

However this is a gauge dependent statement, and is true only when one makes the reduction to an action-at-a - distance theory in the Lorentz gauge. In the transverse gauge, both the Gaunt operator and V_R are combined in the Breit operator as a manifestation of the no retardation tranverse current-current interaction, and the Coulomb potential is treated exactly.

As was pointed out in the previous paragraph the decoupling of the radiation field was done approximately to $O(v^2/c^2)$. Primakoff and Holstein[7] noted that when one goes beyond this approximation, the elimination of the field coordinates introduces novel three-body action-at-a distance potentials $V_3(r_i, r_j, r_k)$, such that V_3 cannot be factored into pairwise terms. The above authors pointed out that expansion of the vector potential (1.1.4) beyond the no-retardation limit introduces terms

proportional to the acceleration of the field source. If the i'th particle "feels" the vector potential, proportional to the j'th particle's acceleration, which in turn (via Newton's third law) depends upon the coordinate of particle k, the mutual interaction energy of the three particles must have contributions proportional to $V_3(i,j,k)$. Expanding the transverse potential A(r,t) in (1.1.4) to first order in the retardation and proceeding in the same manner as in the Darwin reduction described above, the authors reproduced the Darwin Hamiltonian with an additional term, given by

$$H_3 = \sum_{i,j,k} e_k e_j^2 e_i / (8m^3c^4 |r_{kj}||r_{ji}|) \times$$

$$\{ \bar{p}_k \cdot \bar{p}_i + \bar{p}_k \hat{r}_{ji} \; \bar{p}_l \hat{r}_{ji} + \bar{p}_k \cdot \hat{r}_{kj} \; \bar{p}_i \cdot \hat{r}_{kj}$$

$$+ \; \hat{r}_{kj} \cdot \hat{r}_{ji} \; \bar{p}_k \cdot \hat{r}_{kj} \; \bar{p}_i \cdot \hat{r}_{ji} \}$$

(1.1.11)

where $\bar{p}_i$ is the canonical momentum of the i'th particle.

Section 1.2 The Brown - Ravenhall disease.

Let us again backtrack to the Breit equation given in (1.1.7). Breit successfully calculated the fine structure of helium by using the Breit operator to first order in perturbation theory[9]. However, when the Breit operator was evaluated to second order[9], anomalously large contributions inconsistant with the experimental data arose. The reason for this failure is given by Bethe[13], who points out that the Breit operator itself is a pertubative approximation to order e^2, for the transverse photon exchange between two electrons. It is therefore "illegal" to iterate B(1,2) beyond e^2, instead one must calculate the full e^4 transverse photon exchange terms in QED pertubation theory.

Even if one accepts the above constraint on the use of the Breit operator, the Breit equation suffers from a more profound flaw that is independent of the above considerations. Twenty years after the introduction of the Breit equation, Brown and Ravenhall[5] pointed out that interacting multi-particle equations based on the single particle Dirac equation such as (1.1.7), do not in fact possess reasonable physical solutions. Their reasoning follows from the fact that the zero order bound states of the Hamiltonian, h(1) + h(2) are degenerate with an infinite set of degenerate continuum states, see Fig.(1a). If one now adiabatically, turns on an interelectronic

interaction $\lambda V(1,2)$, λ being a small pertubation parameter, the unperturbed bound states will immediatly sink into a morass of continuum states , i.e. bound state solutions of (1.1.7) are unstable .The above ailment popularly known as the Brown Ravenhall (B&R) disease, or by the clinical name of continuum dissolution (CD) [14] seems to have an important exception which we describe below.

Consider again a two electron(fermion) equation (1.1.7), where h(i) is now the <u>free</u> electron Dirac Hamiltonian, and V(1,2) is some attractive electron-electron potential. Such a Hamiltonian has recently been introduced by R.W. Childers[15] as a possible prototype for a two quark system. He points out the difficulties associated with the Breit operator, however he does not make mention of the apparent CD phathology associated with this equation. In fact by deriving radial equations for an s state, where V(1,2) is the ordinary Coulomb potential, he seems to get a viable set of equations that accommodate acceptable bound state solutions in direct contradiction to the claims of B&R. Let us now see why this system is immune to the B&R disease. Suppose we have two fermions with masses, $m_1 > m_2$, the spectrum of h(1) +h(2) is now given by,

$$E = \pm\sqrt{p_1^2 + m_1^2} \pm \sqrt{p_2^2 + m_2^2} \tag{1.2.12}$$

where p_1, p_2 are the momenta of the fermions. This system conserves total linear momentum $\vec{P} = \vec{p}_1 + \vec{p}_2$. In the center of momentum frame, $|\vec{p}_1| = |\vec{p}_2|$. With this additional constraint, the energy spectrum is now given in Fig.1(b). We notice that there exists a positive energy mass gap between $m_1 + m_2$ and $(m_1 - m_2)$ that is not degenerate with the continuum states in contrast to Fig.1(a), where there is no gap. In this region bound states will be stable with respect to CD. However once an additional particle is introduced (or in the case for the Breit equation where there is an infiintely heavy nucleus manifest as a central field) conservation of linear momentum is no longer a strong enough condition to prevent the onset of the Brown Ravenhall disease.

Brown and Ravenhall where able to construct an acceptable relativistic multielectron equation by starting from first principles namely, QED. The resulting wave equation is similar to the Breit equation except, the interelectronic potential V(1,2) is now sandwiched between a set of positive energy (with respect to h(1) + h(2)) projection operators. If we now turn on the interelectronic potential, the presence of the projection operators prevents the mixing of the bound states of h(1)+h(2) with the negative energy continuum, therefore CD is prevented.

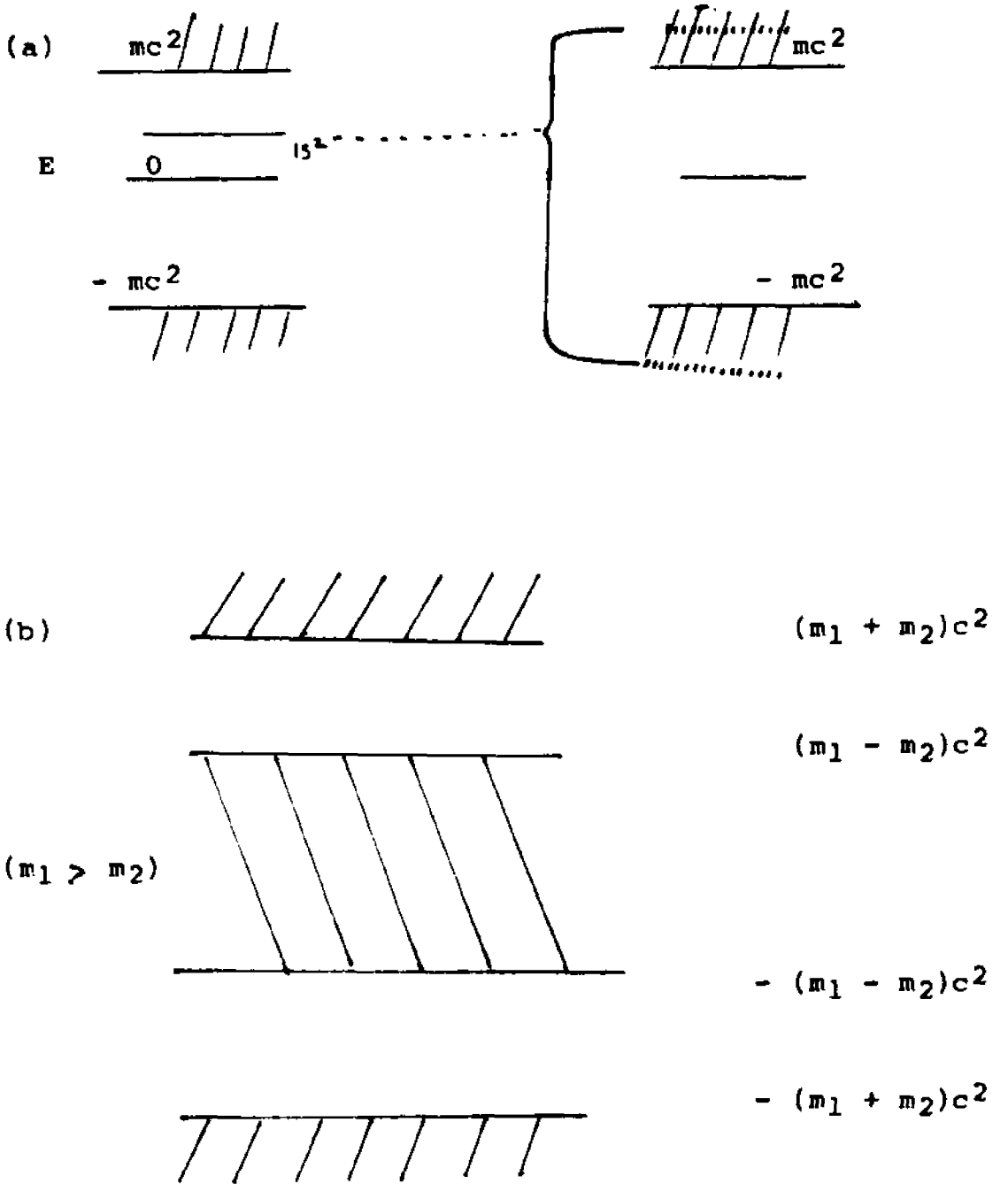


Figure 1. (a) The Brown - Ravenhall disease; a bound state degenerate with an infinite set of continuum states. (b) The continuum energy spectrum (1.2.12); a system that accepts bound states.

Section 1.3 Derivation of configuration space equations.

We review, the reduction from a given non-relativistic Fock space Hamiltonian to configuration space, for bosons interacting via an arbitrary two-body potential, $v(x_{12})$.

The Hamiltonian for the system is given by,

$$H = \int dx\ \psi^{+}(x)\ h(x)\ \psi(x) \ +$$

$$1/2 \int dx_1 \int dx_2\ \psi^{+}(x_1)\psi^{+}(x_2)\ v(x_{12})\ \psi(x_2)\psi(x_1)$$

(1.3.1)

where the $\psi(x)$, $\psi^{+}(x)$ are boson field destruction and creation operators respectively, $h(x)$ is the non-interacting configuration space Hamiltonian. The field operators obey the usual equal time commutation relations

$$\left[\psi(x)\ ,\psi^{+}(x')\right] = \delta(x-x')$$

$$\left[\psi(x)\ ,\psi(x')\right] = 0$$

$$\left[\psi^{+}(x)\ ,\psi^{+}(x')\right] = 0.$$

(1.3.2)

The field operators can be expanded in terms of some complete set of eigenstates $\varphi_n(x)$, of $h(x)$.

$$\psi(x) = \sum a_n \varphi_n(x)$$

$$\psi^\dagger(x) = \sum a_n^\dagger \varphi_n^\dagger(x) \qquad (1.3.2)$$

The a_n, $a_n^\dagger$ are destruction and creation operators satisfying

$$\left[a_n , a_{n'}^\dagger\right] = \delta_{nn'}$$

$$\left[a_n , a_{n'}\right] = 0$$

$$\left[a_n^\dagger , a_{n'}^\dagger\right] = 0. \qquad (1.3.3)$$

The vacuum state $|0\rangle$ is defined such that $a_n|0\rangle = 0$ for all n. The number operator is given by,

$$N = \int dx\ \psi^\dagger(x)\psi(x) = \sum_s a_s^\dagger a_s = \sum_s N_s. \qquad (1.3.4)$$

The operator N_s counts the number of bosons in a given mode s. The total number of bosons N is the sum over the occupation number of all modes.

We now construct a general N-body state $|N\rangle$ by the application of $\psi^{+}(x)$, on the vacuum, and summing over all configurations via an amplitude $\chi(x_1 x_2 \ldots x_n)$, i.e.

$$\Psi_N = \int dx_1\, dx_2 \ldots dx_n\, \chi(x_1 x_2 \ldots x_n)\, \psi^{+}(x_1)\psi^{+}(x_2)\ldots\psi^{+}(x_n)\,|0\rangle\,. \tag{1.3.5}$$

The number operator N commutes with the total Hamiltonian H, therefore $|\Psi_N\rangle$ has the most general form for an N-body eigenstate of H. We get an eigenvalue equation in configuration space by treating χ as a variational parameter[12] below i.e

$$\delta\chi\left\{\langle\Psi_N|H|\Psi_N\rangle - E\langle\Psi_N|\Psi_N\rangle\right\} = 0. \tag{1.3.6}$$

Treating $\delta\chi$ and $\delta\chi^{+}$ as independent variations, the variation $\delta\chi^{+}$ results in the wave equation,

$$\sum_{i=1}^{N} h(i)\,\chi(x_1 x_2 \ldots x_n) + \sum_{i<j} v(x_{ij})\,\chi(x_1 x_2 \ldots x_n) = E\,\chi(x_1 x_2 \ldots x_n) \tag{1.3.7}$$

We now generalize the above procedure in order to get an approximate relativistic cofiguration space eigenvalue equation for electrons interacting via some two-body potential. As a starting point we write down a Fock-space hamiltonian for interacting fermions,

$$H = \int dx \sum_{\alpha\beta} \psi^{\dagger}_{\alpha}(x)\, h^{\alpha}_{\beta}(x)\, \psi^{\beta}(x) +$$

$$1/2 \sum_{\substack{\alpha\beta \\ \mu\nu}} \iint dx_1 dx_2 : \psi^{\dagger}_{\alpha}(x_1)\, \psi^{\dagger}_{\beta}(x_2)\, v^{\alpha\beta}_{\mu\nu}(x_{12})\, \psi^{\mu}(x_2)\, \psi^{\nu}(x_1) : \qquad (1.3.8)$$

The above Hamiltonian is similar to (1.3.1) with the following modifications:

a) The free part H_0 contains a single particle Dirac type configuration space spinor operator $h^{\alpha}_{\beta}(x)$. Unless otherwise specified we shall consider $h^{\alpha}_{\beta}(x)$ to be the Dirac Hamiltonian in a Coulomb field (see appendix A.1.).

b) The wave operators are four component spinors and conjugate spinors that obey anti-commutation relations,

$$\left\{ \psi^{\dagger}_{\alpha}(x) \, , \, \psi^{\beta}(x') \right\} = \delta^{\beta}_{\alpha}(x-x')$$

$$\left\{ \psi^{\dagger}_{\alpha}(x) \, , \, \psi^{\dagger}_{\beta}(x') \right\} = 0$$

$$\left\{ \psi^{\alpha}(x) \, , \, \psi^{\beta}(x') \right\} = 0$$

$$(1.3.9)$$

We have explicitly introduced the spinor components above, as a matter of convenience all spinor components will be implicit unless otherwise stated. We can avoid confusion by treating the $\psi(x)$ as a four component column matrix and $\psi^{\dagger}_{\rho}(x)$ as a row matrix. Products of operators will be positioned such that matrix multiplication is implied i.e., the product $\psi^{\dagger}(x)\,\psi(x)$ will be a scalar since a row matrix multiplies a column matrix from the left, whereas $\psi(x)\,\psi^{\dagger}(x)$ is a 4x4 square matrix (spinor) operator.

We can decompose the wave operators

$$\psi(x) = \sum a_n \varphi_n(x)$$

$$\psi(x) = \sum a_n^{\dagger} \varphi_n^{\dagger}(x) \qquad (1.3.10)$$

where the $\varphi_n(x)$, $\varphi_n(x)$ are eigenspinors of $h(x)$ and $h^{\dagger}(x)$ respectively. The $a_n^{\dagger}$, a_n obey anticommutation $\{a_n, a_n\} = 1$, relations, (all other anticommutators vanish). The a_n, $a_n^{\dagger}$, have the usual interpretation of destruction and creation operators. We can define the vacuum again as $a_n|0\rangle = 0$. With this choice of the vacuum $N_s = a_s^{\dagger} a_s$ is again the number operator for the mode s. Using (1.1.10) the zero order Hamiltonian becomes,

$$H_0 = \sum_{n}^{(+)} |E_n| a_n^+ a_n - \sum_{n}^{(-)} |E_n| a_n^+ a_n$$

(1.3.11)

the sum $\sum^{(-)}$ is over the negative energy eigenvalues, of h(x) and $\sum^{(+)}$ the sum over positive eigenvalues. It is at once obvious that the free Hamiltonian H_0 is not bounded from below. For free particles experiencing an external pertubation this would be a catasthrophe since the pertubation would induce transitions into a bottomless pit i.e. the system would be unstable. Dirac was able to rectify this problem for the quantum mechanical single particle theory, by requiring all negative energy states to be filled. The Pauli principle prevents the positive energy particles from falling into the filled negative energy sea therefore making the system stable. Of course, now one no longer has a single particle theory. Second quantinization of the Dirac equation provides a convenient framework for Dirac's prescription, since we are now dealing with an intrinsic many-body theory. In fact a simple redefinition of the Fock space vacuum is sufficient to construct a theory that does not suffer from the above mentioned difficulties.

Let us first decompose,the fields

$$\psi(x) = \sum^{(+)} b_n \varphi_n(x) + \sum^{(-)} a_n^+ \varphi_n(x)$$

$$\psi(x) = \sum^{(+)} \varphi_n^+(x) b_n^+ + \sum^{(-)} \varphi_n^+(x) a_n$$

(1.3.12)

where

$$\{a_n^\dagger, a_{n'}\} = \delta_{nn'} \quad , \quad \{b_n^\dagger , b_{n'}\} = \delta_{nn'},$$

(1.3.13)

all other commutators vanish.

We define the vacuum by requiring $b_n|0\rangle = 0$,and $a_n|0\rangle = 0$ for all n. The decomposition (1.3.12) will give for H_0.

$$H_0 = \sum_n^{(+)} |E_n| b_n^\dagger b_n + \sum_n^{(-)} |E_n| a_n^\dagger a_n - \sum_n^{(-)} |E_n|$$

(1.3.14)

This form for H_0 contains an infinite c-number term which can be eliminated by a redefinition of the vacuum. In the above definition of the vacuum the $N_n^{e^-} = b_n^\dagger b_n$, and $N_s^{e^+} = a_s^\dagger a_s$, are number operators for particles occupying the mode n, and for antiparticles occupying the mode s. Both the particles and antiparticles have a positive energy spectrum thus H_0 is now bounded from below by the vacuum, i.e. the state with no particles or antiparticles. The number operator for fermions is the sum over all the N_n^{e-} for particles(electrons) and the N_s^{e+} for antiparticles(positrons) i.e.

$$N = \sum_{n}^{(+)} N_n^{e-} + \sum_{s}^{(-)} N_s^{e+}.$$

(1.3.15)

In the Heisenberg picture, equations of motion for $\psi(x,t)$ and the conjugate field $\psi^{\dagger}(x,t)$ give the conservation law,

$$d/dt\left(|e|\ (\psi^{\dagger}(x,t)\psi(x,t)\right) = |e|\bar{\nabla}\cdot(\ \psi^{\dagger}(x,t)\bar{\alpha}\,\psi(x,t)).$$

(1.3.16)

This is the usual charge-current conservation law where, $Q = -|e|\int dx\ \psi^{\dagger}(x)\psi(x)$ is the total charge of the system. Using the decomposition (1.3.12) we get,

$$Q = -|e|\sum_{n}^{(+)} N_n^{e-} + |e|\sum_{s}^{(-)} N_s^{e+}$$

(1.3.17)

The total charge being the sum of the electron charge ,and the positron charge. The spectrum of Q is

$q = (0, \pm 1, \pm 2, \ldots \pm n)\,|e|$.

For the above system $[Q,H] = 0$, but $[H,N] \neq 0$, therefore an eigenstate of H can have a definite charge, but it is meaningless to say that this state has a definite number of fermions. The noncommutivity of N with H is of course due to the fact that the interaction term in H can can create or destroy fermion (electron-positron) pairs. We must express the eigenstate Ψ_N with charge $q = -|e|N^{e-}$,(non relativistically we would call this an N-electron system) as,

$$|\Psi_N\rangle = |\Psi_0\rangle + |\Psi_1\rangle + |\Psi_2\rangle + \ldots \tag{1.3.18}$$

where $|\Psi_0\rangle$ contains N electrons, $|\Psi_1\rangle$ contains N electrons plus a pair, $|\Psi_2\rangle$ contains N electrons plus two pairs etc. The configuration space expansion of the above kets will require the introduction of an infinite set of amplitudes $\chi^i(x_1x_2\ldots,x_1',x_2'\ldots)$ (in reality χ is a multidimensional spinor that transforms as a direct product of single particle spinors; spin indices will be implicit in our discussion) defined by

$$\Psi_0 = \int dx_1 dx_2 \ldots dx_n$$

$$\psi(x_1)\psi(x_2)\ldots\psi(x_n)\ \chi^0(x_1,x_2\ldots x_n)\ |0\rangle$$

$$\Psi_1 = \int dx_1 dx_2 \ldots dx_n \int dx_1' dx_2'$$

$$\psi^+(x_1)\psi^+(x_2)\ldots\psi^+(x_n)\ \psi(x_1')\psi^+(x_2')\ \chi(x_1,x_2\ldots x_n,x_1'x_2')$$

$$+ \text{ etc.} \tag{1.3.19}$$

The amplitudes χ^i would obey an infinite set of coupled non-linear equations for the eigenvalue E if a complete solution of $H|E\rangle = E\,|E\rangle$ is sought. Instead we shall truncate the series (1.3.19) to the first term treating χ^0 as a variational parameter as was done in

equation (1.3.6) for the non-relativistic case. The above approximation is reasonable since physicaly it would give all the effects where pairs are not present, we will call this the no-pair approximation.

Using the no pair ansatz above we can get a configuration space equation, by considering an arbitrary variation of χ° below.

$$\delta_{\chi^{\circ}}\{\langle\Psi|H|\Psi\rangle - E\langle\Psi|\Psi\rangle\} = 0 . \qquad (1.3.20)$$

Contracting the fermion operators, we get

$$\delta_{\chi^{\circ}}\Big\{\int dx_1'\ldots dx_n' \int dx_1 \ldots dx_n \; 2\,\chi^{\dagger}(x_1'\ldots x_n')$$

$$\sum_i \int dx \Lambda_+(x_i', x) h(x) \Lambda_+(x, x_i) + \sum_{i<j} \int dz_1 \int dz_2 \times$$

$$\Lambda_+(x_i', z_1)\Lambda_+(x_j', z_2) V(z_{12}) \Lambda_+(z_2, x_j)\Lambda_+(z_1, x_i)$$

$$- E\Lambda_+(x_1', x_1) \ldots \Lambda_+(x_n', x_n)\Big]\chi(x_1\ldots x_n)\Big\} = 0$$

$$(1.3.21)$$

where the positive energy projection operators are given by

$$\Lambda_+(x,x') = \langle 0|\psi(x)\psi^+(x')|0\rangle = \sum_s^{(+)} \varphi_s(x)\varphi_s^+(x')$$

(1.3.22)

Carrying out the variation we get,

$$\left(\sum_i^N \Lambda_+(i)h(i) + \sum_{i<j} \Lambda_+(i)\Lambda_+(j)V(i,j)\Lambda_+(j)\Lambda_+(i)\right) x$$

$$\omega(x_1\ldots x_n) = E\,\omega(x_1\ldots x_n)$$

(1.3.23)

where the function ω is defined by,

$$\omega(x_1,\ldots x_n,) =$$

$$\int dx_1 \ldots dx_n \Lambda_+(x_1',x_1)\ldots \Lambda_+(x_n',x_n)\,\chi(x_1\ldots x_n),$$

(1.3.24)

and where we have used the shorthand notation,

$$\Lambda_+(i)f(i) = \int dx_i' \Lambda_+(x_i,x_i')f(x_i').$$

(1.3.25)

As was mentioned in section 1.2, the presence of the projection operators prevents the onset of the Brown Ravenhall disease, however as shown above, these need not be put in by"hand", but fall naturally out of the formalism if the correct reduction from QED to

configuration space is made. One may go beyond the no pair approximation by performing a unitary transformation H $H' = U H U^{+}$, such that H' is approximately diagonal with respect to the electron number operator N^{e-} within the required degree of approximation. Such a transformation will introduce new higher order electron interaction terms that contain energy denominators of propagating virtual pairs. However, these energy denominators will never vanish. Therefore even when one goes beyond the no pair approximation the resulting wave equation will never suffer from the Brown Ravenhall malady.

Chapter 2

Having sketched the outline for constructing relativistic configuration space equations compatible with hole theory, we now proceed to apply this method for the QED Hamiltonian. In order to get the QED Hamiltonian into a form similar to (1.3.1), one must decouple the radiation and matter fields. This can be achieved, approximately, by a unitary transformation on the QED Hamiltonian. When the transition to configuration space is made,two and three-body potentials arise. A comprehensive review of this procedure is given. Essentialy this chapter is a review of the papers by Mittleman[6]. Section 2.1, deals mainly with two body potentials, while three body potentials are discussed in section 2.2.

Section 2.1 The Schwinger transformation

The QED Hamiltonian in the coulomb gauge is given by,

$$H_{qed} = H_0^R + H_0^M + H_C + H_I \qquad (2.1.1)$$

where H_0^R , H_0^M are the non-interacting Hamiltonians for transverse photons, and fermions(electrons, positrons) respectively. H_C is the Coulomb interaction term given by,

$$H_C = 1/2 \iint dx_1 dx_2 : \psi^{\dagger}(x_1)\psi^{\dagger}(x_2)\ e^2/x_{12}\psi(x_2)\psi(x_1): \qquad (2.1.2)$$

(from now on we will denote e^2/x_{12} by $V_C(x_{12})$). H_I is the fermion-transverse photon interaction term given by

$$H_I = -\int dx\ \bar{J}(x)\cdot\bar{A}(x)$$

where,

$$\bar{J}(x) = e: \psi(x)\bar{\alpha}\ \psi(x): \ . \qquad (2.1.3)$$

The equal time anticommutation relations for the fermion fields $\psi, \psi^{\dagger}$ have been given by (1.3.9).The Hermitian photon field obeys the transversality condition $\bar{\nabla}.\bar{A} = 0$. We decompose the photon field in a plane wave representation,

$$A(x) = \sqrt{2c/Vk} \sum_{\kappa,\lambda} \left(a^{\dagger}_{k\lambda} \epsilon_{\lambda} e^{i\bar{k}\cdot\bar{x}} + a_{k\lambda} \epsilon_{\lambda} e^{-i\bar{k}\cdot\bar{x}} \right)$$

$$(k \equiv |\bar{k}|),$$

(2.1.4)

where the $a_{k',\lambda'}$ $a_{k\lambda}$ obey commutation relations,

$$\left[a_{k\lambda}, a^{\dagger}_{k',\lambda'} \right] = \delta(k,k')$$

$$\left[a_{k\lambda}, a_{k',\lambda'} \right] = 0$$

$$\left[a^{\dagger}_{k\lambda}, a^{\dagger}_{k',\lambda'} \right] = 0.$$

(2.1.5)

the photon vacuum is defined by $a_{k\lambda}|0\rangle = 0$ for all k, and λ . The $a^{\dagger}_{k\lambda}$, $a_{k\lambda}$ are creation and destruction operators for photons with wave numbers k and polarization λ . The H_0^M term has been discussed in the previous chapter, we noted that H_0^M is diagonal in the number representation of electrons and positrons. Similarly H_0^R is diagonal in the number representation of photons. Consider an eigenstate of $H_0 = H_0^M + H_0^R$, i.e a state with a definite number of electrons and photons, slowly turning on the Coulomb and photon

interaction terms, a cloud of photons and electron-positron pairs will "dress" this zero order eigenstate due to the virtual processes induced by H_I + H_C . We can no longer claim that the dressed state contains a definite number of photons and electrons.

The Schwinger unitary transformation,[16] $H \rightarrow H' = e^{i\sigma} H e^{-i\sigma}$ where the generator, σ is given by,

$$\sigma = -1/2 \int_{-\infty}^{\infty} d\tau \, \epsilon(\tau) \, e^{iH_0\tau} \, H_I \, e^{-iH_0\tau}$$

$$\epsilon(\tau) \equiv \theta(\tau) - \theta(-\tau)$$

(2.1.6)

explicitly illustrates the effects of the dressing due to virtual photon processes induced by H_I. Let us consider the Schwinger transformation in more detail. We have ,

$$\sigma = -1/2 \int_{-\infty}^{\infty} d\tau \int dx \, \epsilon(\tau) \, J_a(x,\tau) \, A_a(x,\tau) \, e^{-\eta|\tau|}$$

$$J_a(x,\tau) = eiH\tau \, J_a(x) \, e^{-iH\tau} \quad ,$$

$$A_a(x,\tau) = e^{iH\tau} \, A_a(x) \, e^{-iH\tau} \quad .$$

(2.1.7)

$e^{-\eta|\tau|}$ is a convergence factor, $\lim \eta \rightarrow 0$ is implied after all integrations are done. The repeated spatial index a is implicitly assumed to be summed over all it's values.

Using the relation $e^{i\sigma} O\, e^{-i\sigma} = \sum_n i^n/n!\, C_n[\sigma, O]$ where the C_n are repeated commutators i.e $C_0=1$, $C_1=[\sigma,O]$, $C_2 = [\sigma, [\sigma, O]]$ etc. we get,

$$H' = \sum_n i^n/n! \left(C_n[\sigma, H_0] + C_n[\sigma, H_I] + C_n[\sigma, H_C] \right)$$

$$= H_0 + i[\sigma, H_0] + i^2/2! [\sigma, [\sigma, H_0]]$$

$$+ H_I + H_C + i[\sigma, H_I] + O(e^3) + \ldots$$

(2.1.8)

We have truncated the infinite series to include terms that are only first order in the parameter e^2.

Let us evaluate the commutator $i[\sigma, H_0]$, by noting,

$$i[\sigma, H_0] = 1/2 \int d\tau\, \epsilon(\tau) \frac{\partial}{\partial \tau} \left(e^{iH_0\tau} H_I\, e^{-iH_0\tau} \right) e^{-\eta|\tau|}$$

(2.1.9)

Integrating by parts, we get,

$$-1/2 \int_{-\infty}^{\infty} d\tau \left(\frac{\partial \epsilon(\tau)}{\partial \tau} \right) H_I(\tau)\, e^{-\eta|\tau|} +$$

$$-1/2 \int_{-\infty}^{\infty} d\tau\, \epsilon(\tau)\, H_I(\tau) \frac{\partial}{\partial \tau} e^{-\eta|\tau|}$$

(2.1.10)

using $\frac{\partial}{\partial \tau}\epsilon(\tau) = 2\delta(\tau)$ and $\frac{\partial}{\partial \tau} e^{-\eta|\tau|} = -\eta\, e^{-\eta|\tau|} \epsilon(\tau)$ we have,

$$i\left[\sigma, H_0\right] = - H_I + \lim_{\eta \to 0} (1/2)\eta \int_{-\infty}^{\infty} d\tau\, H_I(\tau)\, e^{-\eta|\tau|}.$$

(2.1.11)

In the second term above, the limit $\eta \to 0$ will force this term to vanish unless the time integral is proportional to $1/\eta$. However this only occurs for the energy on-shell matrix elements, i.e. real photon transitions. Since we are interested in only virtual photon exchange processes, we can neglect this term in our discussion. Hence,

$$i\left[\sigma, H_0\right] = - H_I. \qquad (2.1.12)$$

Inserting (2.1.12) into our expansion (2.1.8) we get,

$$H' = H_0 + i/2\left[\sigma, H_I\right] + H_C + O(e^3) + \ldots$$

(2.1.13)

We can think of H' as an order e^2 approximation to H. Furthermore, the above expression is diagonal with respect to the photon number representation. The effects due to the exchange of virtual photons manifest themselves in the term $i/2\left[\sigma, H_I\right]$. This term is a sum of two-body and one-body operators in the Fock-space fermion sector. The one-body terms are due to processes where a fermion can emit and

absorb its own photon, these terms must be treated with care via a renormalization program, in order to eliminate unwanted infinite contributions. We shall collectively call all the one-body contributions(both finite and infinite) as self-energy terms. The two-body terms describe processes where different fermions interchange virtual photons. For a general N-fermion system the total two-body contribution to the energy will be proportional to the sum of all possible pairs i.e. $E \sim N^2$; while the one-body contribution could be expected to scale like N. Thus for an atomic system where the number of electrons is on the order of $N \sim 100$, we expect the total two-body energy to be considerably larger than the self-energy corrections. Furthermore, rudimentary evaluation[17] for the non-relativistic self-energy corrections of atomic electrons show that the contribution is proportional to the atomic wave function at the origin, therefore we expect only a few low lying electronic states to give any appreciable self energy correction. For the above reasons we will neglect the one-body parts of H' and concentrate only on the two-body parts of H'. We must mention that the above arguments are no longer valid when we are dealing with highly-ionized high-Z ions, indeed calculations have shown that the self-energy corrections become comparable to the two-body Breit energy for such systems[18]

Let us now expand the commutator

$$i/2\ \left[\sigma, H_I\right] = H_B =$$

$$-\ i/4\ \iint dx\ dx' \int d\tau\, \epsilon(\tau)$$

$$e^{-\eta|\tau|} J_a(x,\tau) J_b(x',\tau)\ \left[A_a(x,\tau), A_b(x',0)\right].$$

(2.1.14)

We have neglected current cummutator terms since these give the aformentioned one-body terms.
The commutator for the photon field is a c-number[19] given by,

$$\left[A_a(x,t), A_b(x',t')\right] = D_{ab}(x-x',t-t')$$

$$-4\pi c\ i/(2\pi)^3 \int d^3k\ /k\ \ e^{i\bar{k}\cdot(\bar{x}-\bar{x}')} \sin ck(t-t')\ (\delta_{ab} - \hat{k}_a\hat{k}_b)$$

where $k = |\bar{k}|$. (2.1.15)

In order to get a configuration space representation for the current operator $\bar{J}(x,t)$ we use the expansion (1.3.12) for the fermion fields, $\psi^{+}(x)$ $\psi(x)$, in terms of the Dirac- Coulomb wave functions $\varphi_n(x)$.

Note: from now on we use a shorthand notation for the electron, positron operators, $b_n = b_n$ when $E_n > 0$, $b_n = a_n$ when $E_n < 0$. Also, $b_n^+ = b_n^+$ when $E_n > 0$, $b_n^+ = a_n$ when $E_n < 0$, see (1.3.2).

Using the above expansion the current operator can be expressed as,

$$J^a(x,t) = \sum_{nn'} b_n^+ b_{n'} e^{iW_{nn'}t} J^a_{nn'}(x),$$

where we define,

$$J^a_{nn'}(x) = \varphi_n(x) \alpha^a \varphi_{n'}(x) \quad , W_{nn'} = E_n - E_{n'}. \tag{2.1.16}$$

The above derivation made use of the identity,

$$\psi(x,t) = e^{iH_0 t} \psi(x) e^{-iH_0 t} = \sum_n b_n e^{-iE_n t} \varphi_n(x) \tag{2.1.17}$$

Alternatively we can express the time dependent current operator in a more convenient form, as

$$J^a(x,t) = :(\psi^+(x) e^{ih(x)t}) \alpha^a (e^{-ih(x)t} \psi(x)): \tag{2.1.18}$$

where h(x) is the single particle configuration space

Hamiltonian for a central field (Coulomb). The brackets allow the $e^{ih(x)t}$, $e^{-ih(x)t}$ to operate only on the $\psi^{\dagger}(x)$, and $\psi(x)$ fields to the left and right respectively. The equivalence between the two expressions (2.1.16) and (2.1.18) can be proved by expanding the exponential operators in (2.1.18) and using the Dirac equation to express the resulting series in powers of the single particle energies. Inserting (2.1.18) and (2.1.15) into (2.1.14) we get for H_B,

$$H_B = 1/2 \int dx_1 \int dx_2 : \psi(x_1)\psi(x_2)\ \tilde{B}\ (x_{12})\ \psi(x_2)\psi(x_1) :$$

where the kernel,

$$\tilde{B}\ (x_{12}) = -ie^2/4 \int_{-\infty}^{\infty} d\tau \epsilon(\tau)\ e^{ih(1)\tau} \alpha_1^a\ D_{ab}(12)\ \alpha_2^b\ e^{-ih(1)\tau}$$

$$+ \ (\ 1 \leftrightarrow 2\ ). \qquad (2.1.19)$$

The numerals 1,2 are shorthand for the spatial coordinates of the fermions. The second term in the above expression represents the symmetrization of the kernel with respect to the particle coordinates.

The above form for H_B is similar to the usual two-body potential operator, i.e (2.1.2) in Fock-space, with the difference that the kernel of the interaction $\tilde{B}(1,2)$ is

now a non-local operator in configuration space rather than the typical multiplicative operator V(1,2). The transition to configuration space is now carried out in an identical manner to that described in the last chapter.

Using the no-pair approximation for H and repeating steps (1.3.20) through (1.3.23) we have a configuration space equation for an N-electron atomic system given by

$$\left\{ \sum_{i}^{N} \Lambda_{+}(i) \;\; h(i)\omega(x_1, x_2, \ldots x_n) + \right.$$

$$\left. \Lambda_{+}(i)\, \Lambda_{+}(j)\, (\, V_C(i,j) + B(i,j))\, \Lambda_{+}(j)\, \Lambda_{+}(i) - E \right\} *$$

$$\omega(x_1, x_2 .. x_n) = 0.$$

(2.1.20)

V_C is the ordinary Coulomb repulsion term while, B(i,j) is a non-local two body potential due to the exchange of transverse photons among the electrons.

It is more convenient to express the potential operator (2.1.19) in the occupation representation. Using the representation (2.1.16) for the current operator in (2.1.14),
we get,

$$H_B = 1/2 \sum_{\substack{nm \\ n'm'}} b_n^+ b_m^+ b_{m'} b_{n'} \left(\eta_{nm,n'm'} + \eta_{mn,m'n'} \right)$$

where,

$$\eta_{nm,n'm'} = -ie^2/4 \int_{-\infty}^{\infty} d\tau \epsilon(\tau) \int dx_1 \int dx_2 \cdot$$

$$\left\{ \varphi_n^+(x_1) \varphi_m^+(x_2) \; e^{iW_{nn'}\tau} \alpha_1^a \; D_{ab}(r,\tau) \alpha_2^b \; \varphi_{n'}(x_1) \varphi_{m'}(x_2) \right\}$$

(2.1.21)

Expressing the photon commutator $D_{ab}(r,\tau)$ given in (2.1.15) by the transform,

$$D_{ab}(r, \;) = \frac{c}{\pi} \left(\nabla^2 \delta ab + \nabla_1^a \nabla_2^b \right) 1/r \int_{-\infty}^{\infty} dk/k^2 \; e^{ikr} \; \sin(ck\tau)$$

where, $r = |x_1 - x_2|$

(2.1.22)

and performing the temporal integral,

$$\int_{-\infty}^{\infty} dt \; \epsilon(t) \; \sin(ckt) \; e^{iW_{nn'}t} e^{-\eta|t|} =$$

$$P/(ck + W_{nn'}) + P/(ck - W_{nn'})$$

(P represents the principal value of the denominators),

(2.1.23)

we have,

$$\eta_{nm,n'm'} = -ie^2/2 \langle n\ m | \{ \alpha_1^a \alpha_2^b (\delta_{ab} + \nabla_1^a \nabla_1^b) c^2/\hbar r \times$$

$$P \int_{-\infty}^{\infty} dk/k\ e^{ikr}\ 1/(ck + W_{nn'})(ck - W_{nn'}) \} | n'\ m' \rangle .$$

(2.1.24)

We evaluate the integral over k to get,

$$\eta_{nm,n'm'} = -e^2/4 \langle n\ m |\ \alpha_1^a\ \alpha_2^b \{ (\nabla^2 \delta_{ab} + \nabla_a' \nabla_b^1)\ \times$$

$$r((2hc/W_{nn'}r)\sin(W_{nn'}r/2hc))^2 \} | n'm' \rangle$$

($\hbar$ is the Planck constant) (2.1.25)

We can define a nonrelativistic limit by setting the quotient $(W_{nn'}r/hc) \ll 1$, (to be more precise, we mean that the expectation value of this operator is small). This limit is realized for low Z atoms, and for positive energy states where the electron velocity $v/c \sim (Z\alpha) \ll 1$. In this limit we can replace the $\sin^2$ term in (2.1.25) by $(W_{nn'}r/2hc)^2$. The matrix element

$\eta_{nm,n'm'}$ then becomes,

$$\eta_{nm,n'm'} = -\ e^2/4r\ (\ \bar{\alpha}_1 \cdot \bar{\alpha}_2\ +\ \bar{\alpha}_1 \cdot \hat{r}_{12}\ \bar{\alpha}_2 \cdot \hat{r}_{12}\ )$$

(2.1.26)

Using the above expression and the corresponding term for $\eta_{nm,n'm'}$, the non - local operator $\tilde{B}(1,2)$ becomes the familiar Breit operator discussed in chapter 1.

An alternative expression for $\eta_{nm,n'm'}$ is obtained by integrating (2.1.25) by parts and then making use of the Dirac equation to get,

$$\eta_{nm,n'm'} = -e^2/2 \langle n\ m \mid \alpha_1 \cdot \alpha_2 \ \cos(W_{nn'} r/\hbar c)/r + W_{mm'}/W_{nn'} \ (1 - \cos(W_{nn'} r/\hbar c))/r \mid n'\ m' \rangle \qquad (2.1.27)$$

In this form $\eta_{nm,n'm'}$ can easily be expressed in terms of two dimensional radial integrals. (see appendix A.3.)

Section 2.2 Three body potentials

We now proceed to construct the three particle potentials by looking beyond the e^2 terms in the expansion (2.1.8). The next terms will be $O(e^3)$, these will be off-diagonal in the photon number, and contribute only to $O(e^6)$ diagonal terms. Some of the e^4 terms will be on diagonal in the photon representation. They are given by,

$$H_{C-T} = -1/2 \left[\sigma, \left[\sigma, H_C\right]\right],$$

and

$$H_{T-T} = -i/8 \left[\sigma, \left[\sigma, \left[\sigma, H_I\right]\right]\right] .$$

(2.2.1)

The subscripts C-T, T-T, refer to " Coulomb - transverse", and " transverse - transverse " parts respectively. This terminology is indictive of the fact that the first part of (2.2.1) describes processes where a virtual Coulomb photon, and transverse photon is exchanged; while in the latter, two transverse photons are exchanged. Concentrating on the H_{C-T} terms first, let us expand the commutator in (2.2.1),

$$H_{C-T} = -1/8 \int_{-\infty}^{\infty} d\tau_1 \epsilon(\tau_1) \int_{-\infty}^{\infty} d\tau_2 \epsilon(\tau_2) \quad J(1) \left[J(2), H_C\right]\left[A(1), A(2)\right]$$

$$+ \text{ (two, one - body terms).} \qquad (2.2.2)$$

All indices and coordinates are implicitly represented by the numerals one, and two. The neglected one and two-body fermion operators correspond to e^4 two, one body potentials, and renormalization terms. We shall ignore these terms and concentrate only on the three - body operators. We expand the fermion commutator, and keep only the resulting two body operator. We get

$$\left[J(x_2, \tau_2), H_C\right] = e^3 \int dx_4 \; \psi^{+}(x_2 \tau_2) \bar{\alpha}_2 \psi(x_4) \left(e^{-ih(2)\tau_2} \; V_C(2,4) \right.$$

$$\left. \psi(x_4)\psi(x_2)\right)$$

$$+ \left(\psi^{+}(x_2)\psi^{+}(x_4) \; V_C(2,4) \; e^{ih(2)\tau_2}\right)\psi(x_4)\bar{\alpha}_2\psi(x_2 \tau_2)$$

$$(2.2.3)$$

where we have used the commutation relations (1.3.9), and (2.1.18). Inserting the above expression into (2.2.1), and putting the resulting three fermion operator into normal ordering, we get,

$$H_{C-T} = 1/6 \int dx_1 \int dx_2 \int dx_3$$

$$: \psi^{+}(x_1)\psi^{+}(x_2)\psi^{+}(x_3) \; \Delta_{C-T}(1,2,3) \; \psi(x_3)\psi(x_2)\psi(x_1) :$$

where,

$$\Delta_{C-T}(1,2,3) = -e^4/8 \int_{-\infty}^{\infty} d\tau_1 \epsilon(\tau_1) \int_{-\infty}^{\infty} d\tau_2 \epsilon(\tau_2)\ e^{ih(1)\tau_1} e^{ih(2)\tau_2}$$

$$\propto {}^{a}_{1} D^{ab}(1,2) \propto {}^{b}_{2}\ e^{-ih(1)\tau_1} e^{-ih(2)\tau_2} V_C(2,3)\ \ e^{-\eta(|\tau_1|+|\tau_2|)}$$

$$+ \text{H.c.} + (\text{all permutations of coordinates}) \qquad (2.2.4)$$

The above expression is not very enlightening, therefore as was done for the non-local Breit operator (1.1.19) we express the above kernel in the occupation representation. Expanding the wave operators in the occupation representation we have,

$$H_{C-T} = \sum b_n^{\dagger} b_l^{\dagger} b_m^{\dagger} b_{m'} b_{l'} b_{n'} \quad V^{C-T}_{nml,n'm'l'} \quad + H.c.$$

where,

$$V^{C-T} = \langle n\ m\ l | \Delta_{C-T} | n'\ m'\ l' \rangle =$$

$$-e^4/8 \quad \int dx_1 \int dx_2 \Big\{ \varphi_n^{\dagger}(x_1) \varphi_l^{\dagger}(x_2) \sum_s$$

$$\int_{-\infty}^{\infty} d\tau_i \, \epsilon(\tau_i) \int_{-\infty}^{\infty} d\tau_k \, \epsilon(\tau_k) \; e^{ih(1)\tau_i} \, e^{ih(2)\tau_k} \, \alpha_1^a D(x_{12}, \tau_i - \tau_k) \alpha_2^b$$

$$e^{-ih(1)\tau_i} \, e^{-ih(2)\tau_k} \quad \varphi_n(x_1) \, \varphi_s(x_2)$$

$$\int dx_3 \int dx_4 \, \varphi_s^{\dagger}(x_4) \, \varphi_m^{\dagger}(x_3) V_C(3,4) \, \varphi_{l'}(x_4) \varphi_{m'}(x_3)$$

(2.2.5)

where we have used the completeness property, $\sum_s \varphi_s(x_2) \, \varphi_s(x_4) = \delta(x_2 - x_4)$. After operating the exponential factors on the surrounding spinors we evaluate the time integrals,

$$\int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \; \epsilon(t_1)\, \epsilon(t_2)\, e^{iW_{nn'} t_1}\, e^{iW_{ls}\, t_2} \operatorname{sinc}k(t_1 - t_2)$$

$$= 4ick \left(W_{nn'}, -W_{ls}\right) P\left[1/(ck+W_{nn'})(ck-W_{ls})(ck-W_{nn'})(ck+W_{ls})\right] .$$

(2.2.6)

Rearranging the above fraction, and inserting into (2.2.25) we get,

$$V^{C-T}_{nlm,n'l'm'} = -e^2/8 \quad \langle n\ l | \propto_1^a \propto_2^b$$

$$4ic^2/\ (W_{nn'} + W_{ll'})(\nabla^2 \delta_{ab} + \nabla_1^a \nabla_2^b) \Big\{ 1/r\ P \int_{-\infty}^{\infty} dk/k$$

$$e^{ikr}\left[1/(ck+W_{nn'})(ck-W_{nn'}) - 1/(ck+W_{ls})(ck-W_{ls})\right]\Big\} | n's \rangle \ \times$$

$$\langle s\ m \mid V_C(3,4) \mid 1'\ m' \rangle .$$

(2.2.7)

Comparing the above k - integration with the corresponding integral in (2.1.23) we get,

$$V^{C-T}_{nlm,n'l'm'} =$$

$$\sum_s \left[(\ \eta_{nl,n's} - \eta_{ln,s'n'})/(W_{nn'} + W_{ls}) \right] C_{sm,l'm'}$$

where the η matrix elements were defined in (2.1.25), and

$$C_{sm,l'm'} \equiv \langle s\ m | V_C(1,2) | 1'\ m' \rangle .$$

(2.2.8)

Let us now turn our attention toward the transverse-transverse three body potentials contained in H_{T-T}. Expanding the multiple commutators we have,

$$-i/64 \int_{-\infty}^{\infty}\int\int d\tau_1\epsilon(\ )\,d\tau_2\epsilon(\ )\,d\tau_3\epsilon(\ )\ e^{-\eta(|\tau_1|+|\tau_2|+|\tau_3|)}$$

$$\Big[J(1)A(1),\ \Big[\,J(2)A(2),\ \Big[J(3)A(3),J(4)A(4)\Big]\Big]\Big]\ .$$

(2.2.9)

Where again all spatial indices and integrations are implicit. The index 4 does not have a time coordinate. We are only interested in the terms that give us the three-fermion operators. After some commutator algebra we get,

$$H_{T-T} = -i/64 \int_{-\infty}^{\infty} d\tau_1\epsilon(\tau_1)\ \ldots\ \times$$

$$\Big(3\ J(1)J(2)\Big[J(3),J(4)\Big]\ +\ J(3)J(4)\Big[J(1),J(2)\Big]\Big)\,D(2,3)\ D(1,4).$$

(2.2.10)

Evaluating the current-current commutators we can rewrite the above,

$$H_{T-T} = 1/6 \int dx_1 \int dx_2 \int dx_3$$

$$:\psi^{\dagger}(x_1)\psi^{\dagger}(x_2)\psi^{\dagger}(x_3)\,\Delta_{T-T}(123)\;\psi(x_3)\psi(x_2)\psi(x_1):$$

$$+ \text{H.c.} + (\text{ all permutations of coordinates})$$

(2.2.11)

where,

$$\Delta_{T-T}(123) = -ie^4/64 \int_{-\infty}^{\infty} d\tau_1 \epsilon(\tau_1) \int_{-\infty}^{\infty} d\tau_2 \epsilon(\tau_2) \int_{-\infty}^{\infty} d\tau_3 \epsilon(\tau_3)\; e^{-\eta(|x_1|+\ldots)}$$

$$\left(e^{ih(1)\tau_1}\, e^{ih(2)\tau_2} \propto_1^a D_{ab}(x_{12}, \tau_1 - \tau_2) \propto_2^b e^{-ih(1)\tau_1} e^{-ih(2)\tau_2}\right) \times$$

$$\left(3\; e^{ih(3)\tau_3} \propto_2^c D_{cd}(x_{23}, \tau_3) \propto_3^d e^{-ih(3)\tau_3}\right.$$

$$\left. + e^{ih(2)\tau_3} \propto_2^c D_{cd}(x_{23}, \tau_3) \propto_3^d e^{-ih(2)\tau_3}.\right.$$

(2.2.12)

Again, as with the H_{C-T} term we can express H_{T-T} in the occupation number representation. Proceeding in the same manner as above we have,

$$H_{T-T} = \sum b^{\dagger}_{n} b^{\dagger}_{l} b^{\dagger}_{m} b_{m'} b_{l'} b_{n'} \; V^{T-T}_{nlm,n'l'm'} + H.c$$

where,

$$V^{T-T}_{nlm,n'l'm'} = -ie^4/64 \int_{-\infty}^{\infty} d\tau_i \epsilon(\tau_i) \int_{-\infty}^{\infty} d\tau_l \epsilon(\tau_l) \int_{-\infty}^{\infty} d\tau_j \epsilon(\tau_j) \sum_{s}$$

$$\langle n\ l \mid e^{iW_{nn'}\tau_i}\ e^{iW_{ls}\tau_l}\ (\alpha^{a}_{1} D_{ab}(x_{12}, \tau_i - \tau_l) \alpha^{b}_{2}) \mid n'\ s \rangle$$

$$\langle s\ m \mid (3\ e^{iW_{mm'}\tau_j} + e^{iW_{se'}\tau_j}\ (\alpha^{c}_{3} D_{cd}(x_{34}, \tau_j) \alpha^{d}_{4}) \mid l'\ m' \rangle .$$

(2.2.13)

By now these integrals certainly look familiar. The integral over $\tau_i - \tau_l$ is of the same type encountered in the V^{C-T} matrix elements, while the integral over τ_j is of the same genre as in (2.1.24). Borrowing previous results we get a compact expression,

$$V^{T-T}_{nlm,n'l'm'} = -1/2 \sum_{s}\ (\eta_{nl,n's} - \eta_{ln,sn})/(W_{nn'} + W_{ls})$$

$$(3\ \eta_{ms,m'l'} + \eta_{sm,lm'})$$

(2.2.14)

Up to now the Schwinger transformation was employed to diagonalize the QED Hamiltonian to $O(e^4)$ with respect to the photon number. The resulting two particle operator in Fock space then became a two particle potential in configuration space when the no pair ansatz was used in the variational equation (1.3.20). It was pointed out in chapter 1, that the no pair ansatz suffers from the deficiency that it does not allow electron - positron pair effects to manifest themselves in configuration space. We will try to remedy this situation in this section.

One recognizes that the two body operator,

$$H_2 = H_C + H_B =$$

$$1/2 \int dx_1 \int dx_2 \, \psi^\dagger(x_1) \psi^\dagger(x_2) \; V(12) \psi(x_2) \psi(x_1)$$

$$\text{where } V(1,2) = V_C(x_{12}) + \tilde{B}(x_{12})$$

(2.2.15)

can be decomposed into a set of different operators that can be characterized by commutation relations with the electron (positron) number operator. If we use the decomposition of the wave operator (1.3.12), then H_2 consists of terms that:

i) scatter two electrons,

ii) scatter one electron, create a pair, or destroy a pair,

iii) two pair terms, and positron scattering terms.

The no pair ansatz then only describes processes of the first type, however the effects induced by ii) should also be manifest when on goes beyond the no pair approximation. In order to do this we make a generalization of the Schwinger transformation[20], in order to decouple the terms of type ii) to $O(e^4)$. Let us be more explicit in our decomposition described above for the H_2. We have,

$$H_2 = \text{terms of type i,iii, } +$$

$$\int dx_1 \int dx_2 \Big[\psi_e^+(x_1)\psi_e^+(x_2)\, V(1,2)\psi_e(x_2))\psi_p^+(x_1)$$

$$+ \qquad \psi_p(x_1)\psi_e^+(x_2)\, V(1,2)\psi_e(x_2)\psi_e(x_1)\Big] \qquad (2.2.16)$$

where we have used (1.3.12), and defined the field operators $\psi_e^+(x)$, $\psi_e(x)$ which create, destroy electrons respectively, and $\psi_p^+(x)$, $\psi_p(x)$ which create, destroy positrons. The Hamiltonian H' now has the form ,

$$H' = H_0 + H_2 + H_2' + O(e^4) \tag{2.2.17}$$

where H_2' are the terms given above, We now employ the Schwinger transformation except that we now replace $H_I(\tau)$ in the generator σ with $H_2'(\tau)$. After carrying out the identical steps given previously we have,

$$H'' = e^{i\sigma} H' e^{-i\sigma}$$

$$= H_0 + H_2 + i/2\left[\sigma, H_2'\right] + \ldots$$

where

$$\sigma = -1/2 \int_{-\infty}^{\infty} d\tau \epsilon(\tau) H_2'(\tau) e^{-\eta|\tau|}. \tag{2.2.18}$$

When evaluating the commutator above, we are interested only in the terms that commute with the electron number operator(the neglected terms appear only in higher order). The resulting terms will be three, two and one electron operators. We are interested only in the three body operators hence,

$$+i/2\left[\sigma, H_2'\right] = -i/4 \int_{-\infty}^{\infty} d\tau \epsilon(\tau) \left[H_2'(\tau), H_2'\right]$$

$$= -i/4 \int_{-\infty}^{\infty} d\tau \epsilon(\tau) \int dx_1 \int dx_2 \int dx_3$$

$$\psi_e^{\dagger}(x_1)\psi_e^{\dagger}(x_2)\psi_e^{\dagger}(x_3)\ e^{-ih(1)\tau}\ e^{-ih(2)\tau} V(1,2)$$

$$e^{ih(1)\tau}\ e^{ih(2)\tau} \bigwedge_{(-)}(2)\ V(2,3)\psi(x_3)\psi(x_2)\psi(x_1) \quad + H.c$$

(2.2.19)

where we have used the commutation relations (1.3.9), and the definition of the negative energy projection operators given in (1.3.24). The above operator in the occupation representation becomes,

$$H_p = 1/2 \sum b_n^{\dagger} b_l^{\dagger} b_m^{\dagger} b_m, b_l, b_n,\ V^p_{nlm,n'l'm'} + H.c$$

where,

$$V^p_{nlm,n'l'm'} = \sum_{s}^{(-)} \langle n\ l | V(1,2) | n'\ s \rangle / (Wnn' + E_l + |E_s|) \times$$

$$\langle s\ m | V(3,4) | l'm' \rangle$$

(2.2.20)

where the energy denominator results from the trivial time integration. We can use (2.1.25) and (2.2.8)for the matrix elements of the two body operator to get

$$V^{P}_{nml,n'm'l'} =$$

$$\sum_{s}^{(-)} (C_{nl,n's} - \eta_{nl,n's} - \eta_{ln,sn})/(W_{nn'} + E_l + |E_s|)$$

$$(C_{sm,l'm'} - \eta_{sm,l'm'} - \eta_{ms,m'l'})$$

(2.2.21)

Adding H_{C-T}, H_{T-T}, and H_P the total three body interaction Hamiltonian is given by,

$$H(3) = 1/6 \int dx_1 \int dx_2 \int dx_3 \; \psi_e^{+}(x_1) \psi_e^{+}(x_2) \psi_e^{+}(x_3)$$

$$S(\Delta_{C-T}(1,2,3) + \Delta_{T-T}(1,2,3) + \Delta_P(1,2,3)) \; \psi_e(x_3) \psi_e(x_2) \psi_e(x_1)$$

$$+ H.c$$

(2.2.22)

where, $\Delta_{C-T}(1,2,3)$, $\Delta_{T-T}(1,2,3)$ are given in (2.2.4), and (2.2.12) respectively, $\Delta_P(1,2,3)$ is the operator in the spatial integral (2.2.19), and S is a symmetrization operator with respect to the particle coordinates. Using the no pair ansatz, and carrying out (1.3.20), one gets the configuration space equation (2.2.19) with an additional configuration space three body potential given by

$$V_3 = 1/6 \sum_{i<j<k} \Lambda_+(i)\Lambda_+(j)\Lambda_+(k) \times$$

$$S(\Delta_{C-T}(i,j,k) + \Delta_{T-T}(i,j,k) + \Delta_P(i,j,k)) \times$$

$$\Lambda_+(k)\Lambda_+(j)\Lambda_+(i).$$

(2.2.23)

Chapter 3

Ambiguities associated with the decoupling transformation discussed in the previous chapter are investigated. The degree of freedom one has in the choice of a decoupling manifests itself in the appearance of non unique two, and three body potentials. It is shown that these potentials differ with respect to time reversal symmetry. A certain class of these ambiguities are resolved in section 3.1. In section 3.2, we make an observation concerning an apparant violation of the Pauli exclusion principle by some of the three-body potentials derived in the last chapter. Finally in the last section, we rederive the Primakoff Holstein three body potential from QED using a "classical limit", where the electrons exchange low frequency or "soft" photons.

Section 3.1 Ambiguities in the photon decoupling transformation

In the previous sections we have employed the Schwinger canonical transformation, on the QED Hamiltonian to decouple the radiation field to $O(e^4)$ in the coupling constant. The crucial property of the Schwinger transformation that allows us to decouple the radiation field is given by equation (2.1.12). The Schwinger transformation obeys this operator identity because the time deritative of the discontinous step function is a delta function i.e,

$$\frac{\partial}{\partial \tau}\epsilon(t) = 2\delta(t) \qquad (3.1.1)$$

$\epsilon(t)$ is not the only function that obeys this equation, another independent function is given by $-2\theta(-t)$. Instead of the Schwinger transformation let us consider the transformation induced by the generator

$$\sigma = \int_{-\infty}^{\infty} d\tau\, \theta(-\tau)\, H_I(\tau)\, e^{-\eta|\tau|} \qquad (3.1.2)$$

We now evaluate the commutator,

$$i\left[\sigma, H_0\right] = -\int_{-\infty}^{\infty} d\tau\ \theta(-\tau) \quad H_I(\tau) e^{-\eta/|\tau|} = -H_I$$

(3.1.3)

where we have integrated by parts and used the property of the step function, $\frac{\partial}{\partial\tau}\theta(-\tau) = -\delta(\tau)$ (we have again neglected the derivative of the adiabatic convergence factor). Therefore the transformation defined by the generator (3.1.2) will also diagonalize the QED Hamiltonian with respect to the photon number to $O(e^4)$. As a matter of fact we can define an even more general transformation

$$H \rightarrow H' = e^{i\sigma(a)}\ H\ e^{-i\sigma(a)}$$

where,

$$\sigma(a) = \int_{-\infty}^{\infty} d\tau\ f(\tau) H_I(\tau)\ e^{-\eta/|\tau|} \quad f(\tau) = -1/2\,\epsilon(\tau)a + (1-a)\theta(-\tau)$$

(3.1.4)

(a) being an arbitrary real parameter. It is obvious that $\sigma(a)$ also obeys the operator relation (3.1.2). We now have a situation where the decoupling of the radiation field, is not a unique procedure, which in turn suggests that the two, three body potentials derived in the previous section are also not unique. The decoupling transformation given by (3.1.4) can be parametrized by the arbitrary constant a.

For a = 1, we should recover the results obtained in the previous section since this choice corresponds to the Schwinger transformation. Let us investigate the dependence of the two body potentials on this parameter. We recall from section 2, that the form of the nonlocal two body potential is given by

$$V(1,2) = V_C(1,2) + B(1,2) \tag{3.1.5}$$

where B(1,2) was defined in (2.1.19). A new two body potential can be derived by the replacement of the $\epsilon(\tau)$ step function in (2.1.19) with $a\,\epsilon(\tau) - 2(1-a)\,\theta(-\tau)$, i.e.

$$B(1,2) \rightarrow B_a(1,2) = -ie^2/4 \int_{-\infty}^{\infty} d\tau \left[\epsilon(\tau)a - 2(1-a)\theta(-\tau)\right] \times$$
$$e^{ih(1)\tau} \alpha_1^a D_{ab}(1,2) \alpha_2^b e^{-ih(1)\tau} + (1 \leftrightarrow 2) \tag{3.1.6}$$

Let us look at the form of the potential $B_a(1,2)$ for various values of the parameter a. For a = 2, we can recast the $B_{a=1}(1,2)$ potential in the same form as (2.1.19) except by replacing the photon propagator $D(x_{12},t)$ by a retarded photon propagator $D_R(x_{12},t) = 2\theta(t)\, D(x_{12},t)$. The retarded propagator vanishes for $t < 0$, likewise for the case a = 0 we get the advanced

propagator $D_A(x_{12},t) = -2\theta(-t)D(x_{12},t)$ whereas for a = 1 the propagator is symmetrical in time. We thus notice that the parameter (a) just picks out the various temporal boundary conditions for the electrodynamic Greens function [21]. In the literature one usually finds that the choice for the retarded propagator is made in order to have causal solutions for the physical problems at hand. This is usually a sensible choice when is one dealing with scattering problems where there is a clear distinction between past and future, however this is no longer true when we are dealing with bound state solutions of a quantum mechanical system such as an atom. In a classic paper[22], Feynman and Wheeler, analyzed in detail causality problems that are encountered in classical action at distance theories. In fact, they showed that only solutions that are symmetric in time will not violate causality,(this is true only for a static universe[23]). Therefore, at this stage, we will not make any a - priori choice in the value of the parameter (a) but, instead, see how far we can carry the formalism until we get to an obvious motivation for choosing any particular value of (a) over another.

Let us first look at the form of the two body potential in the occupation representation. This was done for the Schwinger transformation (a = 1) in section 2 , for the more general case, the time integral in (2.1.23) now becomes ,

$$P\left(1/(ck+W_{nn'}) + 1/(ck-W_{nn'}) \right) \rightarrow$$

$$P(1/(ck+W_{nn'})+1/(ck-W_{nn'}))+(1-a)\pi i\left[\delta(ck+W_{nn'})-\delta(ck+W_{nn'}) \right].$$

(3.1.7)

performing the k space integral as in (2.1.24), we get instead of the η matrix elements defined in (2.1.25),

$$\eta_{nm,n'm'} \rightarrow \eta_{nm,n'm'} + \Omega_{nm,n'm'}(1-a)$$

where,

$$\Omega_{nm,n'm'} = ie^2/2 \langle n\ m | \left(\nabla^2 \delta_{ab} + \nabla_1^a \nabla_2^b \right)$$

$$(c\hbar/W_{nn'})^2/r\ (\sin(Wnn'r/hc)\ |\ n'\ m'\rangle$$

(3.1.8)

At first sight it might seem that the appearance of the imaginary factor makes $B_a(1,2)$ a non - Hermitian operator, but it can easily be proved that $B_a(1,2)$ is a perfectly acceptable Hermitian operator, since

$$\tilde{B}_a^{+}(1,2) =$$

$$-ie^2/4 \int_{-\infty}^{\infty} d\tau\, f(\tau)\ e^{ih(1)\tau}\, \alpha_1^a\, D(12,\tau)\, \alpha_1^b\, e^{-ih(1)\tau}$$

$= B_a(1,2)$ where we have used, $\overset{+}{D}(1,2\tau) = - D(1,2\tau)$

(3.1.9)

Let us now define an operator $\Gamma(a)$ which is the difference of the potential derived in section 2, (a = 1) and the potential for any arbitrary value of (a). This operator in a sense " measures" the degree of ambiguity of the two body potential . After a little algebra and making use of the identity $\epsilon(\tau) = \theta(\tau) - \theta(-\tau)$ we have,

$$\Gamma_a(1,2) =$$

$$-ie^2/4 \int_{-\infty}^{\infty} d\tau\, (1-a)\, e^{ih(1)\tau}\, \alpha_i^a D_{ab}(r_{12},\tau)\, \alpha_i^b\, e^{-ih(1)\tau} + (1 \leftrightarrow 2)$$

(3.1.10)

Let us now take matrix elements of the above operator with respect to the Dirac - Coulomb wave functions, we get,

$$\langle n\ m | \Gamma_a(1,2) | n'\ m' \rangle =$$

$$(1-a)\left(\Omega_{nm,n'm'} + \Omega_{mn,m'n'}\right) \quad ,$$

(3.1.11)

where the Ω matrix elements are defined above,

We notice that for energy on-shell matrix elements i.e., $(W_{nn'} + W_{mm'}) = 0$ the $\langle n\ m | \Gamma_a(1,2) | n'\ m' \rangle$ vanish,

because the functions $\Omega_{nm,n'm'}$ are odd with respect to the sign of the energy difference. We thus come to the important conclusion that our ambiguity in the non local potential $B_a(1,2)$ appears in only the off shell matrix elements of this operator.

We can get a better handle on the physical situation presented here if we investigate the time invariance properties of the operator $B_a(1,2)$. We introduce the single particle relativistic time reversal operator[24] given by,

$$T = -i\alpha_1\alpha_3 K \tag{3.1.11}$$

where the four dimensional spinor operators α_1 α_3 are given by

$$\alpha_1 = \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix}$$

$$\alpha_3 = \begin{pmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{pmatrix} \tag{3.1.12}$$

σ_x and σ_z being the two dimensional Pauli operators. K is the nonrelativistic time reversal, anti-unitary operator. The multiparticle T operator is defined as a product of the single particle time reversal operators.

In order to investigate the time inversion properties of the $B_a(1,2)$ operator let us first investigate the behavior of the photon propagator (2.1.15) under time inversion i.e,

$$D_{ab}(x_{12},t) \rightarrow T\, D_{ab}(x_{12},t)\, T^{+} =$$

$$K\left[2ic/(2\pi)^2 \int d^3\bar{k}/k\ (\delta_{ab} - \hat{\kappa}_a \hat{\kappa}_b)\, e^{i\bar{k}\cdot\bar{r}} \sin(ckt)\right] K$$

$$= 2ic/(2\pi)^2 \int d^3\bar{k}/k\ (\delta_{ab} - \hat{\kappa}_a \hat{\kappa}_b)\, e^{-ikr} \sin(ckt)$$

$$= - D_{ab}(x_{12},t).$$

(3.1.13)

The time inversion behavior of the Dirac matrices are,[24]

$$\alpha^a \rightarrow T^{+} \alpha^a T$$

$$= - \alpha^a.$$

(3.1.14)

Using these intermediate results we can now make a time reversal transformation on $\tilde{B}_a(1,2)$. Representing

this operator in the form ,

$$\tilde{B}_a(1,2) = \tilde{B}(1,2) + \Gamma_a(1,2)$$

(3.1.15)

We have ,

$$T\left(-ie^2/4\int_{-\infty}^{\infty} d\tau\, g(\tau)\; e^{ih(1)\tau}\alpha_1^a D_{ab}(x_{12},\tau)\alpha_2^b\, e^{-ih(1)\tau}\right)T^+$$

$$= +ie^2/4\int_{-\infty}^{\infty} d\tau\, g(\tau)\; e^{-ih(1)\tau}\alpha_1^a(-D_{ab}(x_{12},\tau))\alpha_2^b\, e^{+ih(1)\tau}$$

(3.1.16)

where $g(\tau)$ is an arbitrary real scalar, and we have used the time invariance property of the Dirac - Coulomb Hamiltonian $h(1)$. The function $g(\tau) = \epsilon(t)$ for the $\tilde{B}(1,2)$ operator, and $g(\tau) = 1$ for the $\Gamma_a(1,2)$ operator. We therefore have,

$$T\,\tilde{B}_a(1,2)\,T^+ = T\,\tilde{B}(1,2)\,T^+ + T\,\Gamma_a(1,2)\,T^+$$

$$= \tilde{B}_a(1,2) - \Gamma_a(1,2)$$

(3.1.17)

We thus conclude that the two body potential is time reversal invariant only for the choice a = 1 since Γ_a changes sign under time reversal. We know that QED is a time reversal invariant theory, however by making a unitary photon decoupling transformation we are in essence picking an ansatz for the Fock space eigensolution that does not have the same symmetry property as the Hamiltonian. In this way we are "breaking" the time reversal symmetry of the QED Hamiltonian for any choice $a \neq 1$.

The above ambiguity in the two body potential has also been mentioned by Nambu[25], he uses integrability conditions in order to attempt to resolve this ambiguity. Also K.N.Huang[26] points out that ambiguities in the position of the poles in the k space integral of the virtual photons, results in different expressions for the interelectronic potential. Both authors do not give any clear cut resolution to these ambiguities. In addition they rely on S matrix theory in order to obtain two body potentials, this method does not guarantee Hermitian potentials. The canonical transformation method does not suffer from this drawback. We will now show that for systems with bound states the above ambiguity is resolved, the Schwinger transformation (a=1) being the only well defined canonical transformation.

Consider the action of the operator $U = e^{i\sigma(a)}$ on an N electron state vector $|N\rangle$.

$$U\,|N\rangle = (1 + i\sigma + i^2/2\,\sigma^2 + \ldots)|N\rangle$$

(3.1.19)

Let's consider the third term in the above expansion, and for the moment consider the special case a=0. Using the definition (3.1.4) we have,

$$i^2/2 \int_{-\infty}^{0} dt_1\, H_I(t_1) \int_{-\infty}^{0} dt_2\, H_I(t_2)\, e^{\eta(t_1 + t_2)}\,|N\rangle$$

(3.1.20)

We can rewrite the above expression as,

$$\left\{ i^2/2 \int_{-\infty}^{0} dt_1 \int_{-\infty}^{0} dt_2\; H_I(t_1)H_I(t_2)\, e^{\eta(t_1 + t_2)} + (t_1 \leftrightarrow t_2)\right\}|N\rangle.$$

(3.1.21)

Inserting a complete set of fermion states on the left hand side, and carrying out the time integrations, we get,

$$\sum_{N'} -i^2/2\; i/(W_{nn'} - 2i\eta\;)\,|N'\rangle\langle N'| \int_{-\infty}^{0} ds \left\{ H_I\, e^{i(H - W_{nn'})s} \cdot \right.$$

$$\left. + H_I e^{-i(H - W_{nn'})s}\, e^{\eta s}\right\}|N\rangle$$

(3.1.22)

When the unrestricted summation includes the state $|N\rangle$ and $|N\rangle$ is a bound state, we have

$$\lim_{\eta \to 0} \; i^2/2 \; 1/\eta \; |N\rangle\langle N| \int_{-\infty}^{0} ds \; H_I e^{-iHs} \; H_I \; e^{\eta s} \; |N\rangle$$

(3.2.23)

As the adiabatic factor η goes to zero, the integral $\int_{-\infty}^{0} ds$ is well defined since η will determine the location of the poles in the k space integral over the virtual photons. However, the $1/\eta$ factor outside the integral diverges in this limit. When we carry out the same procedure for the general transformation $U(a) = e^{i\sigma(a)}$, the t_1 integrals in (3.1.21) have the form,

$$\int_{-\infty}^{\infty} dt \; (-1/2 \; \epsilon(t) a + (1-a) \; \theta(-t) \; e^{-\eta|t|} e^{iW_{nn'}t} =$$

$$+i/2 \left\{ a \left[1/(W_{nn'} - i\eta) + 1/(W_{nn'} + i\eta) \right] - 2(1-a) \; 1/(W_{nn'} - i\eta) \right\}$$

(3.2.24)

When $W_{nn'} = 0$ the above integral is defined only if a=1 (Schwinger transformation) if we follow the convention that the limit $\eta \to 0$ is taken after everthing else is evaluated.

The above singularities are reminiscent of similar singularities encountered when the Dyson operator $U(0, \pm\infty) = P\left[\exp(\mp i \int_0^{\pm\infty} dt H_I(t))\right]$ (P is the time ordering operator) is evaluated with a Hamiltonian containing bound states. Gellman and Low[27] showed that these singularities can be removed by a renormalization of the state $|N\rangle$. In the language of diagrams, this entails the cancellation of disconnected diagrams[28]. In our formalism such a renormalization

would destroy the unitary property of the decoupling transformation. We therefore conclude that the Schwinger transformation is the natural choice for the decoupling transformation, since it does not give rise to undefined terms when the adiabatic factor vanishes.

So far we have been working in the framework of the Coulomb gauge. if one considers the QED Hamiltonian in the Lorentz gauge, the interaction term $H_I + H_C$ gets replaced by,

$$H_I^{(L)} = e\int dx \; J_\mu A^\mu \tag{3.1.25}$$

where J_μ, A^μ are the covariant four current, and potential repectively. Performing a Schwinger tarnsformation in order to decouple $H_I^{(L)}$, one gets instead of the Coulomb and Breit operator (2.1.19), a new two body potential whose matrix elements are given by[20],

$$V^L_{n1,n'1'} = \langle n1 \left| -1/2r \; e^2 \; (1 - \alpha_1 \cdot \alpha_2) \right.$$

$$\left. \cos(W_{nn'} r/\hbar c) + \cos(W_{11'} r/\hbar c) \right| n'1' \rangle \tag{3.1.26}$$

for on shell matrix elements ($W_{nn'} + W_{11'} = 0$) these reduce to the corresponding matrix elements of the two body potentials derived previously. The ambiguity again appears only in the off shell matrix elements. However,

the Coulomb gauge seems to be the more physicaly appealing choice, since the Coulomb interaction is treated exactly to all orders in pertubation theory in this gauge, and it is probably the most important e-e interaction.

Section 3.2 Pauli principle violating diagrams

On closer examination, one notices that the unrestricted sum over the intermediate states in (2.2.8), and (2.2.14) will contain contributions from states that violate the Pauli exclusion principle, i.e. more than one particle is in the same state at the same time. The occurance of Pauli violating diagrams in many-body pertubation theory has been known for sometime[29]. We will delay discussion of the past literature to a later paragraph. For now, let us investigate in detail how these diagrams appear in our formalism.

Let us discuss the contribution to the energy shift in a three electron system due to the presence of virtual pairs. A part of the shift comes from the three body potentials given in (2.2.19). The lowest order shift due to these terms is given by,

$$\triangle E^{(3)} = \langle \Psi | H^P | \Psi \rangle \qquad (3.2.1)$$

where $|\Psi\rangle$ is a three electron system, $1/\sqrt{3!}\ b_a^\dagger b_b^\dagger b_c^\dagger |0\rangle$, a,b,c, being the electron quantum numbers. Expanding the above expression we have,

$$\Delta E^{(3)} = 1/6 \sum_{[P]} \left(U^{P}_{abc,[abc]} - U^{P}_{abc,[bac]} \right)$$

(3.2.2)

where the summation is over all the even permutations of indices in the brackets, and

$$U^{P}_{abc,a'b'c'} = V^{P}_{abc,a'b'c'} + V^{P}_{cab,c'a'b'} +$$

$$V^{P}_{bca,b'c'a'} + V^{P}_{bac,b'a'c'} + V^{P}_{acb,a'c'b'} +$$

$$V^{P}_{cba,c'b'a'} = S(V^{P}_{abc,a'b'c'})$$

(3.2.3)

where we have used (2.2.20).

We will now go on to prove that all the terms in the above expansion violate the Pauli exlusion principle. This fact becomes apparant if we proceed to reexpress the above shift in terms of time ordered Feynman diagrams. The above shift can be rederived by using standard pertubation methods. We can evaluate the total energy shift due to the interaction H_2 given in (2.2.15) by[28]

$$\Delta E^{T} = \lim_{\eta \to 0} -i\eta \int_{-\infty}^{0} dt_1 \int_{-\infty}^{0} dt_2 \, \langle 0 | H_2(t_1) H_2(t_2) | 0 \rangle_{\text{connected}} \, e^{\eta t_1} e^{\eta t_2}$$

(3.2.4)

The shift $\Delta E^{(3)}$ is contained in a subclass of diagrams of ΔE^{T} which are generated by a single Wick contraction of the type $\underbrace{\psi^{+}(t_1)\psi}(t_2)$ in the above expectation value. Evaluating (3.2.4) we get,

$$\Delta E^{(3)} = -i2\eta \int_{-\infty}^{0} dt_1 \int_{-\infty}^{0} dt_2$$

$$b_n^{+}(t_1) b_m^{+}(t_2) b_1^{+}(t_2) b_{1'}(t_1) b_{n'}(t_1) b_{m'}(t_2)$$

$$\sum_{s}^{(-)} \langle ns\,|V(12)|\,n'1'\rangle \langle 1m\,|V(34)|\,sm'\rangle\; e^{-i\Delta W(t_1 - t_2)}$$

(3.3.5)

where we have used,

$$\underbrace{\psi^{+}(x_1 t_1)\psi}(x_2 t_2) = \langle 0|\psi^{+}(x_1 t_1)\,\psi(x_2 t_2)|0\rangle$$

$$= \sum_{s}^{(-)} \varphi_s^{+}(x_1)\,\varphi_s(x_2) e^{-i|E_s|(t_1 - t_2)},$$

$b_n(t) = e^{iE_n t} b_n$, and V is given by (2.2.15), and

$$\Delta W = (E_m - E_{m'}) - (E_{1'} + |E_s|)$$

(3.3.6)

The Fock space operator in the above shift can be expressed as a time ordered diagram, Fig.2a. In this diagram,

the initial states n',l',m' are scattered into the final states n,l,m, under the interaction V, with the propagation of a virtual electron positron pair between the interaction times t_1,t_2. After doing the time integrations and, evaluating the expectation value one recovers the shift (3.2.1). This shift is now expressed as a set of thirty six diagrams of the type in Fig.2a, where now the the initial and final states are all permutations of the quantum numbers a,b,c,.There is a minus sign for diagrams where the incoming states are an odd permutation of the outgoing states. We call these exchange diagrams, whereas for even permutations we have direct diagrams. If the diagrammatic representation is taken seriously, one notices that every diagram in the above expansion contains two electrons in the same state between the interaction times t_1,t_2. That is, each term in the shift (3.2.4) violates the Pauli exclusion principle. At first sight this is a startling conclusion. After all, we have imposed the anticommutation relations (1.3.9) on our fields to insure the validity of the Pauli principle. The resolution of this paradox is provided if one looks at additional terms we have not yet considered in the shift (3.2.1). If we perform an additional Wick contraction of the type $\underbrace{\psi(t_1)\ \psi^{+}(t_2)}$, i.e if we include the propagation of a virtual electron, we get an additional shift, that comes from two particle diagrams. We get

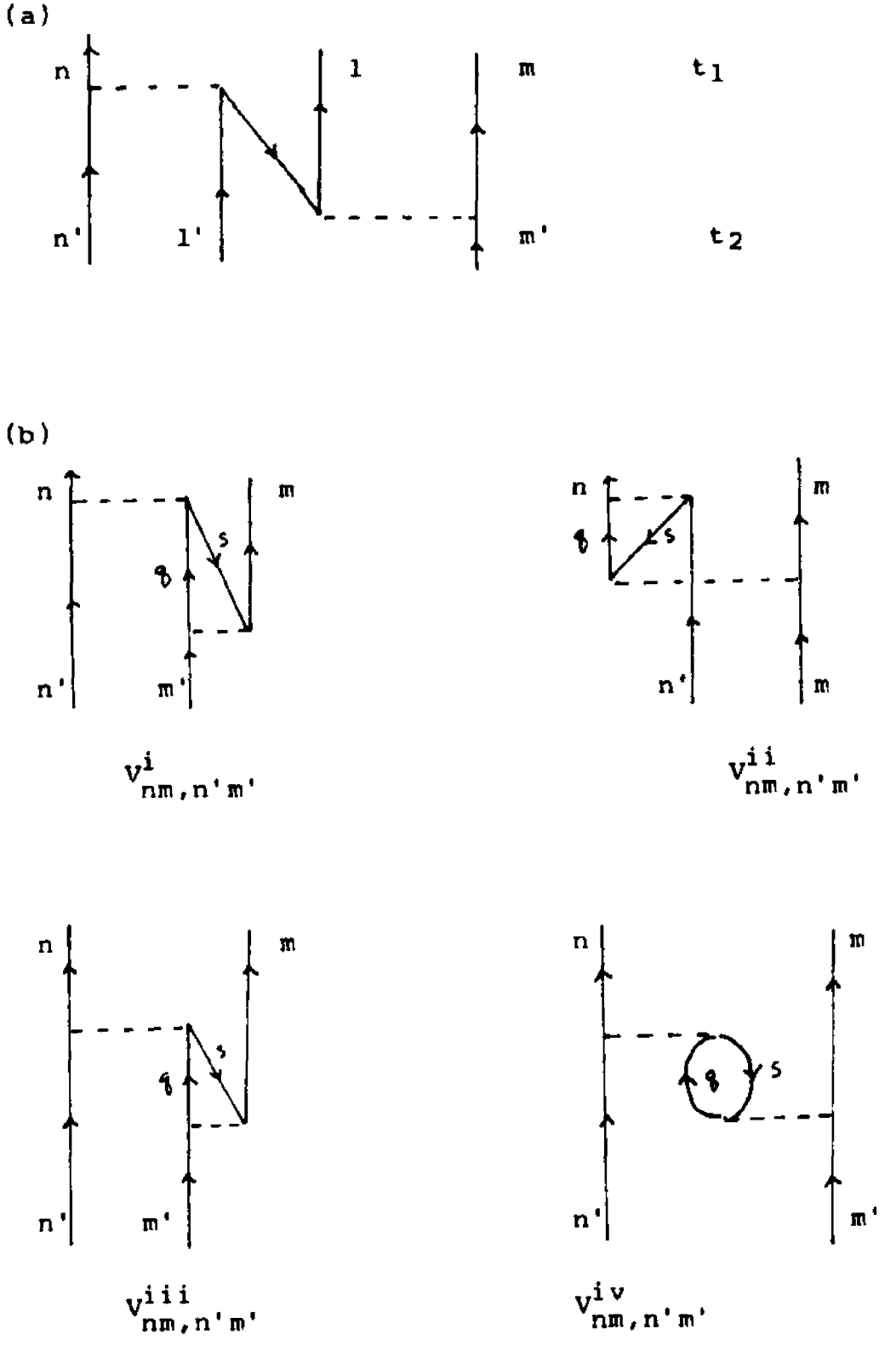


Figure 2. (a) Diagramatic representation of the three body shift (3.2.3): (b) diagramatic representation of the two body matrix elements (3.2.5).

$$\Delta E_2 = \sum \langle \Psi | b_n^{\dagger} b_1^{\dagger} b_{1'} b_{n'} \; v^{(j)}_{n1,n'1'} | \Psi \rangle$$

where,

$$v^{(i)}_{n1,n'1'} = \sum_{s}^{(+)} \sum_{q}^{(-)} \langle ns|V(12)|q1'\rangle\langle q1|V(34)|n's\rangle \; / \Delta W^{(i)}$$

$$v^{(ii)}_{n1,n'1'} = \; " \; \langle ns|V(12)|qn'\rangle\langle q1|V(34)|s1'\rangle \; / \Delta W^{(ii)}$$

$$v^{(iii)}_{n1,n'1'} = \; " \; \langle ns|V(12)|n'q\rangle\langle 1q|V(34)|s1'\rangle \; / \Delta W^{(iii)}$$

$$v^{(iv)}_{n1,n'1'} = \; " \; -\langle ns|V(12)|n'q\rangle\langle q|V(34)|1's\rangle \; / \Delta W^{(iv)} \; .$$

(3.2.7)

These are represented diagramatically in Fig.2b. The energy denominators $\Delta W^{(j)}$ again correspond to the difference between the final and intermediate state energy for each diagram. Taking the above expectation value one gets,

$$\Delta E_{(2)} = 1/6 \sum_{j} S(\; v^{(j)}_{ab,[ab]} - v^{(j)}_{ba,[ab]})$$

$$= 1/6 \sum_{j} (\; v^{(j)}_{ab,[ab]} - v^{(j)}_{ba,[ab]}) +$$

$$(\; v^{(j)}_{ac,[ac]} - v^{(j)}_{ca,[ac]}) + (\; v^{(j)}_{bc,[bc]} - v^{(j)}_{cb,[bc]})$$

(3.2.8)

where, $V^{(j)}_{ab,[ab]} = V^{(j)}_{ab,ab} - V^{(j)}_{ab,ba}$.

As in the three body matrix elements we define direct, and exchange terms of the two body matrix elements, according to whether the diagrams have even or odd permutations of the initial states with respect to the final states.

Let us now look at a particular group of terms in the shift (3.2.1) that are given by,

$$U_{abc,abc} = S\left(\sum_{s}^{(-)} \langle as|V(12)|ab\rangle\langle bc|V(34)|sc\rangle / \Delta W \right)$$

(3.2.9)

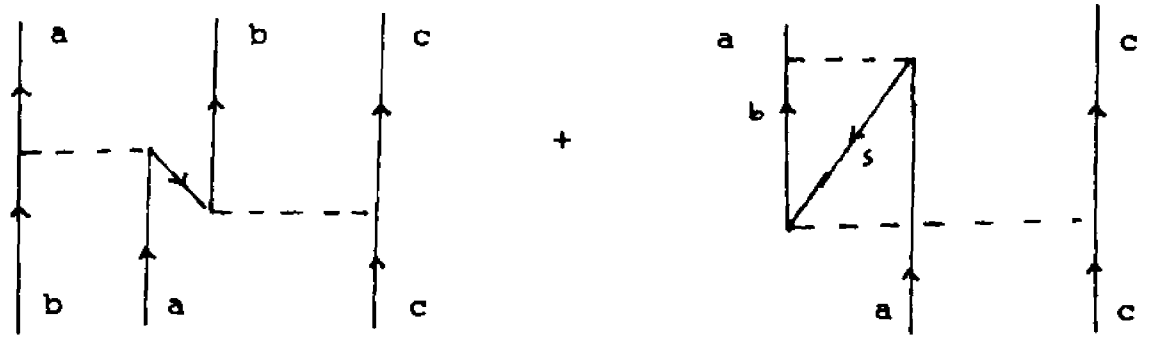
where S is the symmetrization operator defined in (3.2.3). We also look at the direct two body term ,

$$S(V^{(iv)}_{ac,ac}) =$$

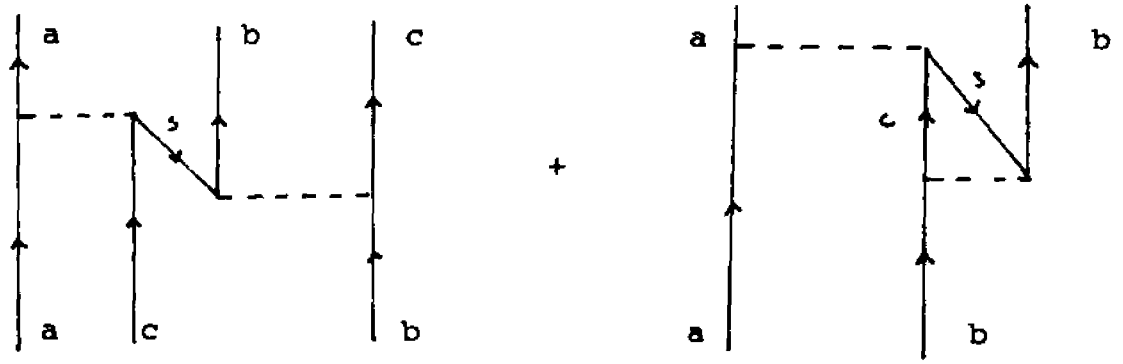
$$- S\left(\sum\sum \langle as|V(12)|a'q\rangle\langle ql|V(34)|sc\rangle / \Delta W^{(iv)} \right)$$

(3.2.10)

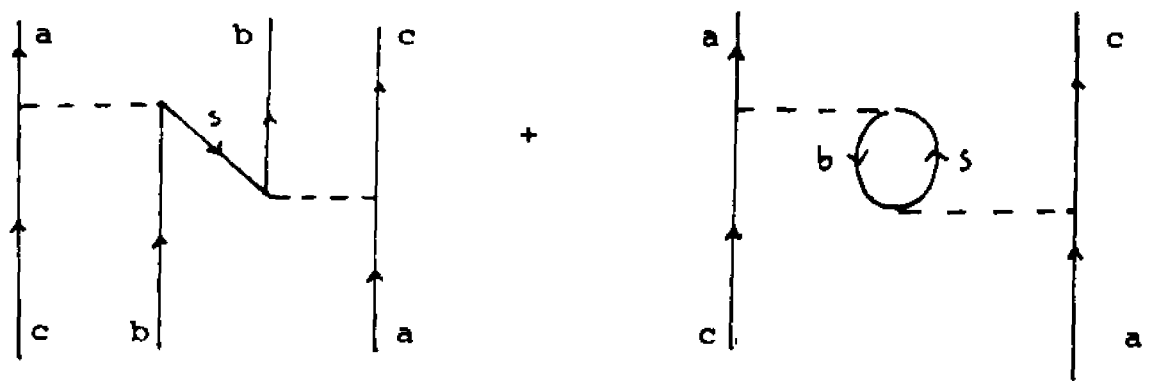
For q = b the two body term will cancel the three body term above. This cancellation is illustrated on the top line of Fig.3, the minus sign in front of the direct two body matrix element $S(V^{(iv)}_{ac,ac})$ comes from the closed fermion loop in the corresponding diagram. The thirty remaining diagrams of the three body shift are likewise cancelled by two body diagrams, this is illustrated in Fig 3.



$-U_{abc,bac}$ Direct terms

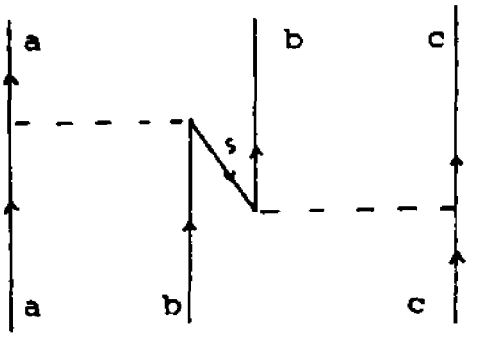


$-U_{abc,acb}$ Direct terms



$-U_{abc,cba}$ Exchange terms

Figure 3. Cancellation of the three body (pair) energy shift with two particle diagrams. Each set of diagrams above are permutated with respect to the particle coordinates generating thirty six diagrams.



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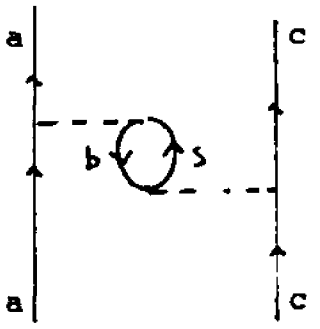
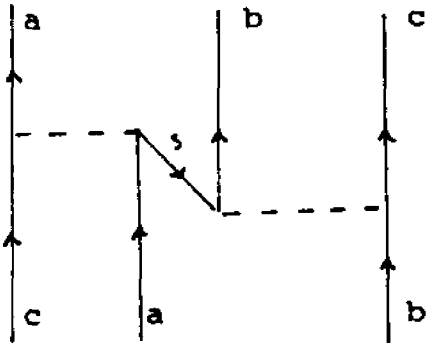


$U_{abc,abc}$ Direct terms



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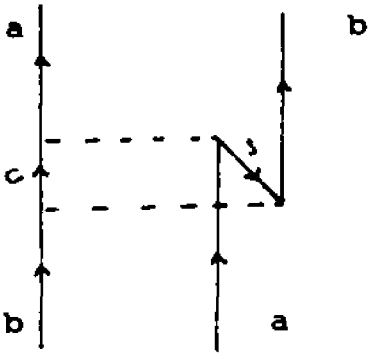
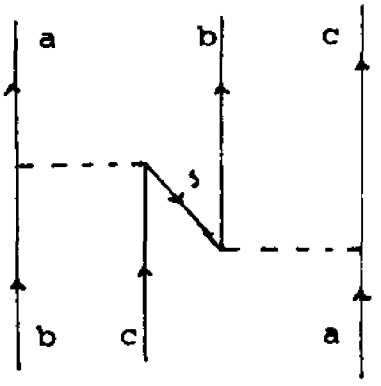


$U_{abc,cab}$ Exchange terms



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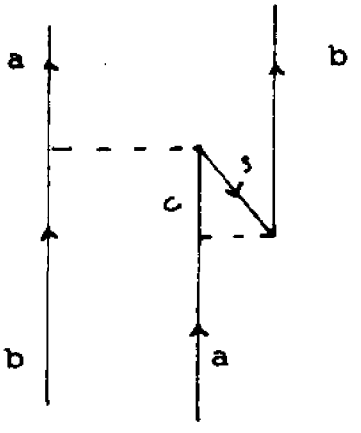

$U_{abc,bca}$ Exchange terms

We must now decide whether the three body terms that violate the Pauli principle should be discarded, or taken seriously. First let us discuss some of the past literature concerning this point. In a series of papers, Kelly[29] points out that the largest contribution to the correlation energy of a nonrelativistic atom in fact come from diagrams that violate the Pauli exlusion principle. The existance of these terms was shown to be a result of the cancellation of disconnected diagrams in the pertubation series[29]. Thus the mere presence of Pauli principle violating diagrams should not be the cause of great alarm. On the question concerning the cancellation of these terms with some of the two body diagrams in Fig.3 let us consider the graph below.

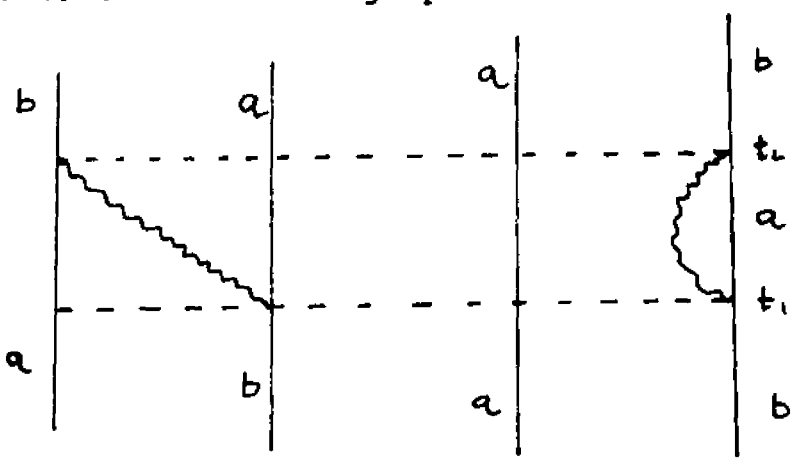

Fig.4. Cancellation of photon exchange diagram.

The diagram on the left describes photon exchange between two electrons, while the one on the right is a self energy diagram. For the labelled states the matrix elements of the two diagrams cancel since they both violate the Pauli

principle. However, it is the usual practice to treat these diagrams as separate entities, in order to carry out a renormalization scheme, even though some matrix elements get counted twice. It is this philosophy we use in dealing with the three body diagrams in Fig. 2. In fact in the next section, we shall show how some of these diagrams reduce to the Primakoff Holstein, classical three-body potential, when the electrons exchange soft photons.

Section 3.3 Classical limit of the three body potentials

We would now like to make the connection between the three body potentials derived in chapter 2, and the classical three body potential (1.1.11) first derived by Primakoff and Holstein, and also rederived by Chanmugan and Schweber[30] for nonrelativistic quantum mechanical particles interacting with a quantized electromagnetic field. The above authors pointed out that the classical potentials are the result of the emission (absorbtion) of two photons from the first particle via the A^2 term, and the subsequent absorbtion(emission) of these photons with the second and third particles respectively via the $\tilde{p}\cdot\bar{A}$ terms.(See Fig.5a)

We can no longer make this identification in the relativistic case since the fermionic current interacts linearly with the radiation field. However, it is well known[31] that the diagram in Fig.5b, describing the scattering of an electron with momentum p, and a photon with momentum hk, goes into the nonrelativistic expression (Thomson scattering) in the limit $p/mc,\ hk/mc \ll 1$. In the same manner we expect the three body term in Fig. 5c to go over into the classical expression (1.1.11) in this limit. We will now verify this expectation, first we wish to isolate the terms in the Hamiltonian (2.1.1) that are responsible for this diagram. The interaction term (2.1.3) can be divided up into,

$$\int dx\ \bar{J}(x)\cdot\bar{A}(x) = \int dx\ [\ \bar{J}_{ee}(x) + \bar{J}_{pp}(x)]\cdot\bar{A}(x)$$

$$+\int \bar{J}_{ep}(x)\cdot\bar{A}(x)\ dx$$

(3.3.1)

where $\bar{J}_{ee}$, $\bar{J}_{pp}$ scatter electrons, and positrons respectively, and $\bar{J}_{ep}$ creates(destroys) pairs. The electron scattering terms in Fig. 5b, are given by the iteration of the pair current above. We can explicitely construct the operator for this process, by introducing a unitary transformation similar to the Schwinger transformation, where now the generator is given by,

$$\sigma_1 = -1/2 \int_{-\infty}^{\infty} d\tau\ \epsilon(\tau)\ \bar{J}_{ep}(\tau)\cdot\bar{A}(0)$$

(3.3.2)

Using the relation,

$$i[\sigma_1, H_0] = - H_I(ep) - 1/2 \int_{-\infty}^{\infty} d\tau\ \epsilon(\tau)\ \bar{J}(\tau)\cdot\bar{A}(0)$$

(3.3.3)

Where $H_I(ep)$ is shorthand for the last term in (3.3.1) and, $\dot{A}(0) = \frac{\partial}{\partial\tau} A(\tau)\Big|_{\tau=0}$. The relevant term responsible for the process in Fig. 5b, is given by,

$$H_2^{(cl)} = i/2\left[\sigma_1, H_I(ep)\right] =$$

$$-i/4 \int_{-\infty}^{\infty} d\tau \int dx \int dy \; \epsilon(\tau) \left[J^a_{ep}(x,\tau), J^b_{ep}(y,\tau) \right] A^a(x,0) A^b(y,0)$$

(3.3.4)

We have neglected contributions coming from the latter term in (3.3.3) since these are small in the soft photon limit. Evaluating the commutator by contracting the positron fields, and doing the time integrals, we have,

$$H_2^{(cl)} = -1/2 \sum_{nn'} \sum_{s}^{(-)} b_n^+ b_{n'} \times$$

$$\int dx \int dy \quad \frac{\varphi_n(x) \; \bar{\alpha}_1 \cdot \bar{A}(x) \varphi_s(x) \varphi_s(y) \; \bar{\alpha}_2 \cdot \bar{A}(y) \varphi_{n'}(y).}{(E_n + |E_s|)}$$

(3.3.5)

(In order to simplify the discussion let us consider $h(x) = c\bar{\alpha} \cdot \bar{p} + mc^2$ as the zero order Hamiltonian, therefore the $\varphi_n(x)$, $\varphi_s(x)$ are free electron, and positron spinors respectively.) For slow electrons $p_n/mc << 1$, and $hk/mc << 1$ we can replace the denominator in (3.3.5) by $2mc^2$. This can be proved by evaluating a matrix element above using free particle spinor wave functions. A typical term will be proportional to,

$$\frac{\delta(p_n - p_s + k)\langle U^{\dagger}(p_n)\,\bar{\alpha}\cdot\epsilon_{k\lambda}\,U(p_s)\rangle}{\sqrt{(p+k)+2mc}} \approx$$

$$\delta(p_n - p_s + k)\langle U^{\dagger}(p_n)\,\bar{\alpha}\cdot\epsilon_{k\lambda}\,U(p_s)\rangle/2mc^2$$

(3.3.6)

where U(p) are the momentum space spinors, and $\epsilon_{k\lambda}$ is the polarization vector of the field $\bar{A}$. Using the completeness relation,

$$\sum_{s}^{(-)} \varphi_s(x)\,\varphi_s(y) = I\,\delta(x-y) - \sum^{(+)} \varphi_s(x)\,\varphi_s(y)$$

(3.3.7)

we get,

$$H_2^{(c1)} = 1/2mc^2 \sum_{nn'} b_n^{+} b_{n'} \int dx_1$$

$$\varphi_n^{+}(x_1)\,\alpha_1^{a}\,A^{a}(x_1)\,\alpha_1^{b}\,A^{b}(x_1)\,\varphi_{n'}(x_1)$$

(3.3.8)

where we have neglected the contribution coming from the sum over the positive energy electrons, since the α matrices couple the large components of these terms with the small components of $\varphi_n(x)$ .Therefore they give $O((p/mc)^2)$ corrections to (3.3.5).

Finally we can get the three body operator in Fig.5c, by iterating the electron scattering terms in (3.3.1) via

another Schwinger transformation with the generator given by, $\sigma = -1/2\int_{-\infty}^{\infty} d\tau\, \epsilon(\tau)\, \bar{J}_{ee}(\tau)\cdot\bar{A}(\tau)$. The relevant three-body operator will be contained in the term, $H_3^{(c1)} = i^2/2\left[\sigma,\left[\sigma,\, H_2^{(c1)}\right]\right]$. Evaluating the photon commutators we get,

$$1/8mc^2 \sum_{\substack{n l m \\ n' l' m'}} b_n^+ b_l^+ b_m^+ b_{m'} b_{l'} b_{n'} \int_{-\infty}^{\infty} d\tau_1\, \epsilon(\tau_1) \int_{-\infty}^{\infty} d\tau_2\, \epsilon(\tau_2) e^{iW_{nn'}\tau_1} e^{iW_{ll'}\tau_2}$$

$$\int dr_1 dr_2 dr_3\, \varphi_n^+(r_1)\, \varphi_l^+(r_2)\, \varphi_m^+(r_3)\, \alpha_1^{\mu} D^{\mu a}(r_1\tau_1, r_3)\alpha_2^a$$

$$\alpha_2^{\nu} D^{\nu b}(r_2, r_3)\alpha_3^b\, \varphi_{n'}(r_1)\, \varphi_l(r_2)\, \varphi_{m'}(r_3). \qquad (3.3.9)$$

Carrying out the time integrals, and using the nonrelativistic approximation, $W_{nn'} r_{12}/hc,\ W_{ll'} r_{23}/hc \ll 1$, where $r_{12} = |r_1 - r_2|$, we have

$$H_3^{(c1)} = 1/8mc^2 \sum b_n^+ b_l^+ b_m^+ b_{m'} b_{l'} b_{n'}$$

$$\langle nml |\ \{\alpha_1\cdot\alpha_l/r_{12} + (\alpha_1\cdot\hat{r}_{12}\ \alpha_2\cdot\hat{r}_{12})/r_{12}\}\ *$$

$$\{\bar{\alpha}_2\cdot\bar{\alpha}_3/r_{23} + (\bar{\alpha}_2\cdot\hat{r}_{23}\ \bar{\alpha}_3\cdot\hat{r}_{23})/r_{23})\}\ |n'm'l'\rangle \qquad (3.3.10)$$

Interchanging r_1 , r_2 , and using the anticommutation relations $\{\alpha^a, \alpha^b\} = 2\delta^{ab}$ we get,

$$H_3^{(cl)} = 1/8mc^2 \sum b_n^+ b_l^+ b_m^+ b_{m'} b_{l'} b_{n'} V^3_{nml,n'm'l'}$$

where, $V^3_{nml,n'm'l'} = \langle nml | Q(1,2,3) | n'm'l' \rangle$

$$e^4 \langle nml | (\bar{\alpha}_1 \cdot \bar{\alpha}_3 + \bar{\alpha}_1 \cdot \hat{r}_{13} \, \bar{\alpha}_3 \cdot \hat{r}_{13} + \bar{\alpha}_1 \cdot \hat{r}_{32} \, \bar{\alpha}_3 \cdot \hat{r}_{23} +$$

$$\hat{r}_{13} \cdot \hat{r}_{23} \; \bar{\alpha}_1 \cdot \hat{r}_{13} \, \bar{\alpha}_3 \hat{r}_{23}) / (r_{13} \; r_{23}) | n'l'm' \rangle$$

(3.3.11)

One can now get the configuration space three body potential from the above operator by, proceeding in the same manner as in (1.3.20) thru (1.3.23). We get

$$V^3(1,2,3) =$$

$$\sum_{i<j<k} e^4/8mc^2 \; \Lambda_+(i) \, \Lambda_+(j) \, \Lambda_+(k) \, Q(1,2,3) \, \Lambda_+(k) \, \Lambda_+(j) \, \Lambda_+(i)$$

(3.3.12)

If we make the identification $p_i/mc \rightarrow \alpha_i/c$, the operator $\frac{e^4}{8m^3c^4} Q(1,2,3)$ reduces to the Primakoff Holstein potential (1.1.11).

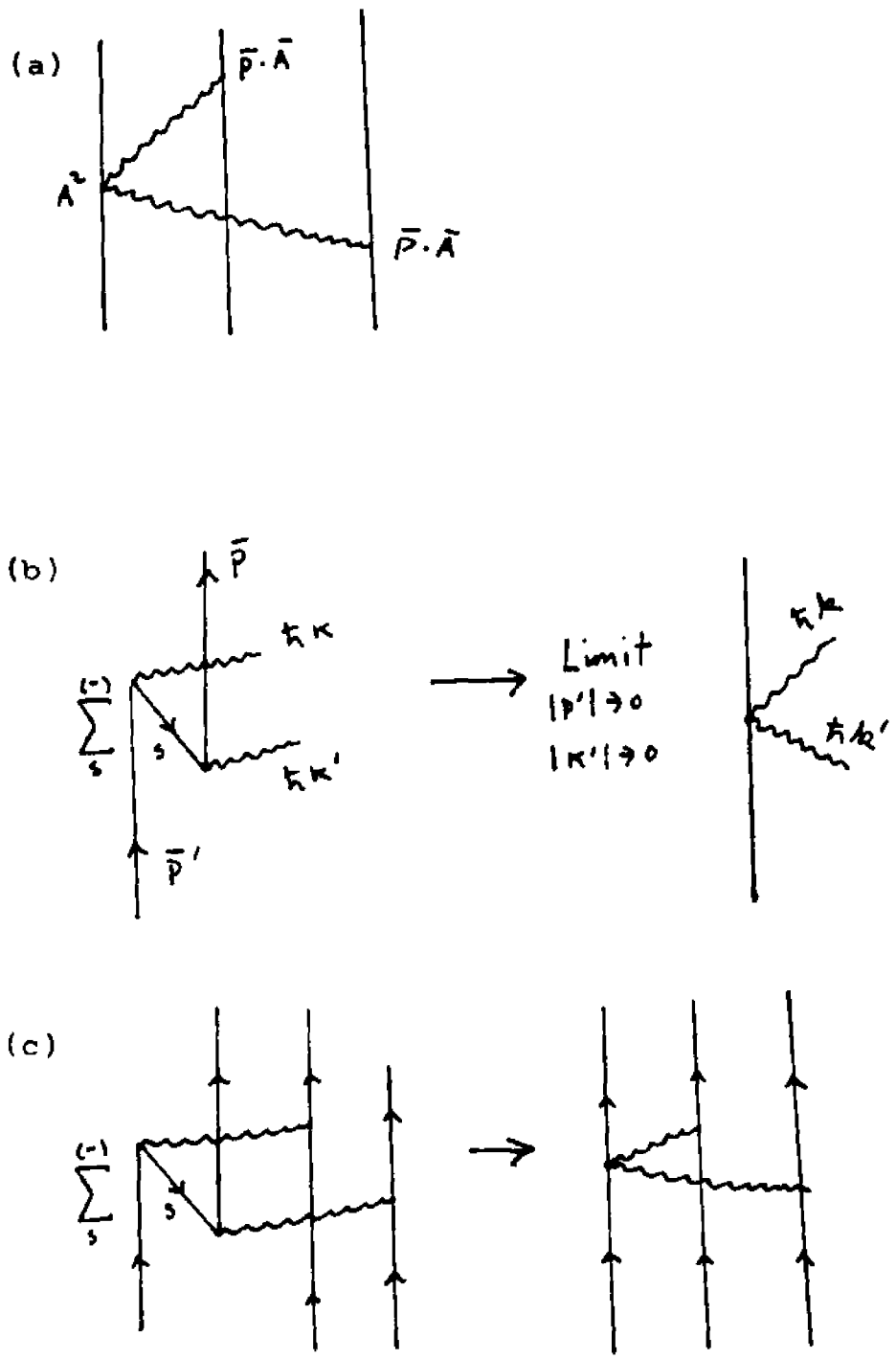

Fig 5. (a) Nonrelativistic diagram giving rise to the Primakoff-Holstein potential: (b) the Thomson scattering limit: (c) The nonrelativistic limit of three-body potentials (due to virtual pair creation) into the Primakoff-Holstein potential.

Section 4.1 Evaluation of the three body energy shift in lithium like ions

The main result of the previous sections is given by equation (2.2.23); the expression for the total three body potential in configuration space. It is the purpose of this part of the thesis to determine whether these three body potentials become important for the atomic structure of heavy atoms. In order to make progress in this direction we consider a much simpler and naive system; a high Z ($Z\alpha \sim 1$), three electron ion, and calculate the energy shift of this system due to the presence of the three - body interelectronic potential.

Experimentally one might determine the three body contribution to the shift by looking at the ionization potential in the lithium sequence. We define this potential as the difference of the ground state energy of a helium like ion, and the energy of the three electron ion; both ions having a nuclear charge Ze.

Let us consider the eigenvalue equation for the lithium like ion

$$\left(\sum_i h(i)\,\Lambda_+(i) + \sum_{i<j} V_2(i,j) + \sum_{i<j<k} V_3(i,j,k)\right)\psi = E\,\psi \qquad (4.1.1)$$

where V2, V3 are the two, and three body potentials respectively. V_3 is smaller than V_2 by a factor e^2,

therefore we can express the solution to the above eq. as,

$$\psi = \psi_2 + e^2\psi' + O(e^4) + \ldots \qquad (4.1.2)$$

where ψ_2 is the solution to (4.1.1) with $V_3 = 0$, and ψ' is the first order correction to ψ_2. Furthermore let us consider ψ_2 to be a solution with even parity. The ionization potential can then be defined as

$$IP = IP(2) - \langle\psi_2|V_3|\psi_2\rangle + O(e^2) + \ldots \qquad (4.1.3)$$

where IP(2) would be the ionization potential if the three body potential, $V_3=0$. Layzer and Bachall[32] have developed a pertubation expansion for IP(2) in terms of the expansion parameters 1/Z, and $(Z\alpha)$. This expansion has been utilized with wide success by many authors[32], however we are only concerned with the evaluation of the three body component $\Delta E = \langle\psi_2|V_3|\psi_2\rangle$, of the above expression. For high values of Z we can approximate the ψ_2, by the zero order wave functions ψ_2^0, the states constructed from Dirac - Coulomb wavefunctions. This is valid since the central nuclear field (we neglect the finite nuclear size, which will be justified by our final result) will dominate over the two body interelectronic potential for a

three-electron ion. This is a restatement of the 1/Z, Zα expansion used by Layzer and Bachall, the difference being that we use the full Dirac Coulomb wavefunctions for the zero order states, whereas Layzer-Bachall start from the nonrelativistic wavefunctions in their perturbation expansion. If we are interested in only the the even parity solutions of ψ_2, then we can express ψ_2^0 in terms of the 1s, 2s, Dirac Coulomb wavefunctions, i.e $\psi_2^0 \equiv |\Psi\rangle = (1s^2 2s)\ ^2S$.

Instead of using the configuration space representation of these potentials it is more convenient to calculate the shifts in Fock space. Reexpressing the state $|\Psi\rangle$ in the occupation representation and using the Fock space Hamiltonians, H^{C-T}, H^{P}, H^{T-T}, constructed in chapter two, we have,

$$\Delta E = \langle\Psi|H^{C-T}|\Psi\rangle + \langle\Psi|H^{P}|\Psi\rangle + \langle\Psi|H^{T-T}|\Psi\rangle . \qquad (4.1.4)$$

In order to calculate the above expression for the Coulomb-transverse, and transverse-transverse shift we use an approximation that we call the static limit approximation (SL). Justification for using this, and other approximations are given in the last section of this chapter.

Section 4.2 The Coulomb - transverse contribution

Consider the three-body operator (2.2.5)

$$H_{C-T} = \sum_{\substack{nlm \\ n'l'm'}} b_n^{\dagger} b_l^{\dagger} b_m^{\dagger} b_{m'} b_{l'} b_{n'} V^{C-T}_{nlm,n'l'm'} + H.c \qquad (4.2.1)$$

where the $V^{C-T}_{nlm,n'l'm'}$ are given in (2.2.8). These matrix elements are composed of the $\eta_{nl,n'm'}$ matrix elements given by (2.1.27). We will now consider an approximation for these matrix elements which will be justified in a later section. We approximate (2.1.27) by expanding the cosine terms to second order in a Taylor expansion, we get

$$\eta_{nl,n's} \cong - e^2/2$$

$$\langle n\ l | \alpha_l \cdot \alpha_L\ (1 - w^2_{nn'} r^2_{12}/2h^2c^2)/r_{12} +$$

$$w_{nn'} w_{ls} r_{12}\ /2h^2c^2 \ | n'\ s\rangle \qquad (4.2.2)$$

the $\eta_{nl,n's} - \eta_{ln,sn'}$, factor in (2.2.8) then becomes,

$$e^2/4h^2c^2 \langle n\ 1 | \bar{\alpha}_1 \cdot \bar{\alpha}_2\, r_{12} (W^2_{nn'} - W^2_{1s}) | n'\ s \rangle$$

(4.2.3)

or

$$V^{C-T}_{nlm,n'l'm'} = \alpha^2/4 \sum \langle nl | \bar{\alpha}_1 \cdot \bar{\alpha}_2\, r_{12} (W_{nn'} - W_{1s}) | ns \rangle$$

$$\langle sm | 1/r_{34} | l'm' \rangle, \qquad (\alpha \equiv e^2/\hbar c).$$

(4.2.4)

Using the above expression and the Dirac equation to replace the eigenvalues with operators we get

$$\alpha^2/4 \sum_s \langle nl | \left[h(1), \bar{\alpha}_1 \cdot \bar{\alpha}_2\, r_{12} \right] - \left[h(2), \bar{\alpha}_1 \cdot \bar{\alpha}_2\, r_{12} \right] | n's \rangle$$

$$\langle sm | 1/r_{34} | l'm' \rangle.$$

(4.2.5)

We now use the completness property of the Dirac spinors and include the H.c term in (4.2.1) to get

$$H_{C-T} = \sum_{\substack{nlm \\ n'l'm'}} b^+_n b^+_l b^+_m b_{m'} b_{l'} b_{n'}\, Q^{C-T}_{nlm,n'l'm'}$$

where,

$$Q^{C-T}_{n1m,n'1'm'} = \alpha^2/4 \langle n1m | [[h(1), \bar{\alpha}_1 \cdot \bar{\alpha}_2 r_{12}], 1/r_{23}]$$

$$- [[h(2), \bar{\alpha}_1 \cdot \bar{\alpha}_2 r_{12}], 1/r_{23}] | n'1'm' \rangle =$$

$$\alpha^2/4 \langle n1m | ihc [\bar{\alpha}_2 \cdot (\bar{\nabla}_2 1/r_{23}), \bar{\alpha}_1 \cdot \bar{\alpha}_2 r_{12}] | n'1'm' \rangle$$

(4.2.6)

where we have used the Jacobi identity for the double commutator and,

$$[h(1), 1/r_{23}] = 0 , \qquad [r_{12} , 1/r_{23}] = 0,$$

$$[h(2), 1/r_{23}] = -ihc \, \bar{\alpha}_2 \cdot (\bar{\nabla}_2 1/r_{23}) .$$

(4.2.7)

Finally using the commutation relationship for the Dirac matrices

$$[\alpha_a, \alpha_b] = 2i \epsilon^{abc} \Sigma_c$$

(4.2.8)

we have

$$Q^{C-T}_{n1m,n'1'm'} =$$

$$-\hbar c \alpha^2/2 \langle n1m \mid (\bar{\nabla}_1 1/r_{23}) \cdot (\bar{\alpha}_1 \times \bar{\Sigma}_2 \; r_{12} \;) \mid n'1'm' \rangle .$$

(4.2.9)

We must now evaluate the above matrix elements using 1s, 2s Dirac-Coulomb wave functions . We express the four component wave functions in terms of large and small components (see appendix A.1)

$$\varphi_n(r) = \begin{pmatrix} P_n(r)/r & \chi^{j,m}_{\mu}(\theta,\varphi) \\ iQ_n(r)/r & \chi^{j,m}_{-\mu}(\theta,\varphi) \end{pmatrix}$$

(4.2.10)

P,Q are the large and small radial components of the spinor, with n as the radial quantum number. The χ^{jm}_{μ} are the two component spin-orbit eigenfunctions, with total angular momentum j, and m as the azimuthal quantum number μ is the parity of the spin-orbit functions. In this section we will be dealing only with s wave spinors, with quantum numbers j=1/2, and μ = +1. We introduce a shorthand notation by labeling the spin orbit functions with the superscript denoting only the magnetic quantum number, and the subscript by the parity assignment $\mu = \pm 1$, or by the orbital angular momentum λ , which is related to μ , via , $\lambda = 1/2 - 1/2(\mathrm{sgn}(\mu))$.

We now expand the matrix element given in (4.2.9),

$$
\begin{aligned}
Q^{C-T}_{abc,a'b'c'} = \hbar c\alpha^2/2 \int_0^\infty dr_1 \int_0^\infty dr_2 \int_0^\infty dr_3 \Big\{ & \\
\Big[P_c(r_3)P_{c'}(r_3) \langle \chi_s^c(3) | (\nabla_i 1/r_{23}) | \chi_s^{c'}(3) \rangle & \\
+ Q_c(r_3)Q_{c'}(r_3) \langle \chi_p^c(3) (\nabla_i 1/r_{23}) | \chi_p^{c'}(3) \rangle \Big] \times & \\
\Big[(P_a(r_1)Q_{a'}(r_1)P_b(r_2)P_{b'}(r_2) \times & \\
\langle \chi_s^a(1)\chi_s^b(2) | i(\bar{\sigma}_i \times \bar{\sigma}_1) r_{12} | \chi_p^{a'}(1)\chi_s^{b'}(2) \rangle & \\
- Q_a(r_1)P_{a'}(r_1)P_b(r_2)P_{b'}(r_2) \times & \\
\langle \chi_p^a(1)\chi_s^b(2) | i(\bar{\sigma}_i \times \bar{\sigma}_1) r_{12} | \chi_s^{a'}(1)\chi_s^{b'}(2) \rangle & \\
+ P_a(r_1)Q_{a'}(r_1)Q_b(r_2)Q_{b'}(r_2) \times & \\
\langle \chi_s^a(1)\chi_p^b(2) | i(\bar{\sigma}_i \times \bar{\sigma}_1) r_{12} | \chi_p^{a'}(1)\chi_p^{b'}(2) \rangle & \\
- Q_a(r_1)P_{a'}(r_1)Q_b(r_2)Q_{b'}(r_2) \times & \\
\langle \chi_p^a(1)\chi_p^b(2) | i(\bar{\sigma}_i \times \bar{\sigma}_1) r_{12} | \chi_s^{a'}(1)\chi_p^{b'}(2) \rangle \Big] \Big\} &
\end{aligned}
\tag{4.2.11}
$$

The bra-ket notation above refers to angular integration,

the subscrits s, p, refer to s, p, state spin orbit functions, and r_i is now the radial coordinate of the i'th particle. We now proceed to evaluate the angular integral,

$$\langle \chi^c_\lambda(3) \mid (\nabla_2 1/r_{23}) \mid \chi^c_\lambda(3) \rangle \tag{4.2.12}$$

for $\lambda = 0, 1$. Using eqn.(III-33) in Armstrong[33] we can represent the vector operator $\bar{\nabla}_2(1/r_{23})$ by,

$$\bar{\nabla}_2(1/r_{23}) =$$

$$\sum_k (-1)^k (k(2k+1)(2k-1)/3)] \; (r_2^{k-1}/r_3^{k+1}) \left[C^{(k-1)}(2)C^k(3)\right]^1$$

for ($r_3 > r_2$),

$$\sum_k (-1)^{k+1} ((k+1)(2k+1)(2k+3)/3)] (r_3^k/r_2^{k+2}) \left[C^{k+1}(2)C^k(3)\right]^1$$

for ($r_2 > r_3$)

(4.2.13)

We now consider the matrix element

$$\langle \chi^c_\lambda(3) | [C^{k'}(2)\; C^k(3)]^1_0 | \chi^c_\lambda(3) \rangle \quad ,$$

this is proportional to the reduced matrix element

$$\langle \chi_{\lambda}(3) \| C^{k}(3) \| \chi_{\lambda}(3) \rangle \propto \begin{pmatrix} \lambda & \lambda & k \\ 0 & 0 & 0 \end{pmatrix} \times \begin{Bmatrix} 1/2 & k & 1/2 \\ \lambda & 1/2 & \lambda \end{Bmatrix}$$

(4.2.14)

where we have used the Wigner-Eckart theorem, and (A.2.9). The 3-j symbol selection rules require $\lambda + \lambda + k$ = even, thus for s-waves we require k=0, for p waves the 3-j symbols are nonvanishing for k=0,2 but the 6-j symbol is non-vanishing for k=1,0 therefore only k=0 will give a non vanishing matrix element, thus we need only to consider the k=0 partial wave in the expansion (4.2.13), .i.e

$$\left(\bar{\nabla}_{1} \, 1/r_{23} \right)_{k=0} = -\left[C^{1}(2) C^{0}(3) \right]^{1} \, 1/r_{2}^{2}$$

$$= - C^{1}(2)/r_{2}^{2}$$

(4.2.15)

The r_3 integrations can immediatly be done to give

$$-1/r_{2}^{2} \, C^{1}(2) \, \delta(m_{c}, m_{c'}) \times$$

$$\int_{0}^{r_{1}} dr_{3} \, (P_{c}(r_{3}) P_{c'}(r_{3}) + Q_{c}(r_{3}) Q_{c'}(r_{3})).$$

(4.2.16)

We must now carry out the rest of the angular integrations. The r_3-integration above is a tensor operator proportional to $C^1(2)$, combining this result with (4.2.11), the integrations over the coordinates of particle 1 and 2 will involve the scalar operator f(1,2) defined by,

$$f(1,2) = i\,\bar{\sigma}(1)\,(\,C^1(2) \times \bar{\sigma}(2)\,)\,|r_{12}| \tag{4.2.17}$$

We can express the operator $|r_{12}|$ in a partial wave expansion,

$$|r_{12}| = \sum_{k}^{\infty} v_k(1,2) C^k(1)\cdot C^k(2) \tag{4.2.18}$$

where $v_k(1,2)$ is given in (A.2.11).

We can now recouple the operator f(1,2) using the recoupling formula (A.2.10) to get,

$$\begin{aligned} f(1,2) &= \sum_{k} i(\,\bar{\sigma}(1)\cdot T^1(2))(C^k(1)\cdot C^k(2))\; v_k(1,2) \\ &= \sum_{k,L} (-1)^{k+L} i(\sigma(1) C^k(1))^L\; (T^1(2) C^k(2))^L\; v_k(1,2) \end{aligned} \tag{4.2.19}$$

where we have defined,

$$T^1(2) = C^1(2) \times \sigma(2)$$

(4.2.20)

Although the summation over the indices k,L has an infinite range, selection rules for the matrix elements of our interest will restrict the sum to the k=1,L=1, partial waves. We need only consider matrix elements of the operator

$$f(1,2) = i(\sigma(1)C^1(1))^1 \cdot (T^1(2)C^1(2))^1 v_1(1,2)$$

(4.2.21)

We will now prove the above stated selection rules and proceed to calculate the neccessary matrix elements of f(1,2). A cursory look at the angular integrations in (4.2.11) show that the integration over particle 1 involves initial and final spin-orbit eigenfunctions that differ by one unit of the orbital angular momenta (i.e the initial and final spin orbit states are of opposite parity.) Using (4.2.19) we must perform integrals of the type,

$$\langle \chi^{a}_{\pm\mu}(1) | (\sigma(1)C^k(1))^L_q | \chi^{a'}_{\mp\mu}(1) \rangle .$$

(4.2.22)

These types of matrix elements occur frequently in applications, and in appendix A.3 we defined the coefficient $E^k(j,\mu\,;j',\mu';L)$ for matrix elements

proportional to (4.2.22). In eq.(A.3.12) the selection rules for these coefficients are given by, K=1, L= 0,1 for the quantum numbers in (4.2.22). We now draw attention to the angular integrations over particle 2 in (4.2.11). The relevant tensor operator in this space will be

$$(T^{1}(2) C^{k=1}(2))^{L=0,1}. \tag{4.2.23}$$

The L=0 term is proportional to the scalar product

$$T^{1}(2)\ C^{1}(2) = (C^{1}(2) \times \bar{\sigma}(2))^{1} \cdot C^{1}(2)$$

$$= (C^{1}(2) \times C^{1}(2)) \cdot \bar{\sigma}(2) = 0. \tag{4.2.24}$$

therefore we have proved that, (4.2.21) is the only partial wave of f(1,2) we need to consider.

We now calculate the matrix elements of f(1,2). In (4.2.11) we have a typical angular integral,

$$\langle \chi^{a}_{\pm\mu}(1)\, \chi^{b}_{\pm\nu}(2) \mid f(1,2) \mid \chi^{a}_{\mp\mu}(1)\, \chi^{b}_{\pm\nu}(2) \rangle \tag{4.2.25}$$

where $\mu, \nu = \pm 1$. Using the Wigner-Eckart theorem and (4.2.21) we get for the above integral

$$X^{L=1}(\, m_a m_{a'}; m_b m_{b'})\, x$$

$$i\, v_1(1,2)\, E^{k=1}(1/2\ \pm\mu\ ;1/2\ \mp\mu\ ;L=1)\langle \chi_{\pm\nu} \| (T^1 C^1)^1 \| \chi_{\pm\nu} \rangle$$

(4.2.26)

where we have used (A.3.9), and the definition (A.3.6) for the magnetic quantum number coefficients X^L.
We now need to evaluate the reduced matrix element

$$\langle \chi_{\pm\nu} \| (T^1 C^1)^1 \| \chi_{\pm\nu} \rangle =$$

$$i/\sqrt{2}\ \langle \chi_{\pm\nu} \| (C^1 \times \bar{\sigma}) \times C^1 \| \chi_{\pm\nu} \rangle$$

(4.2.27)

where we have used (4.2.20), and (A.2.5). Expanding the triple vector product we get

$$(\, C^1 \cdot C^1)\bar{\sigma} - C^1(\bar{\sigma} \cdot \bar{C}^1) =$$

$$\bar{\sigma} - C^1(\bar{\sigma} \cdot C^1).$$

(4.2.28)

Therefore (4.2.27) becomes,

$$i/\sqrt{2}\ \langle \chi_{\pm\nu} \| \bar{\sigma} - c^1(\bar{\sigma}\cdot c^1) \| \chi_{\pm\nu} \rangle .$$

(4.2.29)

We now make use of the well known identity,

$$(\bar{\sigma}\cdot c^1)\ |\ j, s=1/2, m, \pm\mu\rangle \quad = |\ j, s=1/2, m, \mp\mu\rangle$$

(4.2.30)

(where we have explicitly reintroduced all the quantum numbers for the spin orbit functions). Thus (4.2.29) becomes

$$i/\sqrt{2}\ (\langle \chi_{\pm\nu} \| \sigma \| \chi_{\pm\nu} \rangle - \langle \chi_{\pm\nu} \| c^1 \| \chi_{\mp\nu} \rangle).$$

(4.2.31)

Let us now evaluate these reduced matrix elements for $\mu = +1, -1$ separately, first for $\mu = 1$ the above equation becomes

$$i/\sqrt{2}\ (\ \langle j=1/2,\ \lambda=0,\ s=1/2 \| \sigma \| j=1/2,\ \lambda=0,\ s=1/2 \rangle\ -$$

$$\langle j=1/2,\ \lambda=0,\ s=1/2 \| c^1 \| j=1/2,\ \lambda=1,\ s=1/2 \rangle\ ).$$

(4.2.32)

We can simplify the above to get

$$i/\sqrt{2} \left[(2) \begin{Bmatrix} 1/2 & 1 & 1/2 \\ 1/2 & 0 & 1/2 \end{Bmatrix} \langle s=1/2 \| \sigma \| s=1/2 \rangle \right.$$

$$\left. - (-2) \begin{Bmatrix} 1/2 & 1 & 1/2 \\ 1 & 1/2 & 0 \end{Bmatrix} \langle \lambda=0 \| c^1 \| \lambda=1 \rangle \right]$$

$$= i\ 2/\sqrt{3} \qquad (4.2.33)$$

where we have used (A.2.8) and (A.2.9).

Also we consider (4.2.31) for $\nu = -1$, we now have

$$i/2 \ (\langle j=1/2, s=1/2, \lambda=1 \| \sigma \| j=1/2, s=1/2, \lambda=1 \rangle -$$

$$\langle j=1/2, s=1/2, \lambda=1 \| c^1 \| j=1/2, s=1/2, \lambda=0 \rangle =$$

$$i/\sqrt{2} \ (-2) \begin{Bmatrix} 1/2 & 1 & 1/2 \\ 1/2 & 1 & 1/2 \end{Bmatrix} \langle s=1/2 \| \sigma \| s=1/2 \rangle$$

$$- (2) \begin{Bmatrix} 1/2 & 1 & 1/2 \\ 0 & 1/2 & 1 \end{Bmatrix} \langle \lambda=1 \| c^1 \| \lambda=0 \rangle$$

$$= -i\ 2/\sqrt{3} \ . \qquad (4.2.34)$$

To summarise,

$$\langle \chi_{\pm\nu} \| (T^1 C^1)^1 \| \chi_{\pm\nu} \rangle = \nu\ i\ 2/\sqrt{3} \ , \text{ for } \nu = \pm 1. \qquad (4.2.35)$$

Combining the above result, and (4.2.26) we get a compact expression for the matrix element of the operator f(1,2)

$$\langle \chi^{a}_{\pm\mu}(1)\,\chi^{b}_{\pm\nu}(2)|f(1,2)|\chi^{a'}_{\mp\mu}(1)\,\chi^{b'}_{\pm\nu}(2)\rangle =$$

$$- X^{L=1}(m_a m_{a'};m_b m_{b'})\; v_1(1,2)\; E^{k=1}(1/2\ \pm\mu\ ;1/2\ \mp\mu\ ;L=1)(2/\sqrt{3})\nu$$

$$= - X^{L=1}(m_a m_{a'};m_b m_{b'})\;\; 4/3\; v_1(1,2)\,\mu\nu$$

(4.2.36)

where we have used (A.3.14), for the value of the E^k coefficients.

Having expressed the matrix elements of f(1,2) above and the integrations over particle 3 given in (4.2.16), we can express the matrix element of the three-body operator (4.2.11) as a three dimensional radial integral. Inserting (4.2.36) and (4.2.16) into (4.2.11) we get

$$Q^{C-T}_{abc,a\,b\,c} = -\mathrm{Ryd}\ (\delta(m_c,m_{c'})\; X^{L=1}(m_a m_{a'};m_b m_{b'})$$

$$R(aa',bb',cc') \qquad (4.2.37)$$

where R(aa',bb',cc') is a three dimensional radial integral defined by,

$$R(aa',bb',cc') = \int_0^{\infty} dx_1 \int_0^{\infty} dx_2 \;\; 4/3 \; v_1(x_1,x_i)^{*}$$

$$(P_a(x_1)Q_{a'}(x_1) + Q_a(x_1)P_{a'}(x_1))^{*}$$

$$(P_b(x_2)P_{b'}(x_2) - Q_b(x_2)Q_{b'}(x_2))^{*}$$

$$(1/x_2^2) \int_0^{x_2} dx_3 \left(P_c(x_3)P_{c'}(x_3) + Q_c(x_3)Q_{c'}(x_3)\right). \qquad (4.2.38)$$

We have rescaled the radial coordinates r_i into the dimensionless coordinates $x_i = r_i / \lambda\!\!\!^{-}$, $\lambda\!\!\!^{-}$ being the Compton wavelength $\hbar/mc$. The radial components P(x), Q(x) are normalized such that

$$\int_0^{\infty} dx \; (P^2(x) + Q^2(x)) = 1 \qquad (4.2.39)$$

The explicit forms for the 1s, 2s radial wave functions are,

$$P_{1s}(x) = N_{1s}(1+\gamma)^{n_r} x^{\gamma} e^{-\lambda_1 x}$$

$$Q_{1s}(x) = -N_{1s}(1-\gamma)^{n_r} x^{\gamma} e^{-\lambda_1 x}$$

$$P_{2s}(x) = N_{2s}(1+W_2)^{n_r} x \; e^{-\lambda_2 x} (c_0 + c_1 x)$$

$$Q_{2s}(x) = -N_{2s}(1-W_2)^{n_r} x^{\gamma} e^{-\lambda_2 x} (a_0 + a_1 x)$$

where,

$$N_{1s} = (2Z\alpha)^{\gamma+1/2}/[2\Gamma(2\gamma+1)]^{1/2}$$

$$N_{2s} = (2Z\alpha)^{\gamma+1/2} \times [(2\gamma+1)/(1+2W_2)(\Gamma(1+2\gamma)]^{1/2}$$

$$W_2 = [(1+\gamma)/2]^{1/2} \qquad = (Z\alpha)/2W_2 \ , \ \lambda_1 = (Z\alpha)$$

$$c_0 = 2W_2 \ , \ a_0 = 2(1+W_2) \ ,$$

$$c_1 = a_1 = -(Z\kappa)(2W_2+1)/[(2\gamma+1)(W_2)]$$

(4.2.40)

The above expression for $Q^{C-T}_{nml,n'm'l'}$ can now be used for the evaluation of the three-body shift (4.1.5) It is convenient to evaluate this shift in Fock-space instead of relying on configuration space methods. The three-body Hamiltonian is given by (4.2.1) where we now use the approximation for $V^{C-T}_{nml,n'm'l'}$ outlined above. We consider an unperturbed three electron system in a Coulomb field with charge Ze ,

$$|\Psi\rangle = 1/\sqrt{3!}\; b_a^+ b_b^+ b_c^+ \; |0\rangle$$

(4.2.41)

The subscripts refer to the radial, angular momentum, orbital and magnetic quantum numbers for each electron. In our case

$$a=(\; j_a=1/2,\; n_a=1,\; \lambda_a=0,\; m_a=1/2\;)$$

$$b=(\; j_b=1/2,\; n_b=1,\; \lambda_b=0,\; m_b=-1/2)$$

$$c=(\; j_c=1/2,\; n_c=2,\; \lambda_c=0,\; m_c=+1/2)$$

(4.2.42)

The shift of the unperturbed state ΔE due to the interaction H^{C-T} is given by

$$\Delta E = \langle\Psi|H_{C-T}|\Psi\rangle$$

(4.2.43)

Using the expression (4.2.6) for H^{C-T} we can write (4.2.43) as a sum of 36 terms

$$\Delta E = 1/6 \sum_{\rho} \left(U_{abc,[abc]} - U_{abc,[bac]} \right)$$

(4.2.44)

where $\sum_{\phi}$ refer to the sum of all cyclic permutations of [abc], and [acb], and $U_{abc,\ abc}$ is the symmetrized three body interaction defined by,

$$U_{abc,a'b'c'} = S\ (\ Q^{C-T}_{abc,a'b'c'}\ ) \qquad (4.2.45)$$

where $Q^{C-T}_{abc,a'b'c'}$ is given in (4.2.37) and the symmetrization operator S, was defined in (3.2.3).

Magnetic quantum number selection rule $\delta(m_c m_{c'})$ for electron 3 in (4.2.37) allows only twenty of the thirty six matrix elements to be non-vanishing. The remaining matrix elements can be catagorized according to the initial and final spin states of electron 1 and 2. We shall define three distinct types of matrix elements,

Type I: These are matrix elements where the initial spin of electron 1 or 2 is opposite to the final spin. We shall call these spin-flip (SF) terms.

Type II: The initial and final spin for each particle is conserved, and electron 1 and 2 have anti-parallel spins. We shall label these as spin-conserving anti-parallel terms (SCAP).

Type III: The spin is conserved for each particle and electron 1 and 2 have parallel spins. We call these, spin conserving parallel (SCP) terms.

We can evaluate the $X^{L=1}$ coefficients for each grouping using a standard table of 3-j coefficients[34]. We have

$$X^{L=1}(SF) = 1/3,\ X^{L=1}(SCP) = 1/6,\ X^{L=1}(SCAP) = -1/6 \qquad (4.2.46)$$

Collecting the diagrams according to their grouping we have.

The spin-flip (SF) terms are,

$$(V_{bca,abc} + V_{bac,cba} + V_{abc,bca} + V_{cba,bac}$$

$$- V_{abc,bac} - V_{bac,abc} - V_{cba,bca} - V_{bca,cba}).$$

The spin conserving anti-parallel (SCAP) terms give

$$(V_{abc,abc} + V_{bca,bca} + V_{bac,bac} + V_{cba,cba}$$

$$- V_{abc,cba} - V_{bca,bac} - V_{bac,bca} - V_{cba,abc})$$

and the spin-conserving parallel (SCP) terms give

$$(V_{cab,cab} + V_{acb,acb} - V_{cab,acb} - V_{acb,cab}).$$

(4.2.47)

Using the angular coefficients given on the previous page for each group we can collect all the above terms and express them as a sum of radial integrals R(nn':ll';mm') defined in (4.2.38), we get

$$+1/3\ (R(11;21;12)+R(12;11;21)+R(11;12;21)+R(21;11;12)$$

$$-R(11;11;22)-R(11;11;22)-R(21;12;11)-R(12;21;11))$$

$$-1/6\ (R(11;11;22)+R(11;22;11)+R(11;11;22)+R(22;11;11)$$

$$-R(12;11;21)-R(11;21;12)-R(11;12;21)-R(21;11;12))$$

$$+1/6\ (R(22;11;11)+R(11;22;11)-R(21;12;11)-R(12;21;11))$$

(4.2.48)

where the numeral 1, and 2 are the radial quantum numbers for the 1s, and 2s wavefunctions respectively.

Adding all the terms and using the symmetry of the radial integrals under the interchange of particle coordinates i.e. R(nn';...;...) = R(n'n;...;...) etc. we can finally express the three-body level shift as

$$\triangle E = -\mathrm{Ryd}/6 \left[R(11;11;22) - R(11;12;12) + R(12;12;11) - R(12;11;12) \right] \qquad (4.2.49)$$

These triple radial integrals are evaluated numerically and tabulated in Table I.

Table I. The Coulomb - transverse contribution to the energy shift (4.2.49).

Z	$\triangle E^{C-T}$ (in Rydbergs)
137	$-.198 \times 10^{-1}$
130	$-.101 \times 10^{-1}$
118	$-.525 \times 10^{-2}$
100	$-.227 \times 10^{-2}$
80	$-.928 \times 10^{-3}$

Section 4.3 Virtual pair contribution

In the previous chapter we discussed the three-body interaction term H_p, due to the presence of virtual electron-positron pairs. In Fock space this term is given by the expression (2.2.20)

$$H_p = 1/2 \sum_{\substack{nlm,\\ n'l'm'}} b^{\dagger}_{n} b^{+}_{l} b^{+}_{m} b_{n'} b_{l'} b_{m'} \left(V^{p}_{nlm,n'l'm'} \right) + (\text{Hermitian conjugate}) \qquad (4.3.1)$$

where,

$$V^{p}_{nlm,n'l'm'} = \sum_{w}^{(-)} \frac{\langle n\ w|V(1,2)|n'\ l'\rangle\langle l\ m|V(3,4)|w\ m'\rangle}{W_{mm'} + E_{\ell} + |w|} \qquad (4.3.2)$$

the summation above represents the integral over the continuum of positron wavefunctions, w being the energy of the positrons. The operator, $V(1,2) = C(1,2) + B(1,2)$ is the sum of the Coulomb interaction and the generalised Breit interaction.

We wish to evaluate the lowest order energy shift of the three electron system discussed in the previous section for values of $(Z\alpha) \sim 1$. We evaluate the shift $\Delta E_p = \langle \Psi | H_p | \Psi \rangle$ where $|\Psi\rangle$ is given in (4.2.41), expanding, we have

$$\Delta E_p = \sum_{[P]} U^P_{abc,[abc]} - U^P_{abc,[bac]} \quad , \tag{4.3.3}$$

where,

$$U^P_{abc,a'b'c'} = S\,(\,V^P_{abc,a'b'c'}). \tag{4.3.4}$$

Instead of evaluating (4.3.3) directly, we decompose the three-body Hamiltonian (4.3.1) into Coulomb-Coulomb, Coulomb-Breit, Breit-Breit, contributions, the corresponding energy shifts can then be defined by,

$$\Delta E_{C-C} = \sum_{[P]} U^{C-C}_{abc,[abc]} - U^{C-C}_{abc,[bac]} \tag{4.3.5}$$

where,

$$U^{C-C}_{abc,a'b'c'} = S\,(\,V^{C-C}_{abc,a'b'c'}) \tag{4.3.6}$$

and,

$$V^{C-C}_{abc,a'b'c'} = \sum_{w}^{(-)} \frac{\langle aw \mid C(1,2) \mid a'b' \rangle \langle bc \mid C(1,2) \mid wc' \rangle}{W_{cc'} + E_b + |w|}. \tag{4.3.7}$$

$$\Delta E_{C-B} = \sum_{[p]} U^{C-B}_{abc,[abc]} - U^{C-B}_{abc,[bac]} \tag{4.3.8}$$

where,

$$U^{C-B}_{abc,a'b'c'} = S\left(V^{C-B}_{abc,a'b'c'} \right) \tag{4.3.9}$$

and,

$$V^{C-B}_{abc,a,'b,'c'} = 2 \sum^{(-)} \frac{\langle aw | C(1,2) | a'b' \rangle \langle bc | \tilde{B}(1,2) | w\ c' \rangle}{W_{cc'} + E_b + |w|} . \tag{4.3.10}$$

$$\Delta E_{B-B} = \sum_{[p]} U^{B-B}_{abc,[abc]} - U^{B-B}_{abc,[bac]} \tag{4.3.11}$$

where,

$$U^{B-B}_{abc,a'b'c'} = S\left(V^{B-B}_{abc,a'b'c'} \right) \tag{4.3.12}$$

and,

$$V^{B-B}_{abc,a'b'c'} = \sum \frac{\langle aw | \tilde{B}(1,2) | a'c' \rangle \langle bc | \tilde{B}(1,2) | wc' \rangle}{W_{cc'} + E_b + |w|} . \tag{4.3.13}$$

The total shift is now expressed as,

$$\Delta E_p = \Delta E_{C-C} + \Delta E_{C-B} + \Delta E_{B-B} . \tag{4.3.14}$$

In order to evaluate the above matrix elements we must have at our disposal the Dirac-Coulomb positron wave function. Borrowing from the appendix A.1, we have,

$$\varphi_w(\vec{r}) = \begin{pmatrix} P_w(r)/r & \chi_\mu^{j,m}(\theta,\varphi) \\ iQ_w(r)/r & \chi_{-\mu}^{j,m}(\theta,\varphi) \end{pmatrix} \tag{4.3.15}$$

The $\chi_\mu^{j,m}(\Omega)$ are angular components for s-wave positrons. The radial components are given by,

$$P_w(r) = -(w-1)^{1/2}\, r\, K(p)\, \mathrm{Im}\left[e^{-ipr}\, e^{i\Omega}\, {}_1F_1(1+\gamma+iy, 1+2\gamma, 2ipr)\right]$$

$$Q_w(r) = +(1+w)^{1/2}\, r\, K(p)\, \mathrm{Re}\left[e^{-ipr}\, e^{i\Omega}\, {}_1F_1(1+\gamma+iy, 1+2\gamma, 2ipr)\right] \tag{4.3.16}$$

where p is the local momentum defined by, $p=(1+w)^{1/2}$, w being the absolute value of the negative continuum energy. Also,

$$K(p) = \frac{e^{\pi y/2}\,|\Gamma(\gamma+iy)|}{(\pi p)^{1/2}\,\Gamma(1+2\gamma)} \quad ,$$

$y = -(Z\alpha)w/p$, and the

the phase factor

$$e^{i\Omega} = (-1+iy/w)(\gamma+iy) \quad , \quad \gamma = (1-(Z\alpha)^2)^{1/2}.$$

(4.3.17)

These wave functions are normalized to the energy scale i.e

$$\int_0^\infty dx\ (P_w(x)P_{w'}(x) + Q_w(x)Q_{w'}(x)) = \delta(w-w')$$

(4.3.18)

Let us first concentrate on the Coulomb-Coulomb, ΔE_{c-c} contribution to the shift (4.3.3). The matrix elements appearing in the expression (4.3.7) have been discussed in appendix A.3, all the bound states are j=1/2, s-wave states, therefore the angular selection rule for the D^L coefficients, (see appendix A.3) require only the j=1/2, s-wave positron wavefunctions to appear in the summation (4.3.7). We thus have for the matrix elements of our interest (s-states), (here we use the subscripts a,b,a',b', to designate the quantum numbers of an arbitrary Dirac - Coulomb spinor)

$$\langle a\ b \mid C(1,2) \mid a'b' \rangle =$$

$$e^2 \, X^{L=0}(\, m_a m_{a'}; m_b m_{b'}) R^C(a\ a'; b\ b'), \tag{4.3.19}$$

where we have used (A.3.5). The radial integral R^C is defined as,

$$R^C(aa';bb') = \int_0^\infty dx_1 \int_0^\infty dx_2 \, (P_a(x_1)P_{a'}(x_1) + Q_a(x_1)Q_{a'}(x_1)) \times$$

$$(P_b(x_2)P_{b'}(x_2) + Q_b(x_2)Q_{b'}(x_2)). \tag{4.3.20}$$

All Coulomb matrix elements are now expressed in terms of these radial integrals. The R^C terms have various symmetries i.e.

a) Symmetry under interchange of the particle cordinates $R^C(aa',bb') = R^C(bb';aa')$.

b) Symmetry under the exchange of initial and final states of each particle, $R^C(aa';bb') = R^C(a'a,b'b)$.

This is due to the reality of all the radial wavefunctions as our phase convention.

Using the expression (A.3.6) for the coefficients that depend upon the magnetic quantum numbers of the shift,

$$X^{L=0}(m_a m_{a'};m_b m_{b'}) = 1/2\,\delta(m_a,m_{a'})\,\delta(m_b,m_{b'})$$

(4.3.21)

we get nonvanishing contributions to (4.3.3) for the terms where the spin is conserved between the initial and final states of each particle. We then get,

$$\begin{aligned}\triangle E_{C-C} = 1/6\ \ (&V^{C-C}_{abc,abc} + V^{C-C}_{cab,cab} + V^{C-C}_{bca,bca} \\ &+ V^{C-C}_{bac,bac} + V^{C-C}_{acb,acb} + V^{C-C}_{cba,cba}) \\ &- (V^{C-C}_{abc,cba} + V^{C-C}_{cab,acb} + V^{C-C}_{bca,bac} \\ &+ V^{C-C}_{bac,bca} + V^{C-C}_{acb,cab} + V^{C-C}_{cba,abc})\end{aligned}$$

(4.3.22)

Expressing the ΔE_{C-C} in terms of the radial integrals R^C, and parametrizing these integrals with the numeral 1 representing the 1s state, the numeral 2 represents the 2s state, and the letter w represents the continuum state with energy w. We also introduce the notation,

$$\Delta R^C = \frac{R^C(ab;cw)}{W_{ab} + E_c + |w|} \tag{4.3.23}$$

We thus have,

$$\begin{aligned}\Delta E_{C-C} = 1/6 \sum_w \Big\{ & R^C(11;w1)\Delta R^C(1w;22) \\ & + R^C(22;w1)\Delta R^C(1w;11) + R^C(11;w2)\Delta R^C(2w;11) \\ & + R^C(11;w1)\Delta R^C(1w;22) + R^C(11;w2)\Delta R^C(2w;11) \\ & + P^C(22;w1)\Delta R^C(1w;11) - (R^C(12;w1)\Delta R^C(1w;21) \\ & + R^C(21;w2)\Delta R^C(1w;11) + R^C(11;w1)\Delta R^C(2w;12) \\ & + R^C(11;w2)\Delta R^C(1w;21) + R^C(12;w1)\Delta R^C(2w;11) \\ & + R^C(21;w1)\Delta R^C(1w;12) \Big\}.\end{aligned} \tag{4.3.24}$$

The summation over w represents the sum over the continuum wave functions with respect to the energy w, of the positrons. We can make a transformation to a new integration variable, p the local momenta of the positrons by the substitution

$$\sum_{w} dw \longrightarrow \int_{0}^{\infty} dp\ p/w\ . \tag{4.3.25}$$

Using the symmetry properties of the R^C integrals we can simplify (4.3.26), thus

$$\begin{aligned}\Delta E_{C-C} = 1/6 \int_{0}^{\infty} dp\ p/w \Big\{ & 4\ R^C(11;1p)\Delta R^C(21;2p) \\ & + R^C(12;1p)\Delta R^C(12;1p) - 2\ R^C(12;1p)\Delta R^C(21;1p) \\ & - R^C(11;2p)\Delta R^C(11;2p) - R^C(21;1p)\Delta R^C(21;1p) \\ & - R^C(11;2p)\Delta R^C(11;2p)\Big\}.\end{aligned} \tag{4.3.26}$$

We now evaluate the Coulomb-Breit contribution to the energy shift,(4.3.8) The operator B(1,2) appearing in the matrix elements (4.3.10) is the non-local Breit operator discussed at length in chapter 2, as a matter of convenience we shall approximate $\tilde{B}(1,2)$ by the local magnetic (Gaunt) operator G(1,2) given by (1.1.19). The justification for this simplification is discussed in section 4.5. Matrix elements for the Gaunt interaction are discussed in appendix A.3. It was pointed out in the previous paragraph that selection rules for the Coulomb operator allow only the s wave positrons to contribute in the summations (4.3.7) and (4.3.10), again as in the case for the Coulomb matrix elements we need only be concerned with the matrix elements of the Gaunt operator between s wave spinors, using (A.3.10) we have,

$$\langle ab|\tilde{B}(1,2)|a'b'\rangle \approx \langle ab\,|\,-e^2\,\bar{\alpha}_1\cdot\bar{\alpha}_1/r_{12}\,|\,a'b'\rangle$$

$$= 2/3\; X^{L=0}(m_a m_{a'};m_b m_{b'})\; e^2 J^-(a\,a';b\,b')$$

$$-\; 4/3\; X^{L=1}(m_a m_{a'};m_b m_{b'})\; e^2 J^+(a\,a';b\,b'). \qquad (4.3.27)$$

Where we have used (A.3.15) and defined the auxillary integrals,

$$J^{(+,-)}(aa';bb') =$$

$$- \int_0^\infty dx_1 \int_0^\infty dx_2 \quad \frac{r_<}{r_>^2} \left(P_a(x_1)Q_{a'}(x_1) \pm P_a(x_1)Q_{a'}(x_1)\right) \times$$

$$\left(P_b(x_2)Q_{b'}(x_2) \pm P_b(x_2)Q_{b'}(x_2)\right). \qquad (4.3.28)$$

The J^+ integrals have the same symmetry properties as the R^C integrals discussed previously, whereas the J^- change sign under the interchange of the initial and final state of a particle.

We now classify our matrix elements in terms of the magnetic quantum number assignments of the Breit matrix elements.

We define as in section 2 the cases,

Case I) Spin conserving parallel (SCP) terms ,where

$m_a = m_{a'}$, $m_b = m_{b'}$, $m_a = m_b$.

$$R_1^B(aa';bb') = 1/3\ J^-(aa';bb') - 2/9\ J^+(aa';bb') \qquad (4.3.29)$$

Case II) Spin conserving anti-parallel (SCAP), where

$m_a = m_{a'}$, $m_b = m_{b'}$, $m_a = -m_b$.

$$R_2^B(aa';bb')$$

$$= 1/3\ J^-(aa';bb') + 2/9\ J^+(aa';bb') \qquad (4.3.30)$$

case III) Spin flip (SF) terms,where

$m_a = -m_{a'}$, $m_b = -m_{b'}$.

$$R_3^b(aa';bb')$$

$$= 4/3\ J^+(aa';bb').$$

(4.3.31)

Collecting all terms in the shift (4.3.8) and catogorizing them according to the groupings defined above, we have

Case I: SCP terms

$$v^{C-B}_{bca,bca} + v^{C-B}_{bac,bac} - v^{C-B}_{bca,bac} - v^{C-B}_{bac,bca}.$$

(4.3.32)

Case II: SCAP terms

$$v^{C-B}_{abc,abc} + v^{C-B}_{cab,cab} + v^{C-B}_{acb,acb} + v^{C-B}_{cba,cba}$$

$$- v^{C-B}_{abc,cba} - v^{C-B}_{cab,acb} - v^{C-B}_{acb,cab} - v^{C-B}_{cba,abc}.$$

(4.3.33)

Case III: SF terms

$$v^{C-B}_{abc,cab} + v^{C-B}_{acb,cba} + v^{C-B}_{cab,abc} + v^{C-B}_{cba,acb}$$

$$- v^{C-B}_{cab,cba} - v^{C-B}_{cba,cab} - v^{C-B}_{abc,acb} - v^{C-B}_{acb,abc}.$$

(4.3.34)

Each of the above matrix elements can now be expressed in terms of the integrals R^C, R_1^B, R_2^B, R_3^B, we get

$$I) \quad \int_0^\infty dp\ p/w \times$$

$$\Big[R^C(11;p1)\triangle R_1^B(2p;12) + R^C(11;p2)\triangle R_1^B(1p;21)$$

$$- R^C(11;p2)\triangle R_1^B(2p;11) - R^C(11;p1)\triangle R_1^B(1p;22)\Big]$$

$$II) \quad \int_0^\infty dp\ p/w \times$$

$$\Big[R^C(12;p1)\ R_2^B(1p;21) + R^C(21;p2)\ R_2^B(1p;11)$$

$$+ R^C(12;p1)\ R_2^B(2p;11) + R^C(21;p1)\ R_2^B(1p;12)$$

$$- R^C(11;p1)\ R_2^B(1p;22) - R^C(22;p1)\ R_2^B(1p;11)$$

$$- R^C(11;p2)\ R_2^B(2p;11) - R^C(22;p1)\ R_2^B(1p;11)\Big]$$

III) $\int_0^\infty dp\ p/w\ ^{k}$

$$\{R^C(11;p2)\triangle R^B_3(1p;21) + R^C(11;p1)\triangle R^B_3(2p;12)$$

$$+ R^C(21;p1)\triangle R^B_3(1p;12) + R^C(21;p2)\triangle R^B_3(1p;12)$$

$$- R^C(22;p1)\triangle R^B_3(1p;11) - R^C(22;p1)\triangle R^B_3(1p;11)$$

$$- R^C(12;p1)\triangle R^B_3(1p;21) - R^C(12;p1)\triangle R^B_3(2p;11)\}$$

($\triangle R$ is defined as in (4.3.23)). (4.3.35)

Finally we evaluate the Breit -Breit energy shift $\triangle E_{b-b}$. Again we make use of the previous approximation for the generalized Breit operator and expression (4.3.27) for the relevant matrix elements. Selection rules now allow both $s^{1/2}$ and $d^{3/2}$ positrons in the intermediate states, we will make a further approximation by considering only the $s^{1/2}$ positron contribution, this will be justified later. Instead of writing out by hand each of the contributions in (4.3.11) we will get a general expression for the V^{B-B} terms as a product of the J^+, J^-, integrals defined in (4.3.28). Inserting the matrix elements (4.3.27) into (4.3.13) we get,

$$V^{B-B}_{abc,a'b'c'} = \int_0^\infty dp\ p/w\ \times$$

$$\Big\{ M_{00}(aa',bb',cc')\ 4/9\ J^{(-)}(aa';pb')J^{(-)}(bp;cc')$$

$$-M_{01}(aa',bb',cc')\ 8/9\ J^{(-)}(aa';pb')J^{(+)}(bp;cc')$$

$$-M_{01}(cc',bb',\partial\partial')8/9\ J^{(+)}(aa';pb')J^{(-)}(bp;cc')$$

$$+M_{11}(aa',bb',cc')16/9\ J^{(+)}(aa';pb')J^{(+)}(bp;cc')\Big\} \qquad (4.3.36)$$

where we have defined the coefficients,

$$M_{ij}(aa';bb';cc') = \sum_s X^{L=i}(m_a m_{a'};m_s m_{b'})X^{L=j}(m_b m_s;m_c m_{c'}).$$

(4.3.37)

Using (A.3.6) for the X^L coefficients, we have

$$M_{00}(aa';bb';cc') = 1/4 \quad \delta(m_a, m_{a'})\delta(m_b, m_{b'})\delta(m_c, m_{c'})$$

$$M_{01}(aa';bb';cc') =$$

$$1/12 \quad \delta(m_a, m_{a'})\delta(m_b, m_{b'})\delta(m_c, m_{c'})\,(-1)^{m_b - m_c}$$

$$+ 1/6 \quad \delta(m_a, m_{a'})\delta(m_b, -m_{b'})\delta(m_c, -m_{c'})\delta(m_b, -m_c)$$

$$M_{11}(aa';bb';cc') =$$

$$1/36 \quad \delta(m_a, m_{a'})\delta(m_b, m_{b'})\delta(m_c, m_{c'}) \quad (-1)^{m_A - m_b}$$

$$+1/18 \quad \delta(m_a, m_{a'})\delta(m_b, -m_{b'})\delta(m_c, -m_{c'})\delta(m_a, -m_c) \quad (-1)^{m_a + m_b}$$

$$+1/18 \quad \delta(m_a, -m_{a'})\delta(m_b, -m_{b'})\delta(m_c, m_{c'})\delta(m_a, -m_b) \quad (-1)^{-m_b - m_c}$$

$$+1/9 \quad \delta(m_a, -m_{a'})\delta(m_c, -m_{c'})\delta(m_b, m_{b'})\delta(m_a, m_b)\delta(m_a, -m_c) .$$

(4.3.38)

Having expressed the energy shifts in terms of the one dimensional integrals R^C, J^+, J^- we proceed to evaluate these integrals and reduce the shifts to a two-dimensional quadrature problem.

In order to carry out the p-integration we must first integrate over the radial coordinates of all the particles, using the expression (4.2.40) for the bound state wave functions and (4.3.16) for the positron wave functions the R^C, J^+, J^-, can be expressed as a linear combination of the generic integral defined by,

$$I_k(\lambda_1 n;\lambda_2 m) = \int_0^\infty dx_1 \int_0^\infty dx_2\, e^{-ipx}\, F(1+\gamma+iy, 2\gamma+1, 2ipx)\cdot$$

$$\left(x^n x_1^{2\gamma} e^{-\lambda_1 x_1}\right)\left(e^{-\lambda_2 x_2} x_2^m x^{2\gamma}\right)\frac{x_<^k}{x_>^{k+1}}. \qquad (4.3.39)$$

The evaluation of this integral will be taken up in a later paragraph. It wil be convenient to first get an expression for the $J^{(+,-)}$ (ap;bc) integrals defined in (4.3.28)

The subscripts a,b,d refer to some bound state radial wavefunction and p refers to the continuum wave function. Let us reexpress the 1s, 2s radial wave functions (4.2.40) as,

$$P_n(x) = x^\gamma e^{-\lambda_n x} L_n(x)$$

$$Q_n(x) = x^\gamma e^{-\lambda_n x} K_n(x) \qquad (4.3.40)$$

where the L_n and K_n are polynomials defined by,

$$L_n(x) = q_n^1 + q_n^2 x$$

$$K_n(x) = r_n^1 + r_n^2 x$$

(4.3.41)

(n=1,n=2 refer to the 1s, 2s radial wavefunctions respectively.) therefore,

$$q_1^1 = N(1s)(1+\gamma)^{1/2} \ , \ q_1^2 = 0$$

$$q_2^1 = N(2s)(1+W_2)^{1/2} \ a_0, \ q_2^2 = N(2s)(1+W_2)^{1/2} \ a_1$$

$$r_1^1 = -N(1s)(1-\gamma)^{1/2} \ , \ r_1^2 = 0$$

$$r_2^1 = -N(2s)(1-W_2)^{1/2} \ b_0, \ r_2^2 = -N(2s)(1-W_2)^{1/2} \ b_1$$

(4.3.42)

Inserting (4.3.40), and (4.3.16) into the integral (4.3.28) we get

$$J^{(+,-)}(ap;bc) = -\,\mathrm{Re}\,K(p)\Big[e^{i\Omega}\,(1+w)^{1/2}\int_0^\infty dx_1\int_0^\infty dx_2\,\frac{x_<}{x_>^2}\,\times$$

$$x_1^{2\gamma}x_2^{2\gamma}\,e^{-\lambda_a x_1 - ipx_1}\,e^{-(\lambda_b+\lambda_c)x_2}\,\times$$

$$\left\{L_b(x_2)K_c(x_2) \pm K_b(x_2)L_c(x_2)\right\}\left(L_a(x_1)\,F(1+\gamma+iy,1+2\gamma,2ipx)\right]$$

$$\left(\begin{matrix}+\\-\end{matrix}\right)$$

$$\mathrm{Im}\,K(p)\Big[e^{i\Omega}\,(1-w)^{1/2}\int_0^\infty dx_1\int_0^\infty dx_2\,x_1^{2\gamma}\,x_2^{2\gamma}\,\frac{x_<}{x_>^2}\;\;e^{-\lambda_a x_1 - ipx_1}\,\times$$

$$e^{-(\lambda_b+\lambda_c)x_2}\,\times$$

$$\left\{L_b(x)K_c(x) \pm K_b(x)L_c(x)\right\}\left(K_a(x)\,F(1+\gamma+iy,2\gamma+1,2ipx)\right]$$

(4.3.43)

The above form can be simplified if we define,

$$\left\{\begin{matrix}H^1_{+-}(ap;bc)\\H^2_{+-}(ap;bc)\end{matrix}\right\} = \int_0^\infty dx_1\int_0^\infty dx_2\Big[x_1^{2\gamma}\;x_2^{2\gamma}\,\frac{x_<}{x_>^2}\;\;e^{-\lambda_1 x_1 - ipx_1}\,e^{-(\lambda_b+\lambda_c)x_2}\,\times$$

$$\left[L_b(x)K_c(x) \pm K_b(x)L_c(x)\right]\times$$

$$\left\{\begin{matrix}L_a(x)\\K_a(x)\end{matrix}\right\}\times{}_1F_1(1+\gamma+iy,1+2\gamma,2ipx)\Big].$$

(4.3.44)

These integrals can now be expressed in terms of the q, and r coefficients, using (4.3.41) and (4.3.42) we get,

$$\begin{Bmatrix} H^1_{+-}(ap;bc) \\ H^2_{+-}(ap;bc) \end{Bmatrix} = \int_0^\infty dx_1 \int_0^\infty dx_2 \Big[x_1^{2\gamma} x_2^{2\gamma} e^{-\lambda_a x_1 - ipx_1} e^{-(\lambda_b+\lambda_c)x_2} \times$$

$$\Big[(q_b^1 r_c^1 \pm q_c^1 r_b^1) + (q_b^1 r_c^2 + q_b^2 r_c^1)$$

$$\pm (q_c^1 r_b^2 + q_c^2 r_b^1) \; x_2$$

$$\pm (q_b^2 r_c^2 + q_c^2 r_b^2) \; x_1^2 \Big] \times$$

$$\begin{Bmatrix} q^1{}_a + q^2{}_a \, x_1 \\ r^1{}_a + q^2{}_a \, x_1 \end{Bmatrix} {}_1F_1(1+\gamma+iy, 1+2\gamma, 2ipx_1) \Big] .$$

(4.3.45)

We now express the H integrals in terms of the I integrals (4.3.39)

$$\begin{Bmatrix} H^1_{+-}(ap;bc) \\ H^2_{+-}(ap;bc) \end{Bmatrix} = (q_b^1 r_c^1 \pm q_c^1 r_b^1) \times$$

$$\Big[I_1(\lambda_a \; n=0; \; \lambda_b+\lambda_c \; m=0) \begin{Bmatrix} q^1{}_a \\ r^1{}_a \end{Bmatrix} + I_1(\lambda_a \; n=1; \; \lambda_b+\lambda_c \; m=0) \begin{Bmatrix} q^2{}_a \\ r^2{}_a \end{Bmatrix} \Big]$$

$$+\left[\left(q_b^1 r_c^2 + q_b^2 r_c^1 \right) \pm \left(q_c^1 r_b^2 + q_c^2 r_b^1 \right)\right] \times$$

$$\left[I_1(\lambda_a\, n=0;\ \lambda_b+\lambda_c\ m=1) \begin{Bmatrix} q^1{}_a \\ r^1{}_a \end{Bmatrix} + I_1(\lambda_a\, n=1;\ \lambda_b+\lambda_c\ m=1) \begin{Bmatrix} q^2{}_a \\ r^2{}_a \end{Bmatrix}\right]$$

$$+ \left(q_b^2\, r_c^2 + q_c^2\, r_b^2\right) \times$$

$$\left[I_1(\lambda_a n=0;\ \lambda_b+\lambda_c\ \ m=2) \begin{Bmatrix} q^1{}_a \\ r^1{}_a \end{Bmatrix} + I_1(\lambda_a\, n=1;\ \lambda_b+\lambda_c\ m=2) \begin{Bmatrix} q^2{}_a \\ q^2{}_a \end{Bmatrix}\right].$$

(4.3.46)

Finally we can express the $J^{(+,-)}$ as,

$$J^{(+,-)}(ap;bc) = - \mathrm{Re}\ K(p)\ e^{i\Omega}\ (1+w)^{1/2}\ H^{1}_{+-}(ap;bc)$$

$$(\pm)\ \mathrm{Im}\ K(p)\ e^{i\Omega}\ (1-w)^{1/2}\ H^{2}_{+-}(ap;bc).$$

(4.3.47)

We now turn our attention toward parametrizing the Coulomb integrals R^C in terms of the I integrals. Inserting (4.3.40) for the radial wavefunctions into the definition for R^C (4.3.20) we get

$$R^C(ap;bc) = K(p) \left[(1+w)^{1/2} \text{ Re } F^2(ap;bc) \right.$$
$$\left. -(w-1)^{1/2} \text{ Im } F^1(ap;bc) \right] \qquad (4.3.48)$$

where the F coefficients are given by,

$$\begin{Bmatrix} F^1(ap,bc) \\ F^2(ap,bc) \end{Bmatrix} = (q_b^1 q_c^1 + r_b^1 r_c^1) \times$$

$$\left[I_0(\lambda_a \, n=0, \, \lambda_b+\lambda_c \, m=0) \begin{Bmatrix} q_a^1 \\ r_a^1 \end{Bmatrix} + I_0(\lambda_a \, n=1; \, \lambda_b+\lambda_c \, m=0) \begin{Bmatrix} q_a^2 \\ r_a^2 \end{Bmatrix} \right]$$

$$+ (q_b^2 q_c^1 + q_b^1 q_c^2 + r_b^2 r_c^1 + r_b^1 r_c^2) \times$$

$$\left[I_0(\lambda_a \, n=0; \, \lambda_b+\lambda_c \, m=1) \begin{Bmatrix} q_a^1 \\ r_a^1 \end{Bmatrix} + I_0(\lambda_a \, n=1; \, \lambda_b+\lambda_c \, m=1) \begin{Bmatrix} q_a^2 \\ r_a^2 \end{Bmatrix} \right]$$

$$+ (q_b^2 q_c^2 + r_b^2 r_c^2) \times$$

$$\left[I_0(\ \lambda_a\ n=0;\ \lambda_b+\lambda_c m=2) \begin{Bmatrix} q_a^1 \\ r_a^1 \end{Bmatrix} + I_0(\ \lambda_a\ n=1;\ \lambda_b+\lambda_c m=2) \begin{Bmatrix} q_a^2 \\ r_a^2 \end{Bmatrix} \right].$$

(4.3.49)

Above we have been able to express the R^C , R_1^B , R_2^B , R_3^B, radial integrals in terms of the more basic integral $I_k(\lambda_1\ n;\ \lambda_2 m)$ defined in (4.3.39). We now proceed to evaluate this double integral, first we reexpress(4.3.39) as the sum,

$$I_k(\ \lambda_1\ n;\ \lambda_2\ m) = \int_0^\infty dx\ x^{n+2}\ e^{-x(\ \lambda_1\ +ip)}\ {}_1F_1(1+\gamma+iy, 1+2\gamma, 2ipx)$$
$$\times \left[1/x^{k+1} \int_0^x dz\ e^{-\lambda_2 z}\ z^{m+k+2} + x^k \int_x^\infty dz\ e^{-\lambda_2 z}\ z^{m-k-1+2} \right].$$

(4.3.50)

We now make the substitution $z = xt$, and $dz = xdt$, to get,

$$I_k(\ \lambda_1 n;\ \lambda_2 m) = \left[\int_0^1 dt\ t^{\ m+k+1+2\gamma} + \int_0^1 dt\ t^{m-k+2\sigma} \right] \times$$
$$\int_0^\infty dx\ x^{n+m+4}\ e^{-x(\ \lambda_1 + \lambda_2 t\ +\ ip)}\ {}_1F_1(1+\gamma+iy, 1+2\gamma, 2ipx)$$

(4.3.51)

The integral over x can be done immediatly. We have

$$\int_0^\infty dx\; x^{n+m+4}\; e^{-x(\lambda_1 + \lambda_2 t + ip)}\; {}_1F_1(1+\gamma+iy, 2\gamma+1, 2ipx) =$$

$$\frac{\Gamma(n+m+4+1)}{(\lambda_1 + \lambda_2 t + ip)^{n+m+4\gamma+1}}\; {}_2F_1\left(1+\gamma+1y, n+m+4\gamma+1, 2\gamma+1, \frac{2ip}{(\lambda_1+\lambda_2 t + ip)}\right)$$

$$\text{for} \quad \left|\lambda_1 + \lambda_2 t + ip\right| > 2ip. \qquad (4.3.52)$$

We now make use of a linear transformation on the hypergeometric function to get for the above integral,

$$\frac{\Gamma(1+n+m+4\gamma)}{(\lambda_1+\lambda_2 t + ip)^{1+m+n+4\gamma}} \times \left(\frac{\lambda_1 + t+ip}{\lambda_2 + t-ip}\right)^{1+\gamma+iy} \times$$

$${}_2F_1\left(1+\gamma+iy, -n-m-2\gamma, 1+2\gamma, \frac{-2ip}{\lambda_1+\lambda_2 t - ip}\right)$$

$$(4.3.53)$$

When the second argument in the above hypergeometric function is a negative integer or zero, ${}_2F_1$ becomes a polynomial and analytic in the entire complex plane (i.e. for all p). We will be dealing only with s-wave positrons where $\gamma = (1 - (Z\alpha))^{1/2}$, we can therefore conveniently express the integrand in (4.5.53) as a complex polynomial for $\gamma = 0$ ($Z = 137$), $\gamma = 1/2$ ($Z = 118$) and $\gamma = 1$ (small Z). Inserting (4.3.53) into

(4.3.51) we have,

$$I_k(\lambda_1 n;\lambda_2 m) = \Gamma(1+n+m+4\gamma)\Big\{\kappa \int_0^1 dt \Big[\frac{t^{m+k+2}}{(\lambda_1+\lambda_2 t+ip)^{1+n+m+4}}$$

$$ {}_2F_1(1+\gamma+iy,-n-m-2\gamma,1+2\gamma, \frac{-2ipt}{\lambda_1+\lambda_2 t-ip}) \Big] \kappa$$

$$e^{-2y\theta_1} e^{i\theta_1(1+2\gamma)}$$

$$+ \int_0^1 dt \Big[\frac{t^{n+k+2}}{(\lambda_1+t(\lambda_2+ip))} e^{-2y\theta_2} e^{i\theta_2(1+2\gamma)} \kappa$$

$$ {}_2F_1(1+\gamma+iy,-n-m-2\gamma,1+2\gamma, \frac{-2ip}{\lambda_2+t(\lambda_1-ip)}) \Big] \Big\}$$

where we have defined,

$$\theta_1 = \arctan(p/(\lambda_1+\lambda_2 t)), \quad \text{and}$$

$$\theta_2 = \arctan(pt/(\lambda_2+\lambda_1 t)). \qquad (4.3.54)$$

The substitution $t \to 1/t$ was used in the second t integral above.

Having reduced the radial integrals R^C, J_-^+ into one dimensional integrals given by, (4.3.48), and (4.3.37) respectively, we can proceed to evaluate the shift (4.3.2) numerically. This is accomplished by the codes RACC, RACB, RABB which evaluate the shifts $\triangle E^{C-C}$, $\triangle E^{C-B}$, $\triangle E^{B-B}$, given in (4.3.5), (4.3.8), and (4.3.11) respectively. Results for the above shifts are presented in Table II, for values $(Z\alpha) = 1$, $(Z\alpha) = .867$.

Table II. The virtual pair contributions to the energy shift given by (4.3.5), in atomic units.

Z	ΔE^{C-C}	ΔE^{C-B}	ΔE^{T-T}
137	$.17 \times 10^{-1}$	$.82 \times 10^{-3}$	$.28 \times 10^{-4}$
118	$.16 \times 10^{-2}$	$\lesssim 10^{-4}$	$\lesssim 10^{-5}$

Section 4.4 The transverse - transverse contribution

We must also evaluate the transverse-transverse contribution to the three-body energy given by the expression (2.2.13)

$$H_{T-T} =$$

$$\sum b^{+}_{n} b^{+}_{l} b^{+}_{m} b_{m'} b_{l'} b_{n'} \; V^{T-T}_{nml,n'm'l'} + \quad H.c \tag{4.4.1}$$

where, $V^{T-T}_{nml,n'm'l'} =$

$$-1/2 \sum_{s} \Delta\eta_{nl,ns} \; (\; 3 \; \eta_{ms,m'l'} + \eta_{sm,lm'} \;),$$

$$\Delta\eta_{nl,ns} = \eta_{nl,ns} - \eta_{ln,sn} \tag{4.4.2}$$

the η matrix elements being defined in (2.1.21). We now make use of the same approximation for $\Delta\eta$ given by (4.2.2), in addition we use the local form for the Breit operator in the η terms. With these approximations, we obtain for $V^{T-T}_{nml,n'm'l'}$,

$$V^{T-T}_{nm1,n'm'1'} = - e^2/4\hbar^2c^2 \sum_s \times$$

$$\langle n1|[h(1) - h(2), \bar{\alpha}_1 \cdot \bar{\alpha}_2 r_{12}]|n's\rangle\langle ms|G(3,4)|m'1'\rangle$$

(4.4.3)

where G(3,4) is the Gaunt operator (see appendix 3).We could proceed to evaluate the above terms in a similar manner to the one used in the evaluation of the transverse - Coulomb term; using a sum rule and evaluating repeated commutators. This procedure becomes quite cumbersome, because of the presence of the G(1,2) operator. Instead we shall proceed to evaluate (4.4.3) by first evaluating all angular integrals in the above matrix elements and then invoking a sum rule for radial components of the Dirac - Coulomb spinors. All initial and final states of the matrix elements of (4.4.2) are s-wave Dirac-Coulomb spinors. Parity selection rules for the Gaunt operator show that the intermediate states in (4.4.3) can only be (j=1/2,s-wave), (j=3/2,d-wave) spinors, the largest contributions come from the s waves since these are closer to the nucleus. We will thus consider only these intermediate states in (4.4.3). Let us first evaluate the term in (4.4.3) given by

$$\sum_{s} \langle n1 | [h(1), \bar{\alpha}_1 \cdot \bar{\alpha}_2 \, r_{12}] | n's \rangle \langle ms | G(3,4) | m'1' \rangle \tag{4.4.4}$$

We first perform the angular integrations for the relevant matrix elements given by,

$$\langle n1 \mid W_{1s} \, \bar{\alpha}_1 \cdot \bar{\alpha}_2 \, r_{12} \mid n\, s \rangle =$$

$$+ 2/3 \int_0^\infty dr_1 \int_0^\infty dr_2 \; v(1,2) \Big\{ \times X^{L=0}(m_a m_a' ; m_b m_s) \times$$

$$YM_{nn'}(1) YM_{1s}(2) W_{1s} - 2X^{L=1}(m_a m_a' ; m_b m_s) YP_{nn'}(1) YP_{1s}(2) W_{1s} \Big\}$$

(4.4.5)

and, $\langle ms | G(3,4) | m'1' \rangle =$

$$- 2/3 \int_0^\infty dr_3 \int_0^\infty dr_4 \; g(3,4) \Big\{ X^{L=0}(m_s m_b' ; m_c m_c') \; YM_{mm'}(3) YM_{s1'}(4)$$

$$- 2X^{L=1}(m_s m_b' ; m_c m_c') \; YP_{mm'}(3) YP_{s1'}(4) \Big\}.$$

(4.4.6)

We use the notation introduced in the previous sections for the coefficients X^L with the arguments m_a, m_a', m_b, m_b', m_c, m_c', m_s, corresponding to the magnetic quantum numbers of states n, n', l, l' m, m' s respectively. were we have used (A.3.8) and $v(1,2)$, $g(2,3)$ are given by (A.2.11). We also have defined the functions,

$$YM_{nn'}(r) = P_n(r)Q_{n'}(r) - Q_n(r)P_{n'}(r) = -YM_{n',n}(r)$$

$$YP_{nn'}(r) = P_n(r)Q_{n'}(r) + Q_n(r)P_{n'}(r) = YP_{n',n}(r).$$

(4.4.7)

In order to exploit sum rules for the radial functions we must reexpress the $YM_{ls}(r)W_{ls}$ and $YP_{ls}(r)W_{ls}$ factors by making use of the radial equations for j=1/2, s-wave Dirac spinors. Using (A.1.10) we have,

$$E_s P_s(r) = \hbar c\,(d/dr + 1/r)Q_s(r) + (mc^2 + u(r))P_s(r)$$

$$E_s Q_s(r) = -\hbar c\,(d/dr - 1/r)P_s(r) - (mc^2 - u(r))Q_s(r)$$

(4.4.8)

therefore,

$$YM_{ls}(r)W_{ls} = W_{ls}(P_1(r)Q_s(r) - P_s(r)Q_1(r)) =$$

$$E_1P_1(r)Q_s(r) - P_1(r)E_sQ_s(r)$$

$$- E_1P_s(r)Q_1(r) + E_sP_s(r)Q_1(r)$$

$$=$$

$$Q_s(r)(\hbar c(d/dr + 1/r)Q_1(r) + (mc^2 + u)P_1(r))$$

$$- P_l(r)(-\hbar c(d/dr - 1/r)P_s(r) - (mc^2 - u)Q_s(r))$$

$$+ \{l \leftrightarrow s\} \quad =$$

$$\hbar c(d/dr(P_l(r)P_s(r) + Q_l(r)Q_s(r)))$$

$$-2/r(P_l(r)P_s(r) - Q_l(r)Q_s(r)))$$

$$+ 2mc^2(P_l(r)Q_s(r) + P_s(r)Q_l(r)$$

(4.4.9)

We introduce the notation,

$$ZP_{ls}(r) = P_l(r)P_s(r) + Q_l(r)Q_s(r) = ZP_{sl}(r)$$

$$ZM_{ls}(r) = P_l(r)P_s(r) - Q_l(r)Q_s(r) = ZM_{sl}(r)$$

(4.4.10)

and thus rewrite (4.4.9), using the above notation

$$YM_{ls}(r)W_{ls} =$$

$$\hbar c\ d/dr(ZP_{ls}(r)) - 2\hbar c/r\ (ZM_{ls}(r)) + 2mc^2(YP_{ls}(r))$$

(4.4.11)

In the same manner we express the factor $YP_{ls}(r)W_{ls}$,

$$YP_{ls}(r)W_{ls} =$$

$$= Q_s(r)(\hbar c(d/dr + 1/r)Q_l(r) + (mc^2 + u)P_l(r)$$

$$- P_l(r)(-\hbar c(d/dr - 1/r\ )P_s(r) - (mc^2 - u)Q_s(r)$$

$$\{l \leftrightarrow s\} =$$

$$\hbar c\ d/dr(ZM_{ls}(r)) + 2hc(Q_s(r)d/dr(Q_l(r)) - P_s(r)d/dr(P_l(r))$$

$$+ 2mc^2 YM_{ls}(r)$$

(4.4.12)

where we have again used the Dirac equation.

Using the above expresions (4.4.11) and (4.4.12) in (4.4.5) and (4.4.6) we can rewrite our matrix elements,

$$\langle n1 \mid W_{ls}\ \bar{\alpha}_1 \cdot \bar{\alpha}_t \mid r_{12} \mid \mid n's \rangle =$$

$$+\ 2/3 \int_0^\infty dr_1 \int_0^\infty dr_2 \times \Big\{ X^0(m_a m_{a'}; m_b m_s) \times$$

$$\Big[-\tfrac{1}{2}hc\,(d(1,2)\,ZP_{ls}(2) - 2v(1,2)/r_2\ ZM_{ls}(2)) +$$

$$2mc^2 v(1,2) YP_{ls}(2) \Big] YM_{nn'}(1)$$

$$- 2X^1(m_a m_{a'}; m_b m_s) \Big[-hc\ d(1,2) ZM_{ls}(2)$$

$$+2hc(Q_s(2)\ (d/dr_2(Q_1(2)) - P_s(2)(d/dr_2(P_1(2)))$$

$$+\ 2mc^2\ YM_{ls}(2) \Big]\ YP_{nn}\ (1) \Big\}$$

(4.4.13)

where we have integrated by parts and introduced the notation $d(1,2) = d/dr_2\ v(1,2)$.

We now derive sum rules for the radial functions appearing in the above matrix elements. We can express the radial equations (4.4.8) as

$$H_{eff} \Psi_s = E_s \Psi_s$$

(4.4.14)

where we define,

$$\Psi = \begin{pmatrix} P_s(r) \\ Q_s(r) \end{pmatrix}$$

(4.4.15)

and

$$H_{eff} = \begin{pmatrix} -\hbar c(d/dr - 1/r) & -(mc^2 - u) \\ mc^2 + u & \hbar c(d/dr + 1/r) \end{pmatrix}$$

(4.4.16)

The completeness property of the eigenstates of (4.4.14) is given by

$$\sum_s \Psi_s(r)\, \Psi_s(r') = \delta(r - r')I \qquad I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

or,

$$\sum_s P_s(r)P_s(r') = \delta(r - r') \quad , \sum_s Q_s(r)Q_s(r') = \delta(r - r')$$

$$\sum_s P_s(r)Q_s(r') = 0 \qquad (4.4.17)$$

We now use the above sum rules to express the various sums that occur in the evalution of (4.4.4). We have,

$$\sum_s ZP_{ls} YP_{s1'} = YP_{11'} \qquad \sum_s YP_{ls} YP_{s1'} = ZP_{11'}$$

$$" \quad ZP_{ls} YM_{s1'} = YM_{11'} \qquad " \quad YP_{ls} YM_{s1'} = -ZM_{11'}$$

$$" \quad ZM_{ls} YP_{s1'} = YM_{11'} \qquad " \quad YM_{ls} YP_{s1'} = ZM_{11'}$$

$$" \quad ZM_{ls} YM_{s1'} = YP_{11'} \qquad " \quad YM_{ls} YM_{s1'} = -ZP_{11'}$$

(4.4.18)

In the above sums the index s, refer to the radial quantum numbers, integrations over coordinates are implicit in the above expressions i.e

$$\sum_s Q_l P_s P_s Q_{l'} =$$

$$\int_0^\infty dr_1 \int_0^\infty dr_2 \sum_s Q_l(r_1) P_s(r_1) P_s(r_2) Q_{l'}(r_2)$$

$$= \int_0^\infty dr_2 \, Q_l(r_2) Q_{l'}(r_2) =$$

$$Q_l Q_{l'} \tag{4.4.19}$$

Including only s-waves in the intermediate states and using (4.4.13), (4.4.6), and (4.4.18) and utilizing the definitions (4.3.37) for the M_{00}, M_{01}, M_{11} magnetic quantum number coefficients, we get for (4.4.4),

$$\left(\frac{2}{3}\right)^2(-1)\int_0^\infty dr_1\int_0^\infty dr_2\int_0^\infty dr_3\ \ g(2,3)\Big\{$$

$$M_{00}(aa',bb',cc')\ \Big[\ -\tfrac{1}{2}hc\ d(1,2)YM_{11},(2)-2\hbar c/r_2\ v(1,2)YP_{11},(2)$$

$$-2mc^2v(1,2)ZM_{11},(2)\Big]\ \ YM_{nn},(1)YM_{mm},(3)$$

$$-2M_{01}(aa',bb',cc')\ \Big[\ -hc\ d(1,2)YP_{11},(2)-2\hbar c/r_2v(1,2)YM_{11},(2)$$

$$+2mc^2v(1,2)ZP_{11},(2)\ \Big]\ \ YM_{nn},(1)YP_{mm},(3)$$

$$-2M_{01}(cc',bb',aa')\ \Big[\ -hc\ d(1,2)YP_{11},(2)\ -\ 2hc\ v(1,2)(P_1,(2)$$

$$d/dr_2(Q_1(2))\ -\ Q_1,(2)d/dr_2(P_1(2))$$

$$-2mc^2\ v(1,2)ZP_{11},(2)\Big]\ YP_{nn},(1)YM_{mm},(3)$$

$$+4M_{11}(aa',bb',cc')\ \Big[\ -hc\ d(1,2)YM_{11},(2)\ +\ 2hc\ v(1,2)(P_1,(2)$$

$$d/dr_2(Q_1(2))\ -\ Q_1,(2)d/dr_2(P_1(2))$$

$$+\ 2mc^2\ v(1,2)\ ZM_{11},(2)\ \Big]\ YP_{nn},(1)YP_{mm},(3)\Big\}\ .$$

(4.4.20)

We now turn our attention to the second term in (4.4.3) given by,

$$\sum_s \langle n1 | \left[h(1), \alpha_1 \cdot \alpha_2 r_{12} \right] | n's \rangle \langle ms | G(3,4) | m'1' \rangle$$

$$= \sum_s W_{nn'} \langle n1 | \alpha_1 \cdot \alpha_2 r_{12} | n's \rangle \langle ms | G(3,4) | m'1' \rangle$$

(4.4.21)

Using expression (4.4.5), and (4.4.6) for the above matrix elements, (Instead of the W_{ls} term in (4.4.5) we now have $W_{nn'}$, as a factor.) and applying the sum rules (4.4.18) we get for (4.4.21),

$$-(2/3)^2 W_{nn'} \int_0^\infty dr_1 \int_0^\infty dr_2 \int_0^\infty dr_3 \, v(1,2) g(2,3) \times$$

$$M_{00}(aa';bb';cc') \, YM_{nn'}(1) \, (-ZP_{11'}(2)) \, YM_{mm'}(3)$$

$$-2M_{01}(aa';bb';cc') \, YM_{nn'}(1) \, ZM_{11'}(2) \, YP_{mm'}(3)$$

$$-2M_{01}(cc';bb';aa') \, YP_{nn'}(1) \, (-ZM_{11'}(2)) \, YM_{mm'}(3)$$

$$+4M_{11}(aa';bb';cc') \, YP_{nn'}(1) \, ZP_{11'}(2) \, YP_{mm'}(3)$$

(4.4.22)

It is convenient to introduce a shorthand notation for the various integrals appearing in (4.4.20), and (4.4.22). We first define various functions,

$$D_1(nn',ll',mm') = g(2,3)d(1,2)YM_{nn'}(1)YM_{ll'}(2)YM_{mm'}(3)$$

$$D_2(nn',ll',mm') = g(2,3)d(1,2)YM_{nn'}(1)YP_{ll'}(2)YP_{mm'}(3)$$

$$D_3(nn';ll';mm') = g(2,3)d(1,2)YP_{nn'}(1)YP_{ll'}(2)YM_{mm'}(3)$$

$$D_4(nn';ll';mm') = g(2,3)d(1,2)YP_{nn'}(1)YM_{ll'}(2)YP_{mm'}(3)$$

$$F_1(nn';ll';mm') = g(2,3)v(1,2)/r_2\ YM_{nn'}(1)YP_{ll'}(2)YM_{mm'}(3)$$

$$F_2(nn';ll';mm') = g(2,3)v(1,2)/r_2\ YM_{nn'}(1)YM_{ll'}(2)YP_{mm'}(3)$$

$$L_1(nn';ll';mm') = v(1,2)g(2,3)\ P_{l'}(2)(d/dr_2(Q_l(2)) + Q_{l'}(2)$$

$$(d/dr_2(P_{l'}(2)))\ YP_{nn'}(1)YM_{mm'}(3)$$

$$L_2(nn';ll';mm') = v(1,2)g(2,3)\ P_{l'}(2)(d/dr_2(Q_l(2)) - Q_{l'}(2)$$

$$(d/dr_2(P_{l'}(2)))\ YP_{nn'}(1)YP_{mm'}(3)$$

$$K_1(nn',ll';mm') = v(1,2)g(2,3)\ YM_{nn'}(1)ZM_{ll'}(2)YM_{mm'}(3)$$

$$K_2(nn';ll';mm') = \quad " \quad YM_{nn'}(1)ZP_{ll'}(2)YP_{mm'}(3)$$

$$K_3(nn';11';mm') = \quad " \quad YP_{nn'}(1)ZP_{11'}(2)YM_{mm'}(3)$$

$$K_4(nn';11';mm') = \quad " \quad YP_{nn'}(1)ZM_{11'}(2)YP_{mm'}(3)$$

$$K_5(nn';11';mm') = \quad " \quad YM_{nn'}(1)ZP_{11'}(2)YM_{mm'}(3)$$

$$K_6(nn';11';mm') = \quad " \quad YM_{nn'}(1)ZM_{11'}(2)YP_{mm'}(3)$$

$$K_7(nn';11';mm') = \quad " \quad YP_{nn'}(1)ZM_{11'}(2)YM_{mm'}(3)$$

$$K_8(nn';11';mm') = \quad " \quad YP_{nn'}(1)ZP_{11'}(2)YP_{mm'}(3)$$

(4.4.23)

where we implicitly consider the D,F,L, and K coefficients as functions of the radial coordinates r_1, r_2, r_3. We introduce a notation, for the integrals over the radial coordinates of the above integrands by preceding each of the coefficients in (4.4.23) by the letter I, i.e

$$ID_1(nn';11';mm') = \int_0^\infty\int_0^\infty\int_0^\infty dx_1 dx_2 dx_3 \; D_1(nn',11',mm')$$

etc. (4.4.24)

(The x_i are the dimensionless coordinates defined in section 4.2.) Using the above definitions in (4.4.20), and (4.4.22) we get,

$$V^{\lambda=0}_{mm',n'm'1'} = 4/9\ kyd\ x$$

$$\{M_{00}(aa';bb';cc')[\ 1D_1 + 2IF_1 + 2IK_1 - W_{nn'}\ IK_5]$$

$$-2M_{01}(aa';bb';cc')[\ 1D_2 + 2IF_2 - 2IK_2 + W_{nn'}\ IK_6]$$

$$-2I_{01}(cc';bb';aa')[\ 1D_3 + 2IL_1 + 2IK_3 - W_{nn'}\ IK_7]$$

$$+4M_{11}(aa';bb';cc')[\ 1D_4 - 2IL_2 - 2IK_4 + W_{nn'}, IK_8]\}$$

(4.4.25)

where we have used a shorthand notation,

$ID(nn';ll',mm') = 1D.$

Given the expression for $V^{T-T}_{nml,n'm'l'}$ we can now write down the shift for the state (4.2.41), we get

$$\Delta E^{T-T} = \sum_{[p]} U^{T-T}_{abc,[abc]} - U^{T-T}_{abc,[bac]}$$

where,

$$U^{T-T}_{abc,a'b'c'} = S\ (2V^{T-T}_{abc,a'b'c'}).$$

(4.4.26)

The factor 2 above, is a consequence of the inclusion of the H.c. term in (4.4.1) in the energy shift.

The evaluation of this shift presents a formidable and lengthy calculation because of the large number of triple radial integrals occuring in (4.4.25). However, a few of these integrals are done by the program TRANS, and these integrals are about an order of magnitude smaller than the triple integrals encountered in section 4.2. This can also be seen by comparing the Coulomb-Coulomb, and Coulomb-Breit shifts in Table II. We can therefore neglect the transverse-transverse shift since it is smaller than the Coulomb-transverse shift discussed in section 4.2.

Section 4.5 The static limit approximation

We would now like to give some justification for the approximations that we have employed in the previous sections. In sections 4.2, and 4.5 we have approximated the matrix elements,

$\Delta\eta_{nm,n'm'} = \eta_{nm,n'm'} - \eta_{mn,m'n'}$ of the non local Breit operator by the matrix elements of a local operator by expanding the cosine terms in (2.1.27) in a power series and keeping the first term. In this section we shall henceforth call this the static limit (SL). This approximation is reasonable for $(Z\alpha) \ll 1$ since by dimensional arguments the expectation value, $\langle \cos(Wr_{12}/\hbar c) \rangle \sim \cos(Z\alpha) \sim 1$, where W is the energy difference of an electron between it's initial and final state. We would now like to see how this approximation fares when we are in the extreme relativistic regime $(Z\alpha) = 1$. In order to do this we need to compare a typical exact three body energy with the result obtained when the SL approximation for $\Delta\eta$ is used. A representative term that occurs in the Coulomb transverse energy discussed in section 4.2 is given by

$$V_3 = \sum_s \Delta\eta_{nm,n's} \, C_{sq,q'm'}/(W_{nn'}+W_{ms}) \qquad (4.5.1)$$

where (n=1,m=1,n'=1). A typical radial integral

(we consider only the Gaunt component) in the $\Delta\eta$ terms is proportional to,

$$\Delta(n) = \int_0^\infty dx_1 \int_0^\infty dx_2 \; P_1(x_1)Q_1(x_1)$$

$$(1-\cos(W_n x_{12})/x_{12}) \Big|_{L=1} \; Q_1(x_2)P_n(x_2)$$

(4.5.2)

where $P_1(x) = e^{-x}$, $Q_1(x) = -e^{-x}$ are the upper and lower radial components of the 1s, Dirac - Coulomb wavefunctions, $P_n(x)$ is the upper component in the state n (s wave), L=1 represents the L=1 radial partial wave of the non local operator, and W_n is the energy eigenvalue of the state n, (note $W_1=0$). For the Coulomb like matrix elements let us consider matrix elements such as,

$$C(n) =$$

$$\int_0^\infty dx_1 \int_0^\infty dx_2 \; P_n(x_1)P_1(x_2)\left(1/x_{12}\right)\Big|_{L=0} \; f^2(x_2),$$

$$f(x) = xe^{-x}.$$

(4.5.3)

The reasons for choosing the above form for f(x) are technical and will be discussed in a later paragraph. We

are now concerned with evaluating,

$$E = \sum_n \Delta(n)\ C(n)/W_n \tag{4.5.4}$$

Let us define the nonlocal operator in (4.5.2) by the symbol $K_w(1,2)$. Using (A.3.16) we can express this operator as, (where from now on, $w = W_n$)

$$K_w(1,2) =$$

$$-3w^2/\pi \int_{-\infty}^{\infty} dk\ \ J_1(kx_1)J_1(kx_2)\ P/(k^2-w^2). \tag{4.5.5}$$

The $P_n(x)$ functions can be expressed as a sum of confluent hypergeometric functions, let us therefore define,

$$I_w(\lambda_1,\lambda_2,\lambda_3,a) = \int_0^{\infty} dx_1 \int_0^{\infty} dx_2$$

$$e^{-\lambda_1 x_1} K_w(1,2)\ e^{-(\lambda_2+\lambda_3)x_2}\ {}_1F_1(a,1,2\ \lambda_3 x_2) \tag{4.5.6}$$

where λ_1, λ_2 , λ_3 , a, are arbitrary parameters. Using the representation (4.5.5), and the representation for the spherical Bessel functions,

$$J_1(kx) = i/2 \int_0^1 dt\ t\ (e^{ikxt} - e^{-ikxt}) \tag{4.5.7}$$

we can represent the I_w as,

$$I_w(\lambda_1,\lambda_2,\lambda_3\ a) = 6w^2/\pi \int_{-\infty}^{\infty} dk \int_0^1 du \int_0^1 dt\ t\ P/(k^2-w^2)\ x$$

$$k/((\lambda_1^2/u^2) + k^2)\ f(k),$$

$$f(k) = i/2\left(\frac{\lambda_2+\lambda_3-i\kappa t}{\lambda_2-\lambda_3-i\kappa t}\right)^a \frac{1}{(\lambda_2+\lambda_3-i\kappa t)}$$

(4.5.8)

If Real(λ_2) < λ_1, and Im(λ_1)=0, the singularities of f(k) lie in the lower half complex k plane. Integrating along an upper semicircle, we pick up the principle value at $k = \pm w$, and a residue at $k = i\,\lambda_1/u$. An additional integration over the u variable can be done to get,

$$I_w(\lambda_1,\lambda_2,\lambda_3\ a) = -3/2 \int_0^1 dt\ t\ (1 - \lambda_1/w\ \arctan(w/\lambda_1))\ x$$

$$\left\{2\ \text{Real}\left(\frac{\lambda_2+\lambda_3-i\omega t}{\lambda_2-\lambda_3-i\omega t}\right)\frac{1}{(\lambda_2+\lambda_3-i\omega t)}\right\}$$

$$+ 3\int_0^1 dt\ t\ (1/3 - (\lambda_1/w)^2 + (\lambda_1/w)^3 \arctan(w/\lambda_1))\ x$$

$$\left(\frac{\lambda_2+\lambda_3+\lambda_1 t}{\lambda_2-\lambda_3+\lambda_1 t}\right)^a \frac{1}{(\lambda_2+\lambda_3+\lambda_1 t)}$$

$$+ 3\int_0^1 dt\ t\ (1/3 - (\lambda_1/wt)^2 + (\lambda_1/wt)^3 \arctan(wt/\lambda_1))\ x$$

$$\left(\frac{t(\lambda_2+\lambda_3)+\lambda_1}{t(\lambda_2-\lambda_3)+\lambda_1}\right)^a \frac{1}{t(\lambda_2+\lambda_3)+\lambda_1}$$

(4.5.9)

We also wish to get an analogous integral that occurs in the Coulomb type matrix element C(n), we define,

$$R_W(\lambda_1,\lambda_2,\lambda_3,a) = \int_0^\infty dx_1 \int_0^\infty dx_2\ e^{-\lambda_1 x}\ e^{-\lambda_2 x} \quad (1/x_>)$$

$$x_1\ x_2\ e^{-\lambda_3 x}\ {}_1F_1(a,1,2\lambda_3 x_2) =$$

$$-1/\lambda_1^2 \left\{ \frac{(\lambda_2+\lambda_3+\lambda_1)^{a-1}}{(\lambda_2-\lambda_3+\lambda_1)^a} - \frac{(\lambda_2+\lambda_3)^{a-1}}{(\lambda_2-\lambda_3)^a} \right\}$$

(4.5.10)

We are now ready to construct the $\triangle(n)$, and C(n) matrix elements from the above defined functions. Using appendix A.1 for the Dirac - Coulomb wave functions for $(Z\alpha) = 1$, we get when P_n is a bound state,

$$\triangle(n) = \lambda^{3/2}\ (1+w/2(1+\lambda)^{1/2} \times$$

$$(-n\ I_W(2,1,\lambda,a=-n+1) + (1+\lambda)/\lambda\ I_W(2,1,\lambda,a=-n))$$

and,

$$C(n) = \lambda^{3/2}\,(1+w/2(1+\lambda))^{1/2} \times$$

$$(-n\,R(2,1,\lambda,a=-n+1) + (1+\lambda)/\lambda) \times R(2,1,\lambda,a=-n)$$

(4.5.11)

where $\lambda = 1/(1+n^2)^{1/2}$, and $w = n/(1+n^2)^{1/2}$. When the P_n are in the positive energy continuum we have,

$$\Delta(p) = 1/2\,K(p)\,(iy) \times$$

$$\left[e^{i\Omega}\,I_w(2,1,p,a=iy) - e^{-i\Omega}\,I_w(2,1,-p,a=-iy)\right],$$

$$C(p) = 1/2\,K(p)\,(iy) \times$$

$$\left[e^{i\Omega}\,R(2,1,p,a=iy) - e^{-i\Omega}\,R(2,1,-p,a=-iy)\right],$$

$$K(p) = (1+w/w)]\; e^{\pi y/2}/(\sinh(\pi\, y))^{1/2}$$

(4.5.12)

where p is the local momentum related to the energy w, by $w = \sqrt{p^2 + 1}$, $y = w/p$, and $\Omega = -\arctan(p)/2$. Finally when P_n is in the negative continuum we have,

$$\triangle(p) = 1/2\ K'(p)\ y\ x$$

$$\left[e^{i\Omega}\ I_w(2,1,a=-yi,p) + e^{-i\Omega}\ I_w(2,1,a=iy,-p)\right]$$

$$C(p) = 1/2\ K'(p)\ y\ x$$

$$\left[e^{i\Omega}\ R(2,1,a=-iy,p) + e^{-i\Omega} R(2,1,a=iy,-p)\right]$$

(4.5.13)

where $K'(p) = (w-1/w)^{1/2} e^{-\pi y/2}/(\sinh \pi y)^{1/2}$.

The evaluation of (4.5.4) can now be carried out by using (4.5.11), (4.512) and (4.513) for the matrix elements $\triangle(n)$, and C(n). The results are calculated in appendix 5 and tabulated in the first column of Table 4, the contributions from the bound states, positive, and negative energy continuum states are listed separately. Let us now again evaluate (4.5.4) by using the SL approximation outlined above. In this approximation the (n)/w term is replaced by the limiting value of $\triangle(n)/w$ when $w \rightarrow 0$. In this limit we replace the $I_w(\lambda_1,\lambda_2,\lambda,a)$ functions listed above by,

$$\tilde{I}_w(\lambda_1,\lambda_2,\lambda_3,a) = (w/\lambda_1)^2 \left\{ -1/2 \left(\frac{\lambda_2+\lambda_3}{\lambda_2-\lambda_3}\right)^a \frac{1}{(\lambda_2+\lambda_3)} + \right.$$

$$3/5\int_0^1 dt\ t \left[\frac{\lambda_2+\lambda_3+\lambda_1 t}{\lambda_2-\lambda_3+\lambda_1 t}\right]^a \frac{1}{(\lambda_2+\lambda_3+\lambda_1 t)}$$

$$\left. 3/5\int_0^1 dt\ t^3 \left[\frac{t(\lambda_2+\lambda_3)+\lambda_1}{t(\lambda_2-\lambda_3)+\lambda_1}\right]^a \frac{1}{(t(\lambda_2+\lambda_3)+\lambda_1)} \right\}.$$

(4.5.14)

The corresponding contributions for the bound, and continuum states are listed in column two of Table 4.2. Before we discuss the above results let us recalculate the approximation to E in (4.5.4) by using the same procedure considered in sections 4.2, and 4.6. When the cosine term in (4.5.2) is expanded to the leading term, we get for (4.5.4),

$$\tilde{E} = \int_0^\infty dx_1 \int_0^\infty dx_2 \sum_n$$

$$\left\{P_1(x_1)\ Q_1(x_1)\ 1/2\ W_n\ x_{12}\Big|_{L=1}\ Q_1(x_2)P_n(x_2)\ \ C(n)\right\}$$

(4.5.15)

Using the Dirac radial equation to eliminate the W_n factor we get

$$W_n C(n) = \int_0^\infty dx_3 \int_0^\infty dx_4 \left[\frac{dQ_n}{dx_3}(x_3) - Q_n(x_3) + P_n(x_3)(1-1/x_3)\, Q_1(x_3) f^2(x_4) \right].$$

(4.5.16)

We can employ the radial wavefunction sum rules (4.4.17), thus our expression for $\tilde{E}$ becomes,

$$\tilde{E} = 1/2 \int_0^\infty dx_1 \int_0^\infty dx_2 \int_0^\infty dx_3\, P_1(x_1) Q_1(x_1)\, v(1,2) \times Q_1(x_2)\,(1-1/x_2) \Big| Q_1(x_2)\, g(2,3)\, f^2(x_3)$$

(4.5.17)

where $v(1,2)$ is the L=1, radial partial wave component of the operator x_{12}, and $g(2,3)$ is the L=0 component for $1/x_{23}$, these are given in (A.2.11). The above triple integral can be done analytically. The value for $\tilde{E}$ calculated from the above expression is $.3536 \times 10^{-2}$, agreeing with the previous result obtained by summing over the intermediate states without making use of completeness. This is gratifying since it gives us an independent check on our integration algorithm discussed in the previous sections.

We notice that the approximation $\tilde{E}$, for (4.5.4) is reasonable accurate for the partial sum over the bound states and the positive energy continuum, but starts to break down in the sum over the positron continuum. The positron wave function is large around the origin for

high values of the momentum p. Therefore the sum (4.5.4) over this range gives an appreciable contribution, the discrepancy between E, and $\tilde{E}$ is now large since the argument in the cosine term in (4.5.2) cannot be accurately approximated by the leading terms of a power expansion. We can get a qualitative idea of the importance of the continuum in the sum (4.5.1) by estimating the matrix elements when the intermediate states can be approximated by the asymptotic expression $P_n(x) \sim \cos(px + \delta)$, where δ is some phase number. the bound state functions behave like, $P(x) \sim x^{\gamma} e^{-(Z\alpha)x}$, near the origin, where $\gamma = \sqrt{1-(Z\alpha)^2}$. The matrix elements in (4.5.2) (when $\Delta\eta$ is approximated in the SL) behave like,

$$\Delta\eta_{nm,n'm'}/(W_{nn'}+W_{ms}) \sim \int_0^{\infty}\int_0^{\infty} dx_1 dx_2 \; x_1^{2\gamma} \; x_2^{\gamma}$$

$$e^{-2(Z\alpha)x_1} e^{-(Z\alpha)x_2} \; P_n(x_2) \; |x_{12}|^{L=1} \; \sim \; 1/p^{3\gamma+1}$$

$$C_{sq,m'q'} \sim$$

$$\int_0^{\infty}\int_0^{\infty} dx_1 dx_2 \; x_1^{2\gamma} \; x_2^{\gamma} \; e^{-2(Z\alpha)x_1} e^{-(Z\alpha)x_2} P_n(x_2) \; 1/|x_{12}|^{L=0}$$

$$\sim 1/p^{3\gamma}$$

or,

(4.5.18)

$$V_3 \sim \int dp \; 1/p^{6\gamma+1},$$

(4.5.19)

We notice that the singularity of the s state Dirac Coulomb wavefunctions at the origin for $(Z\alpha) = 1$, $(\gamma = 0)$ causes the continuum contribution (4.5.13) to diverge. In order to get a convergent sum in for $(Z\alpha) = 1$ for (4.5.4) we have chosen $f(x) = xe^{-x}$ in (4.5.3). This singularity is really academic since it is due to to the fact that we are dealing with a point nucleus. We note that for relatively large Z, $(Z\alpha) = .86$ the γ parameter is already equal to 1/2, and for this case the Coulomb integral in (4.5.13) already converges quickly for large p. For this value of $(Z\alpha)$, the integrand in (4.5.13) goes as $1/p^4$, and the continumm contribution is nonnegligible for small p only, hence the discrepancy between the SL approximation and the exact energy is diminished.

Even though the above results show that the SL starts to break down for $(Z\alpha) = 1$, it is neverthless an adequate order of magnitude approximation to the exact three body energy, itself being quite small. In order to be more precise by what we define as small, let us consider the energy,

$$Q_3 = \sum_{s}^{(+)} \left(\eta_{n1,n's} + \eta_{1n,1's} \right) C_{sm,1m'} / (W_{nn'} + W_{1s}) .$$

(4.5.20)

This expression is similar to V_3 in (4.5.1), however it differs from V_3 by containing a sum of the η matrix elements rather than a difference. In addition the sum over intermediate states is only over the positive energy(electron) states. Such an energy is the result of an iteration of the nonlocal Breit interaction with a Coulomb potential, and would contribute to the three body correlation energy of the system.

We evaluate the analog of (4.5.2) for Q_3 by replacing the $(1-\cos W_n x_{12})/x_{12}$ term with $(1+\cos W_n x_{12})/x_{12}$, and summing only over the positve energy spectrum. The results for the bound state and continuum state contribution are presented in Table 6.(For more details on this calculation, refer to appendix 5.) One notices that the magnitude of this energy is about ten times larger than the results presented in Table 5. We can therefore state with confidence that even though the static limit breaks down at $Z\alpha = 1$, it is a rough guide on the order of magnitude of the three body energy which is small when normalized to a typical three body correlation energy.

Besides the SL approximations discussed above we have also made some other approximations in the evalution of

Table III. Column (A), partial sums of the energy E (in dimensionless units) defined in (4.5.4). Column (B), the partial sums using the SL approximation. Column (C), total sum in the SL approximation by using the completeness property of the radial wavefunctions. Column (D), partial sums of the correlation type contributions, (see 4.5.19).

Partial sums	A	B	C	D
Bound states	$-.5916\ 10^{-3}$	$-.1028\ 10^{-2}$	—	$-.1036\ 10^{-1}$
Positive continuum	$-.5579\ 10^{-3}$	$-.4587\ 10^{-3}$	—	$-.1321\ 10^{-2}$
negative continuum	$-.1124\ 10^{-3}$	$.5024\ 10^{-2}$	—	—
Total sum	$-.1262\ 10^{-3}$	$.3538\ 10^{-2}$	$.3538\ 10^{-2}$	$-.1168\ 10^{-1}$

the three-body energies in the preceding sections. In section 4.4, and 4.5 we have neglected contributions coming from the j=3/2, d wave, intermediate states. For high values of Z the overlap of these functions with the j=1/2, s wave states (being very close to the nucleus)is very small, therefore the resulting radial integrals will be neglible compared to the integrals evaluated in 4.3, and 4.5. In addition we have completely neglected the so called Coulomb retardation term of the Breit operator, and considered only the magnetic Gaunt component. However; this term was used in Hatree - Fock calculations by many authors [11,38], and was shown to have only a few percent contribution, when compared to the magnetic term.

Conclusion and Discussion

Summarizing the numerical results of the previous sections, we note that the total three body energy is on the order of .01 Rydberg for a three electron ion with $Z\alpha \sim 1$. Before discussing the implication of these results let us consider again the Primakoff - Holstein (P-H) potential given by (3.3.11). We can approximate, by dimensional arguments, a typical energy coming from these terms. Consider the term in the P-H potential given by

$$V(1,2,3) = e^4/8mc^2 \left(\frac{\alpha_1 \cdot \alpha_3}{|r_{12}||r_{23}|} \right) + \text{(permutations of coord.)}.$$

Taking the expectation value of V for low lying orbitals in the presence of a nucleus with charge Ze, we can replace $1/|r_{12}||r_{23}| \longrightarrow Z^2/a_0^2$ (a_0 is the Bohr radius), and $\alpha_1 \cdot \alpha_3 \rightarrow (Z\alpha)^2$. We thus expect a contribution to the energy from the P-H potentials to scale like $(Z\alpha)^4$ Ryd. For Z = 137, this energy would have a magnitude one hundred times larger than the contributions that we have calculated. This seems strange: After all, we have shown in Section 3.3 that the P-H potentials are a classical limit of the virtual pair potentials evaluated

in Section 4.3. We now wish to address ourselves to this seemingly paradoxical situation. We pointed out in Section 3.3 that for a nonrelativistic system the sum over "slow" virtual free positrons gave rise to the P-H potentials, however for a high Z (relativistic) atom one must use the full Coulomb Dirac positron wavefunctions in the sum over the intermediate states. For an atom with Z=137, the positrons in the inner regions of the atom will have the approximate form,

$$P_w(r) \approx w\,K(p) \approx w\,e^{-\pi w/p}$$

where $w = \sqrt{p^2+1}$, p is the momentum of the positrons, and where the normalization factor K(p) is given by (4.3.17). We have also used the identity[35] $\Gamma(iy) = 1/(y\,\sinh y)^{1/2}$. The the pair contribution terms of Section 4.3 will then behave in the region $p \lesssim p'$

$$\Delta E(\text{pair}) \approx \int_0^{p'} dp\; e^{-2\pi w/p}\; w \text{ (Ryd.)}$$

since the integral over the bound state wavefunctions is on the order of one. In the exact evaluation of these terms, most of the contribution to the shift came from values of the positron momenta $p \lesssim 5$. Inserting this value into the cutoff value in the integral and approximating

$w \approx p$, we get,

$$\Delta E \approx \left(e^{-2\pi}\ (12)\right) \text{Ryd.} \approx .01 \text{ Ryd.}$$

We note that the small exponential factor in the normalization constant is responsible for making ΔE small. We have a clear physical explanation for the above results by noting that the Coulomb Dirac virtual positrons have a small probability of penetrating into the regions near the nucleus because of the strong Coulomb repulsion. The inner-shell electrons however are highly likely to be in this region. The overlap of the virtual positrons and inner shell electrons is consequently small; hence the matrix elements for the three body potentials due to virtual pairs in high Z atoms are negligible. The above considerations point out the danger in trusting essentially nonrelativistic derivations as a guide to QED processes in an intense field, even as an order of magnitude guide. It must be pointed out that for a very hot plasma, three body potentials of the type discussed above would probable make a large contribution to the energy of the system since the virtual positrons would now have a very large overlap region with the electrons because of mutual attraction.

In sections 4.3 , and 4.4, we discussed the Coulomb - transverse, and transverse - transverse photon exchange, contributions to the three body energy. These terms have

contributions coming from virtual electrons as well positrons. However, the difference ($\eta_{nm,n'm'} - \eta_{mn,n'm'}$) appearing in these terms are small. We have used the static limit (SL) approximations defined in Section 4.5. to replace the above difference with the matrix elements of a local operator. Even though, as was pointed out in this section, this approximation breaks down for $Z\alpha = 1$, the SL approximation actually gives a good order of magnitude estimate to the correct energy for values of $Z\alpha \approx 1$. We thus conclude that three-body potentials are not an important consideration when dealing with the gross atomic structure of heavy atoms. However, three-body potentials could be important in determing the fine structure of few electron ions with intermediate values of Z. The experimental verification of fundamental many body electromagnetic forces could be an important benchmark in our understanding of higher order effects of QED. Finally as was originally pointed out by Primakoff and Holstein[7], three-body potentials are important in nuclear physics; understanding QED three-body potentials would give us insight into the more complex processes in the nucleus.

Appendix

In appendix A.1, we discuss the Dirac-Coulomb wavefunctions that were widely made use of throughout the thesis. Most of the material of this section comes directly out of M.E. Rose's book[36], " RELATIVISTIC ELECTRON THEORY ". In A.2 we give a brief review of some basic results of Racah Algebra, most of the material from this section is taken from Armstrong's book[33]. In A.3, we simplify, and express the matrix elements of the Coulomb, and Breit interaction, for s wave Dirac - Coulomb wavefunctions, into a linear combination of radial integrals. Some of the computer codes used in this thesis are briefly outlined in A.4.

Appendix A.1 The Dirac equation in a central field

The Dirac, eigenvalue equation in a central field u(r), is given by,

$$\left[-i\hbar c\,\bar{\alpha}\cdot\bar{\nabla} + \beta mc^2 + u(r)\right]\psi(r) = E\,\psi(r) \qquad (A.1.1)$$

where $\bar{\alpha}$, β are four by four matrices given by,

$$\bar{\alpha} = \begin{pmatrix} 0 & \bar{\sigma} \\ \bar{\sigma} & 0 \end{pmatrix} \qquad \{\alpha_i, \alpha_j\} = 2\delta_{ij}$$

$$\{\alpha_i, \beta\} = 0$$

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \qquad \beta^2 = I \qquad (A.1.2)$$

where the $\bar{\sigma}$, I are the two by two Pauli, and identity matrices respectively.

We are interested with the eigenstates of (A.1.1) in an attractive Coulomb potential $u(r) = -Ze^2/r$. We shall hence-forth call these Dirac - Coulomb wavefunctions. The Hamiltonian (A.1.1) commutes with the total angular momentum operator,

$$\bar{J} = \bar{L} + \hbar/2\,\bar{\Sigma} \qquad (A.1.3)$$

and, the relativistic parity operator

$$K = \beta P \qquad \text{(A.1.4)}$$

where $\bar{L} = \bar{r} \times \bar{p}$ is the nonrelativistic orbital angular momentum, $\bar{\bar{\Sigma}}$ is the four by four spin matrix,

$$\bar{\bar{\Sigma}} = \begin{pmatrix} \bar{\sigma} & 0 \\ 0 & \bar{\sigma} \end{pmatrix} \qquad \text{(A.1.5)}$$

and P is the space inversion operator.

Eigenstates of J can be constructed from the,spin orbit functions, which are linear combinations of the orbital angular momentum eigenfunctions $Y_\lambda^m(\Omega)$, and the spin 1/2 eigenstates, $|s\ m_s\rangle$,

$$\chi_\mu^{j,m}(\Omega) =$$

$$\sqrt{(j+m)/2j}\ \ Y_\lambda^{m-\frac{1}{2}}(\Omega)\ |s=1/2\ m_s=\tfrac{1}{2}\rangle +$$

$$\sqrt{(j-m)/2j}\ \ Y_\lambda^{m+\frac{1}{2}}(\Omega)\ |s=1/2\ m_s=-\tfrac{1}{2}\rangle$$

if $\lambda = j - 1/2$,

and

$$\chi_{\mu}^{j,m}(\Omega) =$$

$$\sqrt{(j+1-m)/2j+2}\; Y^{m-\frac{1}{2}}(\Omega)\,\big|s=1/2\;\; m_s=\tfrac{1}{2}\big\rangle -$$

$$\sqrt{(j+1+m)/2j+2}\; Y^{m+\frac{1}{2}}(\Omega)\,\big|s=1/2\;\; m_s=-\tfrac{1}{2}\big\rangle$$

if $\lambda = j + 1/2$,

(A.1.6)

where λ is the orbital angular momentum quantum number, μ is the space inversion quantum number ($\mu = 1$ even parity, $\mu = -1$ odd parity.), and m is the azimuthal quantum number. The eigenstates of (A.1.1) must be diagonal with respect to the K operator, therefore they are linear combinations of the spin orbit eigenfunctions with opposite parities (space inversion). Choosing a standard phase convention[29] we can express the most general form for the eigenstates of (A.1.1), (A.1.3),and (A.2.4) as,

$$\big|E\ j\ m\ \mu\big\rangle = \begin{pmatrix} P(r)/r & \chi_{\mu}^{jm}(\Omega) \\ iQ(r)/r & \chi_{-\mu}^{jm}(\Omega) \end{pmatrix}$$

(A.1.7)

The choice for either of the two expressions for χ_{μ}^{jm} in (A.1.6) is uniquely determined for a given value of j, and the parity μ , by the relation $\lambda = j + \mu(-1)^{j+\frac{1}{2}}$.

Making use of the identity,

$$\bar{\sigma}\cdot\hat{r}\,\bar{\sigma}\cdot\bar{\nabla} = \bar{r}\cdot\bar{\nabla} + i\bar{\sigma}\cdot(\bar{r}\times\bar{\nabla}) =$$

$$d/dr - i\frac{\bar{\sigma}\cdot\bar{L}}{\hbar} \qquad (A.1.8)$$

and,

$$\frac{\bar{\sigma}\cdot\bar{L}}{\hbar}\,\chi_{\mu}^{jm} = \frac{1}{\hbar}(J^2 - L^2 - (\hbar\bar{\Sigma}/2)^2)\chi_{\mu}^{jm}$$

$$= -(k+1)\chi_{\mu}^{jm}, \quad k = (-1)^{j+1/2}(2j+1)/2$$

$$\text{and } \bar{\sigma}\cdot\hat{r}\,\chi_{\mu}^{jm} = \chi_{-\mu}^{jm} \qquad (A.1.9)$$

we get for (A.1.1)

$$(d/dx + k/x)P(x) - (W + 1 - \zeta/x)Q(x) = 0$$

$$(d/dx - k/x)Q(x) + (W - 1 - \zeta/x)P(x) = 0 \qquad (A.1.10)$$

where we have used the dimensionless units, $x = r/\lambda$, $E = mc^2W$, $\zeta = Z\alpha$. λ, being the Compton wavelength, and α the fine structure constant. It is clear from the above equation that the radial functions need be

parametrized by the energy eigenvalues W, and the k number which is related to the relativistic parity quantum number, and j.

We now proceed to construct the radial wavefunctions, P(x), and Q(x). Following Rose, we make a transformation,

$$P(z) = (1+W)^{1/2} (\Phi_1(z) + \Phi_2(z)) e^{-\lambda z}$$

$$Q(z) = (1-W)^{1/2} (\Phi_1(z) - \Phi_2(z)) e^{-\lambda z}$$

$$z = 2\lambda x. \quad \lambda = (1-W^2)^{1/2}$$

(A.1.11)

We now consider bound state solutions $0 < W < 1$. Making an additional transformation $\Phi_2 = M(z)/z^{1/2}$, we get a standard second order equation,

$$(d^2/dz^2 M) + \left[-1/4 + (\xi W/\lambda + 1/2)1/z - (\gamma^{1/2} - 1/4)/z^2\right] M = 0$$

(A.1.12)

where,

$$\gamma = \sqrt{k^2 - (z\alpha)^2}$$

(A.1.13)

The solutions of (A.1.12) are given by the Whittaker

functions[35]. For bound states, we require the solutions to be regular at infinity. Matching the solutions regular at the origin with the asymptotic solutions one gets the quantinization condition,

$$W_{nk} = \left[1 + \left(Z\alpha/(n + \kappa) \right)^2 \right]^{-1/2} \tag{A.1.14}$$

where n is a non-negative integer, and $k = \pm 1, \pm 2, .. \pm(n-1), -n$. One can now rexpress the P(x), Q(x) in terms of the Whittaker functions, imposing the normalization condition,

$$\int_0^\infty dx \left(P^2(x) + Q^2(x)\right) = 1 \tag{A.1.15}$$

We borrow the result of Rose,

$$P(x) = N (1+W_{nk})^{1/2} (2\lambda x)^{\gamma} e^{-\lambda x} \,,$$

$$\left\{ -n\, {}_1F_1(-n+1, 2\gamma + 1, 2\lambda x) - (k - \gamma/\lambda)\, {}_1F_1(-n, 2\gamma+1, 2\lambda x) \right\}$$

$$Q(x) = - N (1-W_{nk})^{1/2} (2\lambda x)^{\gamma} e^{-\lambda x} \,,$$

$$\left\{ n\, {}_1F_1(-n+1, 2\gamma + 1, 2\lambda x) - (k - \gamma/\lambda)\, {}_1F_1(-n, 2\gamma+1, 2\lambda x) \right\}$$

(A.1.16)

with the normalization constant,

$$N = \left(\Gamma(2\gamma + n + 1)/n!\, \xi\, (\xi - \lambda k) \right)^{1/2} \left(\lambda^{n/2} / (2^{n} \Gamma(2\gamma + 1) \right)$$

(A.1.17)

To get the continuum solutions for positive energy ($W > 1$) eigenstates of (A.1.1), one gets an analogous equation to (A.1.12),

$$d^2/dz^2 \left(M \right) - \left[\tfrac{1}{4} + \left(\tfrac{1}{2} + i\xi W/p \right)/z + \left(\gamma^2 - \tfrac{1}{4} \right)/z^2 \right] M = 0$$

(A.1.18)

where now $z = 2ipx$, and, $p = \sqrt{W^2 - 1}$, is the local momenta. The solutions to (A.1.18) can again be expressed in terms of the confluent hypergeometric functions. After requiring energy scale normalization ,

$$\int_0^\infty dx \left(P_W(x) P_{W'}(x) + Q_W(x) Q_{W'}(x) \right) = \delta(W - W')$$

(A.1.19)

Rose gets,

$$P(x) = N(1+W)^{1/2}(2px)^{\gamma}$$

$$\text{Real}\quad e^{-ipx}\, e^{i\Omega}\, {}_1F_1(\gamma + 1 + iy, 2\gamma + 1, 2ipx)$$

$$Q(x) = -N(1-W)^{1/2}(2px)^{\gamma}$$

$$\text{Imag}\quad e^{-ipx}\, e^{i\Omega}\, {}_1F_1(\gamma + 1 + iy, 2\gamma + 1, 2ipx)$$

where $y = (Z\alpha)W/p$, and the normalization,

$$N = e^{y/2}\left|\Gamma(\gamma + iy)\right| / \Gamma(2\gamma + 1)\,(\pi p)^{1/2}. \qquad \text{(A.1.20)}$$

The phase factor,

$$e^{i\Omega} = (-k+iy/W)^{1/2}(\gamma + iy)^{1/2} \qquad \text{(A.1.21)}$$

was chosen in order to make the amplitudes real.

We now consider the negative energy ($W < 0$) solutions to (A.1.1). We note that the radial equations (A.1.10) for this sign of the energy correspond to positive energy equation given above if make the replacement $Z\alpha \rightarrow -Z\alpha$, $P(x) \rightarrow Q(x)$, and $k \rightarrow -k$, while keeping the absolute value of the energy. Therefore (A.2.20) is a positron solution with energy W, if we interchange the upper component of the electron wavefunction with the lower component of the positron function, substitute $y \rightarrow -y$.

Appendix A.2 Tensor Operators

A spherical tensor operator is defined as a set of $(2k+1)$ operators A^k_q, which obey commutation relations

$$\left[J_z, T^k_q\right] = q\, T^k_q$$

$$\left[J_+, T^k_q\right] = (k(k+1) - q(q+1))^{1/2}\ T^k_{q+1}$$

$$\left[J_-, T^k_q\right] = (k(k+1) - q(q-1))^{1/2}\ T^k_{q-1}$$

(A.2.1)

where J_z, $J_+ = J_x + iJ_y$, $J_- = J_x - iJ_y$, and J_x, J_y, J_z, being the ordinary angular momentum operators i.e.,

$$\left[J_i, J_j\right] = i\,\epsilon^{ijk}\,J_k.$$

(A.2.2)

Given two spherical tensor operators T^k_q, $T^{k'}_{q'}$, of rank k, k', we can form higher rank tensor operators N^K_Q,

$$N_Q^K = \sum_{qq'} T_q^k \; T_{q'}^{k'} \begin{pmatrix} k & k' & K \\ q & q' & -Q \end{pmatrix} (-1)^{k-k'-Q} \left[K\right]^{1/2}$$

(A.2.3)

where we have defined a shorthand notation,
$\left[k,m\ldots,n\right] = (2k+1)(2m+1)\ldots(2n+1)$.

Common tensor operators are,

$$C_q^j = \sqrt{4\pi/(2j+1)} \; Y_q^j(\Omega) \;, \; C_q^1 = r$$

$$\sigma_q^1 = (\sigma_z \text{ for } q=3, \; \sigma_+, \text{ for } q=1, \; \sigma_- \text{ for } q=2)$$

(A.2.4)

where $\sigma_+ = \sigma_x + i\sigma_y$, $\sigma_- = \sigma_y - i\sigma_y$,
$\sigma_x, \sigma_y, \sigma_z$ are the Pauli matrices.

The C_q^j act on the orbital space while, $\vec{\sigma}$ act on the spin space. The dot and vector products are common tensor operators (scalar, vector) constructed from two rank k tensors, A^k, B^k

$$A^k \cdot B^k = (-1)^k \left[k\right]^{1/2} \; (A^k \, b^k)^0$$

$$A^1 \times B^1 = -i\sqrt{2}\,(A^1 B^1)^1$$

(A.2.5)

The Wigner - Eckart theorem allows us to factor the magnetic quantum number dependence of the matrix elements of tensor operators i.e.,

$$\langle j\ m_j | T^K_Q | j'\ m_{j'} \rangle = (-1)^{j-m} \begin{pmatrix} J & K & J' \\ -m_j & q & m_j \end{pmatrix} \langle j || T^K || j' \rangle$$

(A.2.6)

the $\langle j || T^K || j' \rangle$ are reduced matrix elements and do not depend on the azimuthal quantum numbers. Often used reduced matrix elements are,

$$\langle l || C^k || l' \rangle = (-1)^l \left[l, l'\right]^{\frac{1}{2}} \begin{pmatrix} l & k & l \\ 0 & 0 & 0 \end{pmatrix}$$

$$\langle s=1/2 || \sigma || s=1/2 \rangle = \sqrt{6}$$

(A.2.7)

where $|l\rangle$ is an orbital angular momentum eigenstate, $|s=1/2\rangle$ is a spin 1/2 eigenstate.

Most of the tensor operators we will make use of are operators in the spin-orbit product space. If we have a state $|J\ M; j_1\ j_2\rangle$ where J,M are the quantum numbers in the product space, j_1, j_2 are the lower dimensional angular momenta, we have a useful formula

$$\langle j_1\ j_2\ J \| (T^{k_1}, U^{k_2})^K \| j_1'\ j_2'\ J' \rangle$$

$$= [J, J', K]^{1/2} \begin{Bmatrix} j_1 & j_1' & \kappa_1 \\ j_2 & j_2' & \kappa_2 \\ J & J & K \end{Bmatrix} \times \langle j_1 \| T^{k_1} \| j_1' \rangle \langle j_2 \| U^{k_2} \| j_2 \rangle$$

(A.2.8)

where T^{k_1}, U^{k_2}, operate on the spin and three dimensional space, respectively. If either of the operators is a scalar, then we have,

$$\langle j_1\ j_2\ J \| T^{k_1} \| j_1'\ j_2'\ J' \rangle = \delta(j_2, j_2')\ (-1)^{j_1 + j_2 + J' + k} \times$$

$$[J, J']^{1/2} \begin{Bmatrix} J & k & J' \\ j' & j & j \end{Bmatrix} \langle j_1 \| T^k \| j_1 \rangle$$

for $k_1 = K$, $k_2 = 0$, and

$$\langle j_1\ j_2\ J \| U^{k_2} \| j_1'\ j_2'\ J' \rangle = \delta(j_1, j_1')\ (-1)^{j_1 + j_2 + J + k_2}$$

$$[J, J']^{1/2} \begin{Bmatrix} J & k & J' \\ j' & j & j \end{Bmatrix} \langle j_2 \| U^k \| j_2 \rangle$$

for $k_1 = 0$, $k_2 = K$.

(A.2.9)

If we have a product space constructed from more than

two component spaces then we can form angular momenta states (in the product space) in more than one way, i.e. in a productspace of three particles we can first couple particle 1,and 2 and then couple this state with the third particle , to get $|JM\ (j_1 j_2) j_3\rangle$ or we can also have $|JM\ j_1\ (j_2 j_3)\rangle$ these two states are related by the recoupling formula,

$$|j_1,\ (j_2 j_3) J_{23},\ JM\rangle = \sum_{J_{12}} (-1)^{j_1 + j_2 + j_3 + J} \begin{Bmatrix} j_3 & J & J_{12} \\ j_1 & j_2 & J_{23} \end{Bmatrix} [J_{12}, J_{23}]^{1/2} |(j_1 j_2)\ J_{12},\ j_3\ JM\rangle \ .$$

(A.2.10)

Another useful formula deals with the partial wave expansion[37]

$$f(|r_{12}|) = \sum_k v_k(1,2)\ C^k(1) \cdot C^k(2)$$

where $v_k(1,2) =$

$r_<^k / r_>^{k+1}$ if $f = 1/|r_{12}|$, and

$\left[1/5(2k+1)\ (r_</r_>)^2 - 1/(2k-1)\right] r^k/r^{k-1}$ if $f = |r_{12}|$.

(A.2.11)

In addition we will also make use of the partial wave expansion for the Gaunt operator, this expansion is given by equation (7.18). in ref.(38),

$$- \alpha_1 \cdot \alpha_2 / r_{12} =$$

$$(-1) \sum_{K,L} (-1)^{K+L} \left[\alpha_1 C^K(1)\right]^L \cdot \left[\alpha_2 C^K(2)\right]^L \left(r_<^K / r_>^{K+1} \right).$$

(A.2.12)

Appendix A.3

Matrix elements of the Coulomb, and Breit operators.

We wish to evaluate the matrix elements of the Coulomb operator $1/r_{12}$, and the Gaunt operator, $-\bar{\alpha}_1\cdot\bar{\alpha}_1/r_{12}$, between Dirac - Coulomb spinors. The matrix elements of these operators can in turn be used as the building blocks in evaluating the matrix elements of the generalized Breit operator(2.1.19). Using the representation for the spinors (A.1.7), and the partial wave expansion for the Coulomb operator (A.1.11) we get,

$$\begin{aligned}\langle ab|1/r_{12}|a'\ b'\rangle \;=\; \sum_{\kappa,q}(-1)^q \int_0^\infty dr_1 \int_0^\infty dr_2 \Big\{ r_<^k/r_>^{k+1} \times \\ \Big[(P_a(r_1)P_{a'}(r_1)\ \langle \chi^a_\mu\, C^k_q(1)|\chi^{a'}_{\mu'}\rangle \;+ \\ Q_a(r_1)Q_{a'}(r_1))\ \langle \chi^a_{-\mu}|C^k_q(1)|\chi^{a'}_{-\mu'}\rangle\Big]\times \\ \Big[(P_b(r_2)P_{b'}(r_2)\ \langle \chi^b_\nu|C^k_{-q}(2)|\chi^{b'}_{\nu'}\rangle \;+ \\ Q_b(r_2)Q_{b'}(r_2))\ \langle \chi^b_{-\nu}|C^k_{-q}(2)|\chi^{b'}_{-\nu'}\rangle\Big]\Big\}\ .\end{aligned} \tag{A.3.1}$$

where the matrix elements $\langle\chi|C^k_q|\chi\rangle$ refer to angular integrations, the χ^a_μ are spin orbit functions defined in (A.1.6), the subscripts μ determine the parity of the spin orbit functions,

If $\mu = +1$, the parity is even, if $\mu = -1$ it is odd. Applying the Wigner Ekhart theorem and defining the reduced matrix elements,

$$D^k(a\,\mu\,;a'\,\mu') = \langle j_a\ s=1/2\ \lambda_a(\mu) \| C^k \| j_a\ s=1/2\ \lambda_{a'}(\mu')\rangle$$

$$\lambda_a(\mu) = j_a - \mu/2\ (-1)^{j_a+]}$$

(A.3.2)

we get for (A.3.1)

$$\langle ab \mid 1/r_{12} \mid a'b'\rangle$$

$$= \sum_{\kappa,q} (-1)^{q + j_a + j_b - m_a - m_b} \begin{pmatrix} j_a & k & j_a \\ -m_a & q & m_a \end{pmatrix} \begin{pmatrix} j_b & k & j_b \\ -m_b & -q & m_b \end{pmatrix} \times$$

$$\int_0^\infty dr_1 \int_0^\infty dr_2 \left[r_<^k / r_>^{k+1} \left[(P_a(r_1)P_{a'}(r_1) D^k(a\,\mu\,;a'\,\mu') + \right.\right.$$

$$\left. Q_a(r_1)Q_{a'}(r_1)) D^k(a\,-\mu\,;a'\,-\mu') \right] \times \left[(P_b(r_2)P_{b'}(r_2) D^k(b\,\mu;b'\,\mu') \right.$$

$$\left. \left. + Q_b(r_2)Q_{b'}(r_2) D^k(b\,-\nu\,;b'\,-\nu') \right] \right].$$

(A.3.3)

Using (A.2.9) we can evaluate the D^k coefficients, we get

$$D^k(a\mu;a'\mu') = (-1)^{1/2 + j_a + k} \left[j_a, j_a\right]^{1/2} \begin{Bmatrix} j_a & k & j_{a'} \\ \lambda_a & 1/2 & \lambda_{a'} \end{Bmatrix}$$

$$\left[\lambda_a, \lambda_{a'}\right]^{1/2} \begin{pmatrix} \lambda_a & k & \lambda_{a'} \\ 0 & 0 & 0 \end{pmatrix}$$

(A.3.4)

where we also have used (A.2.7). An important parity selèction rule comes from the 3-j symbol, $\lambda_a + \lambda_{a'} + k$ = even. In our applications, we are faced with matrix elements where at least three of the states in (A.3.1) are s wave states. Let us consider the special case $j_a = 1/2$, $\mu = 1$, $j_{a'} = 1/2$, $\mu' = 1$, $j_b = 1/2$, $\nu = 1$, $j_{b'}$, ν'. We immediatly notice that the $D^k(1/2\,\mu=1;1/2\,\mu'=1)$ coefficient vanishes unless k=0, because of the above stated parity condition and the triange equality $\triangle(1/2,1/2,k)$ (coming from the 6-j symbol) must be simultaniously satisfied. The k = 0 requirement forces $j_{b'} = 1/2$, and $\nu' = 1$, as can be seen by using (A.3.4) for $D^0(1/2\,\mu=1, j_{b'}, \nu')$. We will thus be concerned only with Coulomb matrix elements where all states are s waves. We then get

$$\langle a\,b \mid 1/r_{12} \mid a'b' \rangle = 2\, X^{L=0}(m_a m_{a'}; m_b m_{b'})$$

$$\int_0^\infty dr_1 \int_0^\infty dr_2 \left[P_a(r_1)P_{a'}(r_1) + Q_a(r_1)Q_{a'}(r_1)\right] \times$$

$$\left[P_b(r_2)P_{b'}(r_2) + Q_b(r_2)Q_{b'}(r_2)\right]$$

(A.3.5)

where we have defined ,

$$X^{L}(m_a m_{a'}; m_b m_{b'}) =$$

$$\sum_{q} (-1)^{q + 1 - m_a - m_b} \begin{pmatrix} 1/2 & L & 1/2 \\ -m & q & m \end{pmatrix} \begin{pmatrix} 1/2 & L & 1/2 \\ -m & -q & m \end{pmatrix}$$

(A.3.6)

and evaluated ,

$$D^{k=0}(1/2\,\mu = +1;\ 1/2\,\mu' = +1) = \sqrt{2}.$$

(A.3.7)

We now turn our attention to evaluating the matrix elements with respect to the Gaunt operator. Using the same notation as above and the partial wave expansion (A.1.12) we get,

$$\langle a\ b|-\bar{\alpha}_1\cdot\bar{\alpha}_2/r_{12}\,|\,a'b'\rangle =$$

$$(-1)\sum_{\kappa,L,q}(-1)^{k+L+q}\int_0^\infty dr_1\int_0^\infty dr_2\ \Big\{\ r_<^k/r_>^{k+1}\ i^2\ \kappa$$

$$\Big[\ (P_a(r_1)Q_{a'}(r_1)\ \langle\chi^a_{-\mu}|\big[\sigma C^k(1)\big]^L_q\,|\chi^{a'}_{-\mu'}\rangle$$

$$-\ Q_a(r_1)P_{a'}(r_1)\ \langle\chi^a_{-\mu}|\big[\sigma C^k(1)\big]^L_q\,|\chi^{a'}_{\mu'}\rangle\ \Big]\ \kappa$$

$$\Big[(P_b(r_2)Q_{b'}(r_2)\ \langle\chi^b_{\nu}|\big[\sigma\, C^k(2)\big]^L_{-q}\,|\chi^{b'}_{-\nu'}\rangle$$

$$-\ Q_b(r_2)P_{b'}(r_2)\ \langle\chi^b_{-\nu}|\big[\sigma C^k(2)\big]^L_{-q}\,|\chi^{b'}_{-\nu'}\rangle\Big]\ \Big\}\ .$$

(A.3.8)

We again make use of the Wigner Ekhart theorem and define the reduced matrix elements

$$E^k(a\,\mu\,;a'\,\mu';L) = \langle j_a\ s=1/2\ \ \lambda_a\|\big[\sigma C^k\big]^L\|\ \lambda_{a'}\ \ s=1/2\ j_{a'}\rangle$$

(A.3.9)

we get for (A.3.8)

$$\sum_{q,\kappa,L}(-1)^{q - m_a - m_b + j_a + j_b + k + L}$$

$$\begin{pmatrix} j_a & L & j_{a'} \\ -m_a & q & m_{a'} \end{pmatrix}\begin{pmatrix} j_b & L & j_{b'} \\ -m_b & -q & m_{b'} \end{pmatrix} \times$$

$$\int_0^\infty dr_1 \int_0^\infty dr_2 \left\{ r_<^k / r_>^{k+1} \left[(P_a(r_1)Q_{a'}(r_1)E^k(a\,\mu;a'-\mu';L) \right.\right.$$

$$- \left.\left. Q_a(r_1)P_{a'}(r_1))E^k(a\,-\mu;a\,\mu';L)) \right] \times \right.$$

$$\left[(P_b(r_2)Q_{b'}(r_2)E^k(b\,\nu;b'-\nu';L) \right.$$

$$- \left. Q_b(r_2)P_{b'}(r_2))E^k(b\,-\nu;b'\,\nu';L) \right] \Big\}.$$

(A.3.10)

We use (A.2.8) to evaluate the E^k coefficients,

$$E^k(a\,\mu;a'\,\mu';L) = \left[j_a,k,j_{b'}\right]^{1/2} \begin{Bmatrix} 1/2 & 1/2 & a \\ \lambda_a & \lambda_{a'} & \kappa \\ j_a & j_{a'} & L \end{Bmatrix} \times$$

$$\langle 1/2 \| \sigma^- \| 1/2 \rangle \ \langle \lambda_a \| c^k \| \lambda_{a'} \rangle$$

(A.3.11)

or,

$$E^k(a\ \mu\ ;a'\ \mu';L) = \left[j_a, k, j_{a'}\right]^{1/2} \begin{Bmatrix} 1/2 & 1/2 & 1 \\ \lambda_a & \lambda_{a'} & \kappa \\ j_a & j_{a'} & L \end{Bmatrix} \times$$

$$\sqrt{6}\ (-1)^{\lambda_a} \begin{pmatrix} \lambda_a & \kappa & \lambda_{a'} \\ 0 & 0 & 0 \end{pmatrix} \qquad \text{(A.3.12)}$$

where we have used (A.2.7). Again we shall only be concerned with the matrix elements of the Gaunt operator between s waves. Thus for $j_a = 1/2 = j_{a'} = j_b = j_{b'}$, and $\mu = 1$, $\mu' = -1$, we get using the 9-j symbol and the $\lambda_a + \lambda_{a'} + k$ = even, selection rules, the nonvanishing terms in (A.3.12) for k = 1, and L = 0,1

$$E^{k=1}(1/2\,\mu{=}1;1/2\,\mu'{=}-1;L) \quad =$$

$$E^{k=1}(1/2\ \mu = -1;\ 1/2\ \mu = 1;L)(-1)^L \qquad \text{(A.3.13)}$$

and,

$$E^{k=1}(1/2\ \mu{=}1;1/2\ \mu = -1;L) \quad = \quad \sqrt{2/3} \quad \text{for } L{=}0$$

$$2/\sqrt{3} \quad \text{for } L{=}1. \qquad \text{(A.3.14)}$$

We therefore get,

$$\langle a\ b \mid -\alpha_1\cdot\alpha_2/r_{12} \mid a'\ b'\rangle = (-1)\int_0^\infty dr_1 \int_0^\infty dr_2 \left[r_</r_>^2 \right.$$

$$\left\{ 2/3\ \ X^{L=0}(m_a m_{a'}; m_b m_{b'}) \times \right.$$

$$(P_a(r_1)Q_{a'}(r_1) - Q_a(r_1)P_{a'}(r_1)) \times$$

$$(P_b(r_2)Q_{b'}(r_2) - Q_b(r_2)P_{b'}(r_2))$$

$$- 4/3\ X^{L=1}(m_a m_{a'}; m_b m_{b'}) \times$$

$$(P_a(r_1)Q_{a'}(r_1) + Q_a(r_1)P_{a'}(r_1)) \times$$

$$\left. (P_b(r_2)Q_{b'}(r_2) + Q_b(r_2)P_{b'}(r_2)) \right\} \Big].$$

(A.3.15)

The generalized Breit operator $\eta_{nm,n'm'}$ in (2.1.27) can now be expressed as a linear combination of the Gaunt, and Coulomb matrix elements given above; if the radial partial waves $r_</r_>^{k+1}$ are replaced by the nonlocal operators $-w\,(2k+1)\,j_k(wr_<)y_k(wr_>)$, where w is the energy difference $W_{nn'}$, and j_k, y_k are the spherical Bessel functions of order k, of the first and second kind respectively. Sometimes it is more practical to express these operators by an integral transform,

$$- w\ (2k+1)\ j_k(wr_<)\ y_k(wr_>) =$$

$$- w(2k+1)\ P/\pi \int_{-\infty}^{\infty} dz\ j_k(zr_1) j_k(zr_2)\ z^2/(z^2-w^2)$$

(A.3.16)

Appendix A.4 Computer Codes

The codes RACC, RACB, RABB, evaluate the shifts given in equations, (4.3.5), (4.3.8), and (4.3.11) respectively. These shifts are essentially linear combinations of integrals defined in (4.3.39) and reduced to simplified form in (4.3.35). The function subprogram VI utilizes a Gaussian quadrature formula to evaluate the I_k integrals defined in (4.3.35). The accuracy of VI is tested by looking at the convergence of the results when more points in the Gaussian quadrature are utilized. Results for various parameters of I_k are given in table A.1. Linear combinations of the I_k are used in the function subprograms RC, RB, to construct the radial integrals RC(aa',bb'), J^{+}_{-}(aa',bb') defined in (4.3.20), and (4.3.28) respectively. These in turn are used to construct the basic matrix elements $V^{C-C}_{abc,a'b'c''}$, $V^{C-B}_{abc,,a'b'c''}$, $V^{B-B}_{abc,a'b'c'}$ defined in (4.3.7), (4.3.10), and (4.3.13) respectively. The expressions for these matrix elements are factored into magnetic quantum number coefficients and the radial integrals described above. This factorization is given by equation (4.3.36) for the $V^{B-B}_{abc,a'b'c'}$ matrix elements, we have for the other matrix elements,

$$V^{C-C}_{abc,a'b'c'} = 4M_{00}(aa',bb',cc') \triangle R^C(aa';pb')R^C(bp;cc')$$

$$V^{C-B}_{abc,a'b'c'} = 8/3\ M_{00}(aa',bb',cc') \triangle R^C(aa';pb')J^+(bp;cc')$$

$$-16/3\ M_{01}(aa',bb',cc') \triangle R^C(aa';bp)J^-(bp;cc')$$

(A.5.1)

where we use the notation of section 4.3, the M coefficients are defined in (4.3.37) and the summation over the intermediate states is implied. The coefficients M_{00}, M_{01}, M_{11}, are evaluated in the subprogram functions GA, GB, GC, respectively. Finally the sum over the intermediate states in the above expressions is accomplished by the general purpose and very accurate integration program QUANC8, available at the C.C.N.Y computation center.

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