Relativistic second-order energy functional for finite fermion systems*

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A second-order energy functional is calculated for a finite system of fermions interacting via meson fields. The positive-type projection operator is utilized to relegate most corrections due to holes to higher than second order. The second-order functional is the basis for the relativistic analog of the Hartree-Fock procedure.

I. INTRODUCTION

In the last few years, there have been several papers on the quantum field-theoretic treatment of a system of fermions that interact via virtual-meson exchange. The semirelativistic problem is relatively simple[1]; the relativistic problem has been attacked in several ways.[2-5]

One of the difficulties in dealing with the relativistic problem is the treatment of effects due to the filled infinite "sea" of negative-energy states. In particular, in a finite system one expects that there is a static meson field that acts like a potential for individual fermions. The difficulty arises in calculating effects of this potential on the infinite negative-energy sea. Clearly, the potential must shift the energies of the negative-energy states, and the integral of these shifts over the infinite sea can be large. On the other hand, physical intuition would suggest that the effects of the negative-energy sea are not large; since the sea is undisturbed in the absence of interaction, effects of the sea are of order g^2 and higher. In Ref. 5 it turned out that there were no zeroth-order effects of the sea. However, the technique used there cannot be applied to finite systems, where some single-particle potential is required to produce a suitable unperturbed ground state. Then the problem of the sea again arises.

In this paper, the usual positive-energy projection operator

$$P_+(\vec{p}) = [\epsilon(\vec{p}) + \vec{\alpha}\cdot\vec{p} + \beta m]/2\epsilon(\vec{p}) ,$$
$$\epsilon(\vec{p}) = (\vec{p}^{\,2} + \vec{m}^{\,2})^{1/2} \quad (1.1)$$

will be used to push effects of the negative-energy sea to higher orders of perturbation theory. The mechanism is the requirement that the effective single-particle potential *not* act on the states in the sea; in momentum space it is required to be of the form

$$v_+(\vec{p},\vec{q}) = P_+(\vec{p})v(\vec{p},\vec{q})P_+(\vec{q}) , \quad (1.2)$$

and Fourier transformation gives a corresponding equation in configuration space.

As a check, the second-order energy of infinite fermion matter is recalculated with the projection operator; this forms the subject of Sec. III. The result for infinite matter using the projection operator is identical with the second-order energy given previously.[5] Then Sec. IV gives the analogous calculation for a finite system. As in the nonrelativistic case, the energy is a functional of the occupied single-particle spinor states $f_i(\vec{x})$,

$$E = E^{(0)}\{f_i(\vec{x})\} + g^2E^{(2)}\{f_i(\vec{x})\} + \cdots \quad (1.3)$$

(for simplicity, the calculations are done with only a scalar mediating field; hence, only one coupling constant), where the $f_i(\vec{x})$ must satisfy the extra condition

$$P_+(\vec{p})\tilde{f}_i(\vec{p}) = \tilde{f}_i(\vec{p}) ,$$
$$\tilde{f}_i(\vec{p}) = (2\pi)^{-3/2}\int e^{-i\vec{p}\cdot\vec{x}}f_i(\vec{x})d\vec{x} ; \quad (1.4)$$

that is, the f_i are orthogonal to the states in the unperturbed negative-energy sea.

Of course, once the functionals $E^{(0)}\{f_i\}$ and $E^{(2)}\{f_i\}$ are known, variation with respect to the orthonormal set of spinor functions f_i gives a self-consistent procedure for determining the set of spinor functions f_i that minimizes $E^{(0)} + g^2E^{(2)}$. This procedure is the same as the Hartree-Fock procedure that is applied in the case of nonrelativistic fermions interacting via a two-body potential $V(\vec{x},\vec{y})$; in that case

$$E^{(0)}_{\rm NR} = \sum_{i=1}^{N}\int f_i(\vec{x})\left(-\frac{\nabla^2}{2m}\right)f_i(\vec{x})d\vec{x} ,$$
$$g^2E^{(2)}_{\rm NR} = \tfrac{1}{2}\sum_{i,j=1}^{N}\int f_i^\dagger(\vec{x})f_j^\dagger(\vec{y})V(\vec{x},\vec{y}) \quad (1.5)$$
$$\times[f_j(\vec{y})f_i(\vec{x}) - f_i(\vec{y})f_j(\vec{x})]\,d\vec{x}\,d\vec{y} .$$

In Ref. 1 it was shown that $E^{(0)} + g^2E^{(2)}$ takes a similar form in the semirelativistic case, and it will be seen that the relativistic form of $E^{(0)} + g^2E^{(2)}$ also resembles (1.5). In the nonrelativistic case, the functional $E^{(0)} + g^2E^{(2)}$ has the advantage

of being "variational," in that it gives an upper bound on the energy of the system. This feature is lost in the semirelativistic and relativistic cases.

It might appear at first that the extra condition (1.4) on the spinors would complicate the Hartree-Fock procedure; however, in Sec. V it will be noted that the extra condition actually simplifies the relativistic Hartree-Fock procedure, in that it reduces the number of radial functions from two to one for each relativistic single-particle function in a spherically symmetric potential.

Throughout, the notation, units, metric, and other conventions are as in Ref. 5.

II. THE PROJECTION OPERATOR P_+

Before proceeding to the calculation, it is necessary to make a few remarks about the operator P_+ of Eq. (1.1). In this paper P_+ will be called the positive-*type* projection operator, for the reason that positive-type spinors will sometimes belong to negative eigenvalues of single-particle Hamiltonians. The positive-type part $A_+(\vec{p},\vec{q})$ of an operator $A(\vec{p},\vec{q})$ in momentum space is defined as in Eq. (1.2),

$$A_+(\vec{p},\vec{q}) = P_+(\vec{p})A(\vec{p},\vec{q})P_+(\vec{q}) , \tag{2.1}$$

and it is convenient to define

$$A_R \equiv A - A_+ . \tag{2.2}$$

There is also a negative-type projection operator P_-

$$P_-(\vec{p}) = 1 - P_+(\vec{p}) . \tag{2.3}$$

A spinor f is said to be of positive or negative type if $P_+f=f$ or $P_-f=f$, respectively.

The positive-type parts of the operators β and $\vec{\alpha}\cdot\vec{p}$ are

$$\begin{aligned} \beta_+ &= \frac{m}{\epsilon(\vec{p})} P_+ , \\ (\vec{\alpha}\cdot\vec{p})_+ &= \frac{p^2}{\epsilon(\vec{p})} P_+ . \end{aligned} \tag{2.4}$$

III. INFINITE FERMION MATTER

The Hamiltonian that will be considered is

$$\begin{aligned} H = H_c &+ \int \psi^\dagger(\vec{\alpha}\cdot\vec{p} + \beta m)\psi \\ &+ \tfrac{1}{2}\int [\dot{\phi}^2 + (\nabla\phi)^2 + \mu^2\phi^2] \\ &- g\int \phi(\bar{\psi}\psi - \langle\bar{\psi}\psi\rangle_{00}) , \end{aligned} \tag{3.1}$$

where H_c contains the counterterms necessary for renormalization. As in Ref. 5, the substitution

$$\phi = \phi_\rho + \chi \tag{3.2}$$

is made, with ϕ_ρ a static c-number field (uniform in infinite matter). However, in contrast to Ref. 5, part of the term

$$-g\int \phi_\rho \psi^\dagger \beta\psi \tag{3.3}$$

will now be included in the unperturbed Hamiltonian H_0, namely, the positive-type part

$$-g\int \psi^\dagger(\beta\phi_\rho)_+\psi , \tag{3.4}$$

while the remaining part

$$-g\int \psi^\dagger(\beta\phi_\rho)_R\psi \tag{3.5}$$

will be put into the interaction Hamiltonian H_I. Explicitly,

$$\begin{aligned} H &= H_c + H_{0,\rho} + H_{I,\rho} , \\ H_{0,\rho} &= \int \psi^\dagger[\alpha\cdot p + \beta m - g(\beta\phi_\rho)_+]\psi \\ &\quad + \tfrac{1}{2}\int [\chi^2 + (\nabla\chi)^2 + \mu^2\chi^2] , \\ H_{I,\rho} &= H_{I0,\rho} + H_{I1,\rho} + H_{I2,\rho} + H_{I3,\rho} + H_{I4,\rho} , \\ H_{I0,\rho} &= \tfrac{1}{2}\int \phi_\rho(-\nabla^2 + \mu^2)\phi_\rho , \\ H_{I1,\rho} &= -g\int \chi(\bar{\psi}\psi - \langle\bar{\psi}\psi\rangle_{\rho 0}) , \\ H_{I2,\rho} &= -g\int [\psi^\dagger(\beta\phi_\rho)_R\psi - \langle\psi^\dagger(\beta\phi_\rho)_R\psi\rangle_{\rho 0}] , \\ H_{I3,\rho} &= \int \chi[(-\nabla^2 + \mu^2)\phi_\rho - g(\langle\bar{\psi}\psi\rangle_{\rho 0} - \langle\bar{\psi}\psi\rangle_{00})] , \\ H_{I4,\rho} &= -g\int [\langle\psi^\dagger(\beta\phi_\rho)_R\psi\rangle_{\rho 0} - \langle\psi^\dagger\beta\phi_\rho\psi\rangle_{00}] . \end{aligned} \tag{3.6}$$

The negative-type eigenvalues and eigenvectors of the single-particle operator h_ρ

$$h_\rho = \vec{\alpha}\cdot\vec{p} + \beta m - g(\beta\phi_\rho)_+ \tag{3.7}$$

are the same as the negative-energy eigenvalues and eigenvectors of h_0. The positive-type eigenvalues are [see (2.4)]

$$\begin{aligned} \epsilon_\rho(\vec{p}) &= \epsilon_0(\vec{p}) - gm\phi_\rho/\epsilon_0(\vec{p}) , \\ \epsilon_0(\vec{p}) &= \epsilon(\vec{p}) = (\vec{p}^{\,2} + m^2)^{1/2} . \end{aligned} \tag{3.8}$$

[Note that the positive-type eigenvalue $\epsilon_\rho(\vec{p})$ can be negative; hence the use of the word "type."] The ground state of $H_{0,\rho}$ has all negative-type states filled and positive-type states filled up to momentum p_F with[6]

$$\rho = \gamma p_F^{\,3}/3\pi^2 . \tag{3.9}$$

It follows immediately that for any single-particle

operator A

$$\langle \psi^\dagger A_R \psi \rangle_{\rho 0} = \langle \psi^\dagger A \psi \rangle_{00} , \tag{3.10}$$

and therefore

$$H_{I4,\,\rho} = 0 . \tag{3.11}$$

The unperturbed energy is

$$\langle H_{0,\rho} \rangle_{\rho 0} - \langle H_{0,0} \rangle_{00} = \frac{2\gamma}{(2\pi)^3} \Omega \int \epsilon_\rho(\vec{p}) d_F \vec{p} = \frac{2\gamma}{(2\pi)^3} \Omega \int \epsilon_0(\vec{p}) d_F \vec{p} - \Omega g \phi_\rho \rho_S^{(0)} , \tag{3.12}$$

$$\rho_S^{(0)} = \langle \bar{\psi}\psi \rangle_{\rho 0} - \langle \bar{\psi}\psi \rangle_{00} = \frac{2\gamma}{(2\pi)^3} m \int \frac{d_F \vec{p}}{\epsilon_0(\vec{p})} .$$

In zeroth order $\phi_\rho = 0$ and the energy per unit volume is

$$F_\rho^{(0)} = E_\rho^{(0)}/\Omega = \frac{2\gamma}{(2\pi)^3} \int \epsilon_0(\vec{p}) d_F \vec{p} , \tag{3.13}$$

as in Ref. 5.

The calculation of the second-order energy proceeds as in Ref. 5. With $H_{0,\rho}$ of (3.6) the fermion Green's function G_ρ at density ρ can be written

$$G_\rho(p) = G_0(p) + G_{\rho 0}(p) , \tag{3.14}$$

with $G_0(p)$ the zero-density Green's function:

$$G_0(p) = \frac{i}{(2\pi)^4} \frac{\not{p} + m}{p^2 - m^2 + i0} = \frac{i}{(2\pi)^4} \left[\frac{P_-(\vec{p})}{p_0 + \epsilon(\vec{p}) - i0} + \frac{P_+(\vec{p})}{p_0 - \epsilon(\vec{p}) + i0} \right] \beta . \tag{3.15}$$

The negative-type parts of G_ρ and G_0 are equal, and

$$G_{\rho 0}(p) = \frac{i}{(2\pi)^4} \left[\frac{1}{p_0 - \epsilon_\rho(\vec{p}) + i\eta(\vec{p})} - \frac{1}{p_0 - \epsilon_0(\vec{p}) + i0} \right] P_+(\vec{p}) \beta, \quad \eta(\vec{p}) = \begin{cases} 0_+, & |\vec{p}| > p_F \\ 0_-, & |\vec{p}| \le p_F . \end{cases} \tag{3.16}$$

The function $G_{\rho 0}$ can be split into zeroth-order and second-order parts, with

$$G_{\rho 0}^{(0)}(p) = \frac{i}{(2\pi)^4} \left[\frac{1}{p_0 - \epsilon_0(\vec{p}) + i\eta(\vec{p})} - \frac{1}{p_0 - \epsilon_0(\vec{p}) + i0} \right] P_+(\vec{p}) \beta = -\frac{\not{p} + m}{16\pi^3 \epsilon(\vec{p})} \delta_F(p_0 - \epsilon(\vec{p})) ,$$

$$G_{\rho 0}^{(2)}(p) = \frac{i}{(2\pi)^4} \frac{\epsilon_\rho(\vec{p}) - \epsilon_0(\vec{p})}{[p_0 - \epsilon_\rho(\vec{p}) + i\eta(\vec{p})][p_0 - \epsilon_0(\vec{p}) + i\eta(\vec{p})]} . \tag{3.17}$$

Since $G_{\rho 0}^{(2)}(p)$ is of second order in g, it does not contribute to the second-order energy, and since $G_{\rho 0}^{(0)}$ is identical with $G_{\rho 0}$ of Ref. 5, the second-order exchange energy follows exactly as in Ref. 5:

$$F_{\rho,\mathrm{ex},S}^{(2)} = \frac{\gamma}{2} \frac{g^2}{(2\pi)^6} \int \frac{d_F \vec{p}\, d_F \vec{q}}{\epsilon(\vec{p}) \epsilon(\vec{q})} \frac{(pq) + m^2}{\mu^2 - (p-q)^2} . \tag{3.18}$$

The direct second-order energy comes from $H_{0,\rho}$ and $H_{I0,\rho}$. It is just

$$F_{\rho,D,S}^{(2)} = -\tfrac{1}{2} g \phi_\rho^{(1)} \rho_S^{(0)} .$$

Thus, use of the type projection operator leads to the same second-order energy for infinite matter as was obtained in Ref. 5.

IV. FINITE SYSTEMS

Again the starting point is the Hamiltonian (3.1). Now the substitution

$$\phi = \phi_N + \chi \tag{4.1}$$

and the separation of positive-type parts give, just as in (3.6),

$$\begin{aligned}
H &= H_c + H_{0,N} + H_{I,N} , \\
H_{0,N} &= \int \psi^\dagger [\vec{\alpha} \cdot \vec{p} + \beta m - g(\beta \phi_N)_+] \psi \\
&\quad + \tfrac{1}{2} \int [\dot{\chi}^2 + (\nabla \chi)^2 + \mu^2 \chi^2] , \\
H_{I,N} &= H_{I1,N} + H_{I2,N} + H_{I3,N} + H_{I4,N} , \\
H_{I0,N} &= \tfrac{1}{2} \int \phi_N (-\nabla^2 + \mu^2) \phi_N , \\
H_{I1,N} &= -g \int \chi (\bar{\psi}\psi - \langle \bar{\psi}\psi \rangle_{N0}) , \\
H_{I2,N} &= -g \int [\psi^\dagger (\beta \phi_N)_R \psi - \langle \psi^\dagger (\beta \phi_N)_R \psi \rangle_{N0}] , \\
H_{I3,N} &= \int \chi [(-\nabla^2 + \mu^2) \phi_N - g(\langle \bar{\psi}\psi \rangle_{N0} - \langle \bar{\psi}\psi \rangle_{00})] , \\
H_{I4,N} &= -g \int [\langle \psi^\dagger (\beta \phi_N)_R \psi \rangle_{N0} - \langle \psi^\dagger \beta \phi_N \psi \rangle_{00}] .
\end{aligned} \tag{4.2}$$

The negative-type eigenvalues and eigenvectors of the single-particle operator

$$h_N = \vec{\alpha}\cdot\vec{p} + \beta m - g(\beta\phi_N)_+ \tag{4.3}$$

are the same as the negative-energy eigenvalues and eigenvectors of

$$h_0 = \vec{\alpha}\cdot\vec{p} + \beta m . \tag{4.4}$$

As for the positive-type spectrum, it will be assumed that h_N has at least N discrete eigenvalues (each less than m). Then the ground state of $H_{0,N}$, denoted $|0, N\rangle$, is obtained by filling (in addition to all states of negative type) the N lowest eigenstates of h_N. (It is also possible for h_N to have negative eigenvalues for positive-type states.) The positive-type eigenspinors of h_N will be denoted f_i,

$$\begin{aligned} &h_N f_i = \epsilon_i f_i , \\ &P_+ f_i = f_i . \end{aligned} \tag{4.5}$$

The discrete part of the spectrum of h_N is all that will be needed here; there is also a continuum for $\epsilon_i \geq m$ if ϕ_N has proper asymptotic properties.

It follows directly from the definition of $|N, 0\rangle$ that for any single-particle operator A

$$\langle\psi^\dagger A_R\psi\rangle_{N0} = \langle\psi^\dagger A\psi\rangle_{00} , \tag{4.6}$$

and therefore

$$H_{I4,N} = 0 . \tag{4.7}$$

In zeroth order in g, the contribution to the energy from $H_{0,N}$ is

$$E^{(0)} = \sum_{i=1}^{N} (f_i , (\vec{\alpha}\cdot\vec{p} + \beta m) f_i) , \tag{4.8}$$

where sums are to be understood as including the positive-type states only.

For the second-order terms, ϕ_N must be found to first order. From $H_{I3,N}$ it follows that

$$\begin{aligned} (-\nabla^2 + \mu^2)\phi_N^{(1)}(\vec{x}) &= g\rho_S^{(0)}(\vec{x}) , \\ \rho_S^{(0)}(\vec{x}) &= \langle\bar{\psi}\psi\rangle_{N0} - \langle\bar{\psi}\psi\rangle_{00} \\ &= \sum_{i=1}^{N} f_i^\dagger(\vec{x})\beta f_i(\vec{x}) . \end{aligned} \tag{4.9}$$

The operators P_+ and ∇^2 commute, so that

$$(-\nabla^2 + \mu^2)(\beta\phi_N)_+ = g(\beta\rho_S^{(0)})_+ . \tag{4.10}$$

The direct second-order energy from $H_{0,N}$ is

$$-g\sum_{i=1}^{N}(f_i , (\beta\phi_N)_+ f_i) = -g\sum_{i=1}^{N}(f_i , \beta\phi_N f_i) , \tag{4.11}$$

where the equality follows from (4.5). From $H_{I0,N}$ there is a contribution

$$\tfrac{1}{2}\int \phi_N^{(1)}(-\nabla^2 + \mu^2)\phi_N^{(1)} = \frac{g}{2}\int \phi_N^{(1)}\rho_S^{(0)} . \tag{4.12}$$

Thus the total contribution from these two terms is

$$\begin{aligned} E^{(2)}_{N,D,S} &= -\frac{g}{2}\int \phi_N^{(1)}\rho_S^{(0)} \\ &= -\frac{g^2}{8\pi}\int \rho_S^{(0)}(\vec{x})\frac{e^{-\mu|\vec{x}-\vec{y}|}}{|\vec{x}-\vec{y}|}\rho_S^{(0)}(\vec{y})\,d\vec{x}\,d\vec{y} . \end{aligned} \tag{4.13}$$

The calculation of the exchange term requires the Green's function

$$\begin{aligned} G_N(p, q) &= G_N(p_0, \vec{p}, \vec{q})\delta(p_0 - q_0) \\ &= G_0(p, q) + G_{N0}(p, q) , \\ G_{N0}(p, q) &= G_{N0}(p_0, \vec{p}, \vec{q})\delta(p_0 - q_0) , \\ G_0(p, q) &= G_0(p)\delta(p - q) , \\ G_{N0}(p_0, \vec{p}, \vec{q}) &= \frac{i}{(2\pi)^4}\left(\sum_j \frac{\tilde{f}_j(\vec{p})\tilde{f}_j^\dagger(\vec{q})}{p_0 - \epsilon_j + i\eta_j} - \frac{\delta(\vec{p}-\vec{q})P_+(\vec{p})}{p_0 - \epsilon(\vec{p}, \vec{q}) + i0}\right)\beta , \end{aligned} \tag{4.14}$$

where $\epsilon(\vec{p}, \vec{q})$ is a function that satisfies

$$\epsilon(\vec{p}, \vec{p}) = \epsilon_0(\vec{p}) . \tag{4.15}$$

The completeness relation for the positive-type states is

$$\sum_j \tilde{f}_j(\vec{p})\tilde{f}_j^\dagger(\vec{q}) = \delta(\vec{p}-\vec{q})P_+(\vec{p}) , \tag{4.16}$$

so that

$$G_{N0}(p_0, \vec{p}, \vec{q}) = G_{N0}^{(0)}(p_0, \vec{p}, \vec{q}) + G_{N0}^{(2)}(p_0, \vec{p}, \vec{q}) , \tag{4.17}$$

with

$$\begin{aligned} G_{N0}^{(0)}(p_0, \vec{p}, \vec{q}) &= -\frac{1}{(2\pi)^3}\sum_{j=1}^{N}\tilde{f}_j(\vec{p})\tilde{f}_j^\dagger(\vec{q})\delta(p_0 - \epsilon(\vec{p}, \vec{q}))P_+(\vec{p})\beta , \\ G_{N0}^{(2)}(p_0, \vec{p}, \vec{q}) &= \frac{i}{(2\pi)^4}\sum_j \tilde{f}_j(\vec{p})\tilde{f}_j^\dagger(\vec{q})\left(\frac{1}{p_0 - \epsilon_j + i\eta_j} - \frac{1}{p_0 - \epsilon(\vec{p}, \vec{q}) + i\eta_j}\right)\beta . \end{aligned} \tag{4.18}$$

Here $G_{N0}^{(2)}$ is of second order in g, so that only $G_{N0}^{(0)}$ will contribute to the second-order exchange energy.

The second-order exchange energy comes from the graph of Fig. 1 and the $\delta m_c^{(2)}$ term in H_c, just as in Ref. 5:

$$-2\pi i\delta^{(1)}(0)\Delta E_G^{(2)} = -\tfrac{1}{2}[-(2\pi)^4 ig]^2 \mathrm{Tr}\int [G_N(p,p')G_N(q',q) - G_0(p)\delta(p-p')G_0(q)\delta(q-q')]$$
$$\times D(p-q)d^4p\, d^4q\, d^4p'\, d^4q'\delta(p'-q'-p+q)$$
$$= -[-(2\pi)^4 ig]^2\delta^{(1)}(0)\mathrm{Tr}\int [G_{N0}(p_0,\vec{p},\vec{p}')G_0(q)\delta(\vec{q}-\vec{q}') + \tfrac{1}{2}G_{N0}(p_0,\vec{p},\vec{p}')G_{N0}(q_0,\vec{q},\vec{q}')]$$
$$\times D(p-q)d^4p\, d^4q\, d\vec{p}'d\vec{q}'\delta(\vec{p}'-\vec{q}'-\vec{p}+\vec{q})\,. \tag{4.19}$$

The first term involves the integral that appears in the second-order vacuum self-energy $\Sigma_0^{(2)}$; the second-order part of the first term can be written[5]

$$(2\pi)^4 i\delta^{(1)}(0)\mathrm{Tr}\int G_{N0}^{(0)}(p_0,\vec{p},\vec{p}')\Sigma_0^{(2)}(p)\delta(\vec{p}'-\vec{p})d^4p\, d\vec{p}'$$
$$= -2\pi i\delta^{(1)}(0)\mathrm{Tr}\sum_{j=1}^{N}\int \tilde{f}_j(\vec{p})\tilde{f}_j^{\dagger}(\vec{p})\delta(p_0-\epsilon_0(\vec{p}))\frac{(\not{p}+m)}{2\epsilon_0(\vec{p})}[\delta m_c^{(2)} + (\not{p}-m)\Sigma_{0,1}^{(2)}(\not{p})]d^4p$$
$$= -2\pi i\delta^{(1)}(0)\mathrm{Tr}\sum_{j=1}^{N}\int \tilde{f}_j(\vec{p})\tilde{f}_j^{\dagger}(\vec{p})\beta\delta m_c^{(2)}$$
$$= -2\pi i\delta^{(1)}(0)\delta m_c^{(2)}\int \rho_S^{(0)}(\vec{x})d\vec{x}\,, \tag{4.20}$$

and, as in Ref. 5, this cancels the second-order energy from the $\delta m_c^{(2)}$ term in H_c. The remaining exchange energy comes from the second term in (4.19); it is easily seen to be

$$E_{N,\mathrm{ex},S}^{(2)} = \frac{g^2}{2(2\pi)^3}\sum_{i,j=1}^{N}\int \frac{\tilde{f}_i^{\dagger}(\vec{q})\beta\tilde{f}_j(\vec{p})\tilde{f}_j^{\dagger}(\vec{p}')\beta\tilde{f}_i(\vec{q}')}{\mu^2-(p-q)^2}\delta(\vec{p}-\vec{q}-\vec{p}'+\vec{q}')d\vec{p}\, d\vec{q}\, d\vec{p}'d\vec{q}'\,. \tag{4.21}$$

In the denominator of (4.21), p_0 and q_0 are to be set equal to $\epsilon(\vec{p},\vec{p}')$ and $\epsilon(\vec{q},\vec{q}')$, respectively, according to the δ functions in $G_{N0}^{(0)}(p_0,\vec{p},\vec{p}')$ and $G_{N0}^{(0)}(p_0,\vec{q},\vec{q}')$.

The expression (4.21) for E_{ex} is sensitive to the choice of the function $\epsilon(\vec{p},\vec{q})$. Of course, the actual value of $E^{(\infty)}$

$$E^{(\infty)} \equiv \lim_{N\to\infty}\sum_{n=0}^{N} g^n E^{(n)} \tag{4.22}$$

is independent of the choice of $\epsilon(\vec{p},\vec{q})$. Therefore, it seems logical to choose $\epsilon(\vec{p},\vec{q})$ so that $E^{(2)}$ is stationary with respect to variations of $\epsilon(\vec{p},\vec{q})$. For example, in the parametrizations $\alpha\epsilon(\vec{p}) + \beta\epsilon(\vec{q})$ and $\epsilon(\alpha\vec{p}+\beta\vec{q})$ with $\alpha+\beta=1$, the value that makes E_{ex} stationary $\alpha=\beta=\frac{1}{2}$ by symmetry. The extent to which E_{ex} depends on $\epsilon(\vec{p},\vec{q})$ is a rough measure of the accuracy of the second-order calculation. After all, the term in $[\epsilon(\vec{p},\vec{p}')-\epsilon(\vec{q},\vec{q}')]^2$ is of order g^2 and represents a g^4 correction to E_{ex}, so that it is not inconsistent to omit it entirely from (4.21). The "pure" second-order exchange energy is

$$E_{N,\mathrm{ex},S}^{(2)} = \frac{g^2}{16\pi^3}\sum_{i,j=1}^{N}\int \frac{f_i^{\dagger}(\vec{x})\beta f_j(\vec{x})e^{i\vec{k}\cdot(\vec{x}-\vec{y})}f_j^{\dagger}(\vec{y})\beta f_i(\vec{y})}{\mu^2+\vec{k}^2}\, d\vec{x}\, d\vec{y}\, d\vec{k}\,, \tag{4.23}$$

which, except for the condition that the f_i be of positive type, is just what would have been expected from the form of the nonrelativistic Fock exchange term.

V. P_+ AGAIN

The condition $P_+ f = f$ on a Dirac spinor simplifies the calculation of f in a spherically symmetric potential V_+. In momentum space, with the standard forms

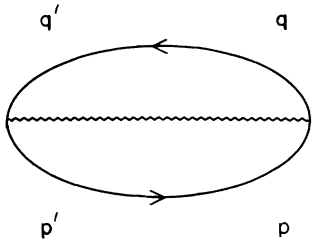

FIG. 1. Second-order energy graph.

$$\beta = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad ,$$
$$\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix} \quad , \tag{5.1}$$

the usual form for a Dirac spinor eigenfunction in a spherically symmetric potential is

$$f^{lj}_m = \begin{pmatrix} g_1^{lj}(p)\, \mathcal{Y}^{lj}_m(\hat{p})/p \\ g_2^{lj}(p)\, \mathcal{Y}^{Lj}_m(\hat{p})/p \end{pmatrix} \quad , \tag{5.2}$$

where $\mathcal{Y}^{lj}_m(\hat{p})$ is the vector coupled space-spin harmonic and L is the "opposite orbital angular momentum"; that is, $L = l \pm 1$ for $j = l \pm \frac{1}{2}$. In (5.2) g_1 and g_2 are independent "radial" functions that are determined by solving coupled integral equations (in configuration space, coupled differential equations). The condition $P_+ f = f$ gives

$$f^{lj}_m = [2\epsilon(\vec{p})]^{-1/2} \begin{pmatrix} [m+\epsilon(\vec{p})]^{1/2} g^{lj}(p) \mathcal{Y}^{lj}_m(\hat{p})/p \\ -p[m+\epsilon(\vec{p})]^{-1/2} g^{lj}(p) \mathcal{Y}^{Lj}_m(\hat{p})/p \end{pmatrix} \quad , \tag{5.3}$$

with a single normalized radial function $g^{lj}(p)$,

$$\int_0^\infty |g^{lj}(p)|^2 dp = 1 \quad . \tag{5.4}$$

This is a considerable simplification for numerical computation.

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