Three-electron atoms from a Bethe-Salpeter equation approach

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The two-electron Bethe-Salpeter equation is reviewed. The transition to a Hamiltonian form is discussed, and the criterion that the first-order energy shift vanish is used to determine the electron-electron potential that appears in the Hamiltonian. A similar program is carried through for the three-electron case. The fundamental idea of Feldman and Fulton [Nucl. Phys. **B195**, 61 (1982)] is used for the transition to the Hamiltonian form, although some changes are necessary. The optimum two-electron interaction is the same as that in the two-electron case. It is necessary to introduce a static three-electron interaction, which then can be determined from the vanishing of the first-order energy shift. It is extremely complicated and unlikely to prove useful in the near future.

I. INTRODUCTION

The use of the Bethe-Salpeter equation[1] (BSE) for the calculation of atomic structure has hardly been pursued since the original appearance of the equation. Essentially all the progress that has been made in the two-body problem has resulted from an approximation of the two-body interaction by a instantaneous (unretarded) potential and the reduction of the resulting equation to a Hamiltonian form.[2] A perturbation theory was then developed in order to obtain corrections to the energy obtained from the Hamiltonian equation. The choice of the instantaneous potential is somewhat arbitrary. It has received some attention in the literature for nonrelativistic (low-z) cases.[3] There does not seem to be any convincing prescription for its choice in the relativistic (high-z) case.

In Sec. II, I review the two-electron problem in which the nucleus is treated as a spectator merely providing an attractive potential for the electrons. A slightly different perturbation theory is introduced in order to make energies explicitly real. The criterion for fixing the instantaneous potential is that the first-order correction to the energy shall vanish. This results in an instantaneous potential which is very similar to the two-body potential obtained from the configuration-space Hamiltonian[4] directly from QED; i.e., without the intermediary step of the BSE.

In Sec. III a similar program is attempted for the three-body BSE. First the explicit three-particle interaction (resulting from the exchange of at least three photons) is neglected. The two-electron interactions are approximated by instantaneous potentials and the reduction to single-time (Hamiltonian) form is accomplished by following the ideas of Feldman and Fulton[5] with some surprising results. Negative energy states do not appear in the single-time three-electron wave functions, a result which is not true for the two-electron case.

The attempt to make the first-order correction to the energy vanish fails in this case since we find that in addition to two-electron terms contributing to the energy shift there are three-electron terms. These cannot be canceled by any choice of the instantaneous two-electron potential. If we determine the two-electron potential from the condition that there be no two-electron contributions to the energy shift, then a two-electron instantaneous interaction is obtained which is the same as that obtained in Sec. II. That is, the presence of the other electron, does not affect the optimum electron-electron interaction.

In Sec. IV we return to the original three-electron BSE and include the three-electron interaction. The transition to the Hamiltonian form is accomplished by allowing for instantaneous three-electron potentials. (These have appeared previously in both a classical[6] and QED formulation of the problem.[7]) The result is a surprisingly simple generalization of the Feldman and Fulton[5] prescription. It is possible to obtain the optimum three-electron static potential which makes the first-order energy shift vanish but it is too complex to even display here. The extension of this program to more than three electrons would appear to be profitless at this time.

II. HELIUMLIKE ATOMS

The BSE for two electrons in a static nuclear potential is well known. It is reviewed briefly here to establish notation and define the different approach taken here. It

can be written, in the Furry picture, as

$$S_1^{-1}(e_1)S_2^{-1}(e_2)\psi(\{e\})$$

$$= \frac{i}{2\pi} \int d^2e'\delta(e_1'+e_2')I_{12}(\{e\},\{e'\})\psi(\{e'\}) , \quad (2.1)$$

where

$$S_i(e_i) = [W/2+e_i-h_i(1-i\eta)]^{-1} . \quad (2.2)$$

Here W is the energy eigenvalue, e_i is fourth component of the ith momentum, h_i is the Dirac Hamiltonian including the nuclear potential, and η the usual positive infinitesimal. A mass operator could also be included in h_i in principle. The two-electron-irreducible interaction I_{12}, in the sense described by Salpeter and Bethe,[1] can also be included to any practical order so that (2.1) is, in principle, exact. In lowest order I_{12} is local and time-translationally invariant so that it becomes a simpler function of its arguments

$$I_{12}^{(0)}(\{e\},\{e'\}) = I_{12}^{(0)}(e_1-e_2-e_1'-e_2') , \quad (2.3)$$

with the spatial dependence suppressed. The δ function on the right of (2.1) serves to keep the "wave function" on shell, which is the only region of $\{e\}$ space that need be considered. The solution of (2.1) is a formidable task so that essentially all investigations proceed by replacing I_{12} by v_{12} a static, or instantaneous, interaction independent of the $\{e\}$ variables. This results in the Schrödinger equation obtained by Salpeter,[2]

$$(W^{(0)}-h_1-h_2-\Omega_{12}v_{12})\Phi=0 , \quad (2.4)$$

where $W^{(0)}$ is the approximate eigenvalue and

$$\Omega_{12}=\Lambda_+-\Lambda_-, \quad \Lambda=\Lambda_++\Lambda_- ,$$

$$\Lambda_+=\Lambda_+(1)\Lambda_+(2) , \quad (2.5)$$

$$\Lambda_-=\Lambda_-(1)\Lambda_-(2) ,$$

where $\Lambda_\pm(i)$ projects onto the positive (negative) energy spectrum of $h(i)$. It is easily shown that

$$\Lambda\Phi=\Phi \quad (2.6)$$

and that the presence of the Ω in (2.4) eliminates the profound difficulties of the Breit equation, which is (2.4) with $\Omega_{12}\rightarrow1$. These difficulties are referred to here as the Brown-Ravenhall disease (BRD). The potential $\Omega_{12}v_{12}$ is not Hermitian but it is easily demonstrated that the ei-

genvalue $W^{(0)}$ is nevertheless real so that the lack of Hermiticity in (2.4) is unimportant. This will be significant below. The static potential v_{12} is, at this point, arbitrary. Its choice has been discussed[3] in the past but a somewhat different point of view is taken here.

The true eigenvalue W is close to $W^{(0)}$ provided that the static potential mimics the effect of I_{12} sufficiently well. In that case the first-order of W, $W^{(1)}$, can be obtained as a linear expression in $(I_{12}-v_{12})$. The requirement that $W^{(1)}$ vanish then leads to an expression for v_{12}. In order to implement this program we first need an expression for $\psi^{(0)}(\{e\})$ in terms of Φ, (2.4), where $\psi^{(0)}$ is the solution of (2.1) with I_{12} replaced by v_{12}. This has been given previously[2] as

$$\psi^{(0)}(\{e\}) = \frac{1}{2\pi i}(S_1+S_2)\Phi , \quad (2.7)$$

where now the eigenvalue occurring in S_1 and S_2 is $W^{(0)}$.

If (2.1) is expanded about $\psi^{(0)}$ and $W^{(0)}$ the first-order result is

$$\left[F(W^{(0)}) - \frac{i}{2\pi} \int d^2e'\delta\left[\sum e'\right]v_{12}\right]\psi^{(1)}$$

$$= -W^{(1)}F'(W^{(0)})\psi^{(0)}+\frac{i}{2\pi} \int d^2e'\delta\left[\sum e'\right]\delta I_{12}\psi^{(0)} , \quad (2.8)$$

where

$$F(W)=(W/2+e_1-h_1)(W/2+e_2-h_2) \quad (2.9)$$

and

$$F'(W)=\frac{d}{dW}F(W) . \quad (2.10)$$

In order to extract $W^{(1)}$ from this equation it is necessary to multiply (2.8) from the left by a function which will make the left side of the equation vanish. This eliminates the dependence upon the unknown first-order wave function, $\psi^{(1)}$. The function which accomplishes this is

$$\tilde{\psi}^{(0)}=\tilde{\Phi}(S_1^\dagger+S_2^\dagger)\left[-\frac{1}{2\pi i}\right] , \quad (2.11)$$

where it is important that the Hermitian conjugate of the propagators (2.2), be used in order to keep $W^{(1)}$ real for Hermitian I_{12}. Operating on (2.8) with $\int d^2e\delta(\sum e)\tilde{\psi}^{(0)}$ from the left yields

$$+ \frac{i}{2\pi}\tilde{\Phi}(W-h_1-h_2-\Omega_{12}v_{12})\int d^2e'\delta\left[\sum e'\right]\psi^{(1)}(\{e'\})$$

$$= -W^{(1)}\int d^2e\,\tilde{\psi}^{(0)}(\{e\})F'(W^{(0)})\psi^{(0)}(\{e\})+\frac{i}{2\pi}\int d^2e\,d^2e'\delta\left[\sum e\right]\delta\left[\sum e'\right]\tilde{\psi}^{(0)}(\{e\})\delta I_{12}\psi^{(0)}(\{e'\}) . \quad (2.12)$$

Then we must have

$$\tilde{\Phi}(W^{(0)}-h_1-h_2-\Omega_{12}v_{12})=0 , \quad (2.13)$$

which yields

$$\tilde{\Phi}=(\Omega_{12}\Phi)^* . \quad (2.14)$$

We now use $W^{(1)}=0$ in order to obtain v_{12}. The $\{e\}$ integrals can be performed by the insertion of the projection operators $\Lambda_\pm$, (2.5), around I_{12} in all possible ways. We simplify by using the lowest order, (2.3), for I_{12} and obtain

$$(\tilde{\Phi},\Omega_{12}v_{12}\Omega_{12}\Phi)=\frac{1}{4\pi}\int_{-\infty}^{\infty}dx\int_0^{\infty}ds\,e^{-\eta s}[\tilde{\Phi}((e^{ish_1}\Lambda_+I_{12}\Lambda_+e^{-ish_1}e^{-isx/2}+e^{-ish_1}\Lambda_-I_{12}\Lambda_-e^{ish_1}e^{+isx/2}$$

$$+e^{-ish_1}\Lambda_+I_{12}\Lambda_-e^{-ish_2}e^{-is(W^{(0)}-x/2)}$$

$$+e^{ish_2}\Lambda_-I_{12}\Lambda_+e^{ish_1}e^{-is(W^{(0)}-x/2)})+(1\leftrightarrow2))\Phi]\,, \tag{2.15}$$

where $I_{12}=I_{12}(x)$ is an even function of its argument. Then the requirement that v_{12} be independent of the state, except for its energy, implies a form for v_{12}. Notice that components of v_{12} such as

$$\Lambda_+(1)\Lambda_-(2)v_{12}\Lambda_+(1)\Lambda_+(2)$$

do not occur, which is the crux of the cure of the BRD. If I_{12} is independent of x then we obtain $v_{12}=\Omega_{12}I_{12}\Omega_{12}$, which then allows for the incorporation of any instantaneous piece of I_{12} into v_{12}. If we compare the component of v_{12} proportional to $\Lambda_+I_{12}\Lambda_+$ to the two-electron potential obtained from a direct transition from Fock space to the Hamiltonian form of the configuration space equation,[4] it is seen that they are the same.

III. LITHIUMLIKE ATOMS

The three-electron BSE has not been dealt with extensively in the literature.[8,5] It can be written as

$$S_1^{-1}S_2^{-1}S_3^{-1}\psi(\{e\})=\frac{i}{2\pi}S_3^{-1}\int d^3e'\delta\left[\sum e'\right]\delta(e_3-e_3')I_{12}(\{e\},\{e'\})\psi(\{e'\})+(1\leftrightarrow3)+(2\leftrightarrow3)$$

$$+\left[\frac{i}{2\pi}\right]^2\int d^3e'\delta\left[\sum e'\right]I^{(3)}(\{e\},\{e'\})\psi(\{e'\})\,, \tag{3.1}$$

where there are now three e_i variables, the on-shell constraint being $e_1+e_2+e_3=0$. The propagators are now

$$S_i^{-1}=\frac{W}{3}+\varepsilon_i-h_i(1-i\eta)\,, \tag{3.2}$$

with the symbols having the same meaning as above. The three pair interactions, of which only the first is written explicitly, contains the same pair interaction I_{ij} as occurred in Sec. II so that in lowest order the first term on the right in (3.1) describes a photon exchange between 1 and 2 while 3 propagates as a spectator. The last term is the intrinsic three-electron interaction which cannot be generated from the iteration of any combination of the first three. Its leading term arises from the exchange of three photons. For the moment we neglect this three-electron term.

The replacement of I_{12} by v_{12} a static interaction yields an equation which is not easily reduced to a Schrödinger equation form. Before turning to this problem we first consider the limitation placed on the form of v_{12} by the requirement that the BRD shall not arise. That is, we adopt the point of view that the BRD is well understood and that a consistent derivation of the Schrödinger equation from QED will preclude its appearance. The disease arises from intermediate states in an expansion of the wave function which are part of a continuum and are degenerate with the initial state. For the two-electron problem, one in the positive energy continuum and one in the negative continuum of h can be arranged to be degenerate with the initial state. The projection operators occurring in (2.5) eliminate that possibility since they result in $\Lambda_+(1)\Lambda_-(2)\Phi=0$. For the more-than-two-electron case

it is clear that any combination of electrons with some in positive and others in negative energy states can form a continuum which will be degenerate with the initial state. Therefore, if the BRD is to be avoided, all electrons must be either in positive energy or in negative energy states. This precludes the occurrence of a part of the static potential of the form

$$\Lambda_-(1)\Lambda_-(2)v_{12}\Lambda_+(1)\Lambda_+(2)$$

and its Hermitian conjugate. A term of this form could take a part of Φ with all electrons in positive states and move a pair to negative states and thereby cause the degenerate configuration which results in the BRD. This restricts the possible static pair interaction to the form

$$v_{12}=\Lambda_+(1)\Lambda_+(2)V_{12}\Lambda_+(1)\Lambda_+(2)$$

$$+\Lambda_-(1)\Lambda_-(2)\bar{V}_{12}\Lambda_-(1)\Lambda_-(2)\,, \tag{3.3}$$

where for generality, V_{12} and $\bar{V}_{12}$ are allowed to be different. We use this form below.

The next step is analogous to (2.7) the relation between the Bethe-Salpeter wave function $\psi^{(0)}$ and the Schrödinger wave function Φ. Feldman and Fulton[5] have given a prescription for the nonrelativistic problem which is essentially the same one used here. The two-electron example can be taken as a prototype. In (2.7) the Schrödinger, or one-time, function Φ must be propagated to a two (unequal) time function $\psi^{(0)}$ in all possible ways. This is accomplished by propagating either the first particle with S_1 or the second with S_2 to different times. The three-electron case is more complex in that propagation of the equal-time function Φ to three unequal times can

be done in more than one way. In order to describe the most general case we need the two-body propagator

$$S_{12}^{-1} = S_1^{-1} + S_2^{-1} - v_{12}$$

$$= \tfrac{2}{3} W^{(0)} + e_1 + e_2 - (h_1 + h_2)(1 - i\eta) - v_{12} , \quad (3.4)$$

which satisfies the integral equation

$$S_{12} = (S_1^{-1} + S_2^{-1})^{-1}(1 + v_{12}S_{12}) . \quad (3.5)$$

Then the Feldman-Fulton[5] prescription is

$$\psi^{(0)}(\{e\}) = \frac{1}{(2\pi i)^2}[(S_1 + S_2)S_{12} + (S_2 + S_3)S_{23}$$

$$+ (S_1 + S_3)S_{13}]\Phi . \quad (3.6)$$

That is, first a pair propagates away from the one-time function Φ and then one of this pair propagates still further in time. This must then be symmetrized in all particles. The use of (3.2), (3.4), and (3.5) and the on-shell constrain allows this to be rewritten as

$$\psi^{(0)}(\{e\}) = \frac{1}{(2\pi i)^2} S_1 S_2 S_3 (X + S_3^{-1} v_{12}S_{12} + S_2^{-1} v_{13}S_{13}$$

$$+ S_1^{-1} v_{23}S_{23})\Phi , \quad (3.7)$$

which proves to be a more useful form. Here

$$X = S_1^{-1} + S_2^{-1} + S_3^{-1} = W^{(0)} - \sum_i h_i(1 - i\eta) . \quad (3.8)$$

The demonstration that this is indeed the correct assumption is accomplished by the substitution of (3.7) into a form simply derivable from (3.1) with $I_{12} \rightarrow v_{ij}$ and $I^{(3)} = 0$,

$$\psi^{(0)}(\{e\}) = \frac{i}{2\pi} S_1(e_1)S_2(e_2)$$

$$\times \int d^3 e' \delta\left[\sum e'\right]\delta(e_3 - e_3')$$

$$\times v_{12}\psi^{(0)}(\{e'\}) + (1 \leftrightarrow 3) + (2 \leftrightarrow 3) , \quad (3.9)$$

where W is replaced by $W^{(0)}$ in all the propagators in (3.7)–(3.9). The performance of the e' integrals on the right will be briefly described.

There are three types of terms. The first arises from the substitution of the X term of (3.7) into the first term on the right of (3.9). Performance of $de_2' de_3'$ results in a term

$$-\frac{i}{(2\pi)^3} S_1 S_2 S_3 v_{12} \int de_1' S_1(e_1')S_2(-e_1' - e_3)X\Phi .$$

$$(3.10)$$

The e_1' integration path is closed in the upper half plane thereby picking up the pole in one or the other of the denominators supplied by the two propagators. Which of the poles is selected depends upon the sign of h_1 and h_2 and it is clear that the integral vanishes if they have opposite signs. The result is

$$-\frac{1}{(2\pi)^2} S_1(e_1)S_2(e_2)S_3(e_3)v_{12}\Omega_{12}S_{12}^{(0)}(e_1 + e_2)X\Phi ,$$

$$(3.11)$$

where

$$S_{12}^{(0)}(e_1 + e_2)$$

$$= [\tfrac{2}{3} W^{(0)} + e_1 + e_2 - (h_1 + h_2)(1 - i\eta)]^{-1} \quad (3.12)$$

and the on-shell condition has been used. The second type of term comes from the second term of (3.7) substituted into the first term on the right of (3.9). Performance of $de_2' de_3'$ results in

$$-\frac{i}{(2\pi)^3} S_1 S_2 v_{12} \int de_1' S_1(e_1')S_2(-e_1' - e_3)v_{12}$$

$$\times S_{12}(-e_3)\Phi . \quad (3.13)$$

The remaining integral is identical with that in (3.10). The on-shell result is

$$-\frac{1}{(2\pi)^2} S_1(e_1)S_2(e_2)v_{12}\Omega_{12}S_{12}^{(0)}(e_1 + e_2)$$

$$\times v_{12}S_{12}(e_1 + e_2)\Phi . \quad (3.14)$$

The third type of term results from the third term of (3.7) similarly substituted into (3.9). After performance of the e_2' and e_3' integrals the result is

$$-\frac{i}{(2\pi)^2} S_1(e_1)S_2(e_2)S_3(e_3)v_{12}$$

$$\times \int de_1' S_1(e_1')v_{13}S_{13}(e_1' + e_3)\Phi . \quad (3.15)$$

The poles of both propagators lie on the same side of the real axis so that the contour can always be closed so as to enclose no poles. The integral therefore vanishes. The fourth type of term arises from the substitution of the last term of (3.7) into the first term on the right of (3.9). This can be obtained from the third type of term, (3.15), by the interchange $1 \leftrightarrow 2$. It also vanishes.

The combination of (3.11) and (3.14) results in

$$-\frac{1}{(2\pi)^2} S_1 S_2 S_3 (v_{12} + S_3^{-1} v_{12}S_{12})\Omega\Phi , \quad (3.16)$$

where use has been made of (3.5), (3.8), and the commutativity of Ω_{12} with S_{12} and S_3 with v_{12}. We have further replaced $\Omega_{12}\Phi$, (2.5), by $\Omega\Phi$, where

$$\Omega = \Lambda_+ - \Lambda_- , \quad (3.17)$$

where $\Lambda_\pm$ are now three-particle projectile operators. This replacement is correct since we have seen that the three particles must all be either in positive or all be in negative energy states in the wave function Φ. The expression (3.16) must now be symmetrized in all pairs in order to form the right side of (3.9) after the substitution of (3.7). The full equation is

$$-\frac{1}{(2\pi)^2}S_1S_2S_3(X+S_3^{-1}v_{12}S_{12}+S_2^{-1}v_{13}S_{13}+S_1^{-1}v_{23}S_{23})\Phi$$

$$=-\frac{1}{(2\pi)^2}S_1S_2S_3(v_{12}+v_{13}+v_{23}+S_3^{-1}v_{12}S_{12}+S_2^{-1}v_{13}S_{13}+S_1^{-1}v_{23}S_{23})\Omega\Phi \ . \quad (3.18)$$

The $\{e\}$ dependence must cancel explicitly since Φ is assumed to be independent of this set. This can only occur if

$$\Omega\Phi=\Lambda_+\Phi \ , \qquad (3.19)$$

that is, Φ contains no negative energy states. Then the equation for Φ follows immediately,

$$\left[W^{(0)}-\sum_i h_i-\sum_{i>j}v_{ij}\right]\Phi=0 \qquad (3.20)$$

and

$$v_{ij}=\Lambda_+V_{ij}\Lambda_+ \ , \qquad (3.20a)$$

so that $\bar{V}_{12}=0$, (33). The absence of the negative energy states in Φ is exactly the result obtained from the transition from the Fock-space Hamiltonian formulation of QED to a configuration space equation[4] of the form (3.20). The explicit appearance of the negative energy states in the two-electron problem, (2.4), is not repeated for three or more electrons.

We can now try to determine the as-yet arbitrary two-electron interaction in a similar way to that used in Sec. II. Equation (3.1) (still neglecting $I^{(3)}$) is perturbed about $W^{(0)}$ and $\psi^{(0)}$, (3.7). The requirement that $W^{(1)}$ be real results in

$$\tilde{\psi}^{(0)}=\tilde{\Phi}(X+S_{12}^\dagger v_{12}S_3^{-1}+S_{13}^\dagger v_{13}S_2^{-1}+S_{23}^\dagger v_{23}S_1^{-1})S_1^\dagger S_2^\dagger S_3^\dagger\frac{1}{(2\pi i)^2} \ , \qquad (3.21)$$

where v_{ij} is taken to be Hermitian and $S_i^{-1}=(S_i^\dagger)^{-1}$ in the $\eta\rightarrow0$ limit. The further requirement that $\psi^{(1)}$ not appear in the final equation for $W^{(1)}$ [as was done in (2.12) for the two-electron case] yields

$$\tilde{\Phi}\left[W^0-\sum_i h_i-\sum_{i>j}v_{ij}\right]=0 \qquad (3.22)$$

or, coupled with (3.20) and (3.20a),

$$\tilde{\Phi}=\Phi^* \qquad (3.23)$$

The expression for $W^{(1)}$ is readily obtained and is explicitly real. The requirement that it vanish and the use of (3.9) yields

$$\int d^3e\ \delta\left[\sum e\right]\tilde{\psi}^0(\{e\})S_1^{-1}(e_1)S_2^{-1}(e_2)S_3^{-1}(e_3)\psi^{(0)}(\{e\})$$

$$=\int d^3e\ \delta\left[\sum e\right]\tilde{\psi}^{(0)}(\{e\})\frac{i}{2\pi}\left[S_3^{-1}(e_3)\int d^3e'\delta\left[\sum e'\right]I_{12}+\cdots\right]\psi^{(0)}(\{e'\}) \ . \quad (3.24)$$

The evaluation of the left side of the equation with the aid of (3.6) and (3.20a) is straightforward but somewhat lengthy. The procedure merely involves repeated contour integrals for two of the e_i parameters. The use of (3.20) or (3.22) results in the expression $(2\pi)^2(\Phi,(v_{12}+v_{13}+v_{23})\Phi)$. The right-hand side of (3.24) is much more complex. The substitution of (3.6) and (3.20a) results in 16 terms which arise from I_{12}. The symmetrization in the electron designation results in 32 more. Most of the original 16 are of the type $(\cdots I_{12}\cdots v_{13}\cdots)$ which are three-body potentials which will be discussed in Sec. IV. The two-electron terms, interpretable as v_{12}, arise from the first two terms in each of (3.6) and (3.20a). For these we use

$$S_1S_2S_3(X+S_3^{-1}v_{12}S_{12})=(S_1+S_2)(S_3+S_{12}) \qquad (3.25)$$

and its Hermitian conjugate. The δ functions in the e parameters can be used, and then a simple change of variables gives

$$\frac{i}{8\pi}\Phi^*\int_{-\infty}^\infty dx\ dy\ dz\,[S_{12}^\dagger(z)+S_3^\dagger(-z)]\left[S_1^\dagger\left[\frac{y}{2}+\frac{x}{4}\right]+S_2^\dagger\left[z-\frac{x}{4}-\frac{y}{2}\right]\right]I_{12}(x)\tfrac{1}{2}[S_3^{-1}(z)+S_3^{\dagger-1}(-z)]$$

$$\times\left[S_1\left[\frac{y}{2}-\frac{x}{4}\right]+S_2\left[z-\frac{y}{2}-\frac{x}{4}\right]\right][S_3(-z)+S_{12}(z)]\Phi \ . \quad (3.26)$$

The y integrals can be done by raising the denominators in which they occur into an exponent by a parametric integral. This gives

$$\frac{i}{4}\Phi^*(W-h_3-h_{12})\int_{-\infty}^{\infty}dx\int_0^{\infty}ds\,e^{-\eta s}\int_{-\infty}^{\infty}dz\,S_{12}^{\dagger}(z)F_{12}(x,s)\frac{\mathcal{P}}{[(W/3)-z-h_3]}S_{12}(z)(W-h_3-h_{12})\Phi\,, \tag{3.27}$$

where

$$F_{12}(x,s)=e^{-isx/2}[e^{ish_1}I_{12}(x)e^{-ish_1}+(1\leftrightarrow2)]\,. \tag{3.28}$$

The z integral in (3.27) can be done by first expanding the S_{12}'s in eigenfunctions of

$$h_{12}=h_1+h_2+v_{12}\,, \tag{3.29}$$

thereby turning S_{12} into a sum over c numbers, which allows the principal value integral in (3.27) to be performed. The result allows an inference from (3.24) which is

$$\Lambda_+v_{12}\Lambda_+=\frac{1}{4\pi}\int_{-\infty}^{\infty}dx\int_0^{\infty}ds\,e^{-\eta s-isx/2}[e^{ish_1}I_{12}(x)e^{-ih_1s}+(1\leftrightarrow2)]\,. \tag{3.30}$$

This should be compared with (2.15), the analogous result for the two-electron case. The $(+,+)$ part of (2.15) is identical with (3.30) showing that this part of the optimum two-electron potential is the same in both cases. The other components of (2.15) do not occur in the lowest-order static pair potential when three (or more) electrons are present. They instead occur as higher-order pair potentials or three-body potentials.

In order to complete the program outlined above we see that it is necessary to introduce three body potentials. This is done in Sec. IV.

IV. INCLUSION OF THREE-ELECTRON INTERACTIONS

In Sec. III the necessity for the inclusion of a three-electron potential arose in two ways. The first was due to the intrinsic three-electron interaction $I^{(3)}$ in (3.1). The second arose from the requirement that the first-order correction to $W^{(0)}$, the eigenvalue of the Hamiltonian equation, (3.20), should vanish. We therefore write the static approximation to the full three-electron BSE as

$$\hat{\psi}^{(0)}(\{e\})=\frac{i}{2\pi}S_1S_2v_{12}\int d^3e'\delta\left(\sum e'\right)\delta(e_3-e_3')\hat{\psi}^{(0)}(\{e\})+(1\leftrightarrow3)+(2\leftrightarrow3)$$

$$+\left[\frac{i}{2\pi}\right]^2S_1S_2S_3v^{(3)}\int d^3e'\delta\left(\sum e'\right)\hat{\psi}^{(0)}(\{e'\})\,. \tag{4.1}$$

Here $v^{(3)}$ is the static-three-electron potential and all the other symbols are unchanged. We must now provide a modification of $\psi^{(0)}$, (3.6) or (3.7), which can allow for the participation of $v^{(3)}$ in the propagation of the single-time function Φ into the multitime functions $\psi^{(0)}$. The clue to providing this is that $v^{(3)}$ is a single-time operator which is meaningful only when it operates on a single-time wave function. This limits the possible forms of the terms in which $v^{(3)}$ can participate. We modify (3.7) as

$$\hat{\psi}^{(0)}(\{e\})=\psi^{(0)}(\{e\})+\delta\psi^{(0)}(\{e\})\,, \tag{4.2}$$

where $\psi^{(0)}(\{e\})$ is given by (3.7) and

$$\delta\psi^0(\{e\})=\frac{1}{(2\pi i)^2}S_1S_2S_3(v+v_{12}S_{12}\gamma_{12}$$

$$+v_{13}S_{13}\gamma_{13}+v_{23}S_{23}\gamma_{23})\Phi\,, \tag{4.3}$$

where v and the γ_{ij} are static operators (independent of $\{e\}$) to be determined below. When (4.2) is substituted into the right side of (4.1) three new types of terms arise: First, from the v_{ij} terms operating on $\delta\psi^{(0)}$, second, from the $v^{(3)}$ term operating on $\psi^{(0)}$, and third from the $v^{(3)}$ term operating on $\delta\psi^{(0)}$.

In the first type, the v_{12} operator of (4.1) operating on

the v term of (4.3) gives

$$\frac{1}{(2\pi i)^2}S_1S_2S_3v_{12}S_{12}^{(0)}\Omega_{12}v\Phi\,. \tag{4.4}$$

The v_{12} operator on the second term of $\delta\psi^{(0)}$ gives

$$\frac{1}{(2\pi i)^2}S_1S_2S_3v_{12}S_{12}^{(0)}\Omega_{12}v_{12}S_{12}\gamma_{12}\Phi\,. \tag{4.5}$$

The last two terms of $\delta\psi^{(0)}$ yield

$$\frac{1}{(2\pi i)^2}S_1S_2S_3v_{12}S_{12}^{(0)}\Omega_{12}(v_{13}D_{13}\gamma_{13}+v_{23}D_{23}\gamma_{23})\Phi\,, \tag{4.6}$$

where

$$D_{ij}=(X-v_{ij})^{-1}\,, \tag{4.7}$$

where X is given in (3.8) and $S_{12}^{(0)}$ in (3.12). All the contour integrals used in obtaining (4.4)–(4.7) were already encountered in Sec. III.

The second type of term, obtained from the operation of the $v^{(3)}$ term of (4.1) on $\psi^{(0)}$ is obtained by using same contour integrals, with the result

$$\frac{1}{(2\pi i)^2}S_1S_2S_3v^{(3)}\Phi\,. \tag{4.8}$$

The third type of term, from the $v^{(3)}$ term of (4.7) operating on $\delta\psi^{(0)}$ again requires only the same contour integrals and results in

$$\frac{1}{(2\pi i)^2}S_1S_2S_3v^{(3)}\frac{\Lambda}{X}$$

$$\times(v+v_{12}D_{12}\gamma_{12}+v_{13}D_{13}\gamma_{13}+v_{23}D_{23}\gamma_{23})\Phi \ . \qquad (4.9)$$

These results are then assembled. The requirement of the cancellation of the explicit dependence on the $\{e\}$ variables places constraints upon the $\{e\}$-independent operators v, $v^{(3)}$, and γ_{ij}. These are

$$v-\gamma_{12}+v_{13}D_{13}\gamma_{13}+v_{23}D_{23}\gamma_{23}=0 \qquad (4.10)$$

plus two additional equations obtained by permutations of the subscripts. These can be combined to give

$$D_{12}\gamma_{12}=D_{13}\gamma_{13}=D_{23}\gamma_{23}\equiv Q \ , \qquad (4.11)$$

which, when substituted back, yields

$$Q = \left[X - \sum_{i>j} v_{ij}\right]^{-1}v=\Delta^{-1}v \qquad (4.12)$$

or

$$\gamma_{ij}=D_{ij}^{-1}Q \ . \qquad (4.13)$$

The equation for Φ that emerges is

$$\left[W^{(0)}- \sum_i h_i - \sum_{i>j} v_{ij}+v-v^{(3)}-v^{(3)}\Delta^{-1}v \right]\Phi=0 \ . \qquad (4.14)$$

The choice $v=v^{(3)}$ makes $v^{(3)}\Delta^{-1}v$ Hermitian. Then (4.14) can be written as

$$\left[W^{(0)}-H_2-v^{(3)}\frac{1}{W^{(0)}-H_2}v^{(3)} \right]\Phi=0 \ , \qquad (4.15)$$

where

$$H_2= \sum_i h_i + \sum_{i>j} v_{ij} \ . \qquad (4.16)$$

The definitions

$$\Phi_\pm=\Phi\pm\chi, \quad \chi=(W^{(0)}-H_2)^{-1}v^{(3)}\Phi \qquad (4.17)$$

can be used to turn (4.15) into a pair of linear eigenvalue equations

$$(W_+^{(0)}-H_2-v^{(3)})\Phi_+=0 \ , \qquad (4.18a)$$

$$(W_-^{(0)}-H_2+v^{(3)})\Phi_-=0 \ , \qquad (4.18b)$$

which gives two different sets of eigenvalues.

We return to $\delta\psi^{(0)}$ (4.3) with the result (4.13) which gives

$$\delta\psi^{(0)}= \frac{1}{(2\pi i)^2}S_1S_2S_3(X +S_3^{-1}v_{12}S_{12}+S_2^{-1}v_{13}S_{13}$$

$$+S_1^{-1}v_{23}S_{23})\frac{1}{(W^{(0)}-H_2)}v^{(3)}\Phi \ , \qquad (4.19)$$

which, using (4.2) and (3.7), gives

$$\hat{\psi}^{(0)}= \frac{1}{(2\pi i)^2}S_1S_2S_3(X +S_3^{-1}v_{12}S_{12}+S_2^{-1}v_{13}S_{13}$$

$$+S_1^{-1}v_{23}S_{23})\frac{1}{(W^{(0)}-H_2)}$$

$$\times \left[v^{(3)}+v^{(3)}\frac{1}{W^{(0)}-H_2}v^{(3)} \right]\Phi \ . \qquad (4.20)$$

The two independent solutions of Φ arising from Φ_+ and Φ_- yield different results. If we choose the Φ_- solutions (i.e., $\Phi_+=0$), then $X=-\Phi$, and the last factor of (4.20) vanishes. This is not an interesting solution for the BSE since the zeroth-order approximation to the BS wave function vanishes. For the other case ($\Phi_-=0$), we obtain $\Phi=\Phi_+$ and (4.15) becomes

$$(W^{(0)}-H_2-v^{(3)})\Phi=0 \qquad (4.21)$$

and (4.20) becomes

$$\hat{\psi}^{(0)}= \frac{1}{(2\pi i)^2}S_1S_2S_3(X +S_3^{-1}v_{12}S_{12}+S_2^{-1}v_{13}S_{13}$$

$$+S_1^{-1}v_{23}S_{23})\Phi \ , \qquad (4.22)$$

which is the form (3.7) originally given by Feldman and Fulton[5] for the nonrelativistic case in which three-body interactions do not occur. We see that the only modification introduced by the three-body static potential is in the Schrödinger wave functions. Its relation to the BS wave function is unchanged by this potential.

The condition that $W^{(1)}$ vanish which was exploited in Sec. III to obtain v_{ij} could now be completed with the determination of $v^{(3)}$. The results are sufficiently lengthy to make their display here impractical.

The program discussed above could be extended to the four-electron case. The complexity of the algebra is greatly increased by the necessity for inclusion of three-electron propagators, S_{123}, etc., in the extension of (4.22) to this case. This probably precludes the useful extension to the many-electron problem.

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