To determine the necessity for d waves at 9.954 MeV, a search was made including only s and p waves. The resulting error per datum point was about 1.5. A phase-shift search was also made at 9.954 MeV, including unsplit d waves. That is, the d waves were varied in the search, but were constrained to be equal. Again, the error per datum point was about 1.5 even though the number of parameters varied increased from 3 to 4. These results provide strong evidence for split d waves at 10 MeV.

As shown in Table VII, at 9.954 MeV the phase shifts give an error per datum point of 0.6. A systematic investigation was made at this energy in order to ascertain the extent a given phase shift could be changed without increasing the error per point beyond 1.0. The procedure was as follows: The value of one phase shift was changed from that given in Table VII by an amount Δ and variation of this phase shift was then suppressed while the computer adjusted the remaining phase shifts to minimize the error function E. This procedure was repeated for several values of Δ (both positive and negative) and the resulting values of E were plotted as a function of the phase shift. Each phase shift was treated in this same manner.

The values of Δ which resulted in an error per point of 1.0 are listed as the uncertainties in Table VII. Note that strong correlations exist between the uncertainties. In particular, although the uncertainties appear to indicate that the d-wave phase shifts overlap, it was found that for every solution the $d_{5/2}$ phase shift was 1.2 to 1.8 deg larger than the $d_{3/2}$ phase shift. Thus, good fits to the data were obtained only for the $d_{5/2}$ phase shift greater than the $d_{3/2}$ phase shift, and it appears that the d-wave splitting is determined more accurately than the absolute values of the d-wave phase shifts.

In all of the above analysis the error per polarization datum point was approximately the same as the error per cross-section point.

VII. CONCLUSIONS

Polarizations in ^{4}He$(\vec{p},p)^4$He measured at four points are in excellent agreement with the measurements of Brown, Haeberli, and Saladin.[8] In order to fit the available data at 10 MeV, small positive split d waves are required with the $d_{5/2}$ phase shift 1 to 2 deg larger than the $d_{3/2}$ phase shift.

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Upper Bounds for Errors of Expectations in the Few-Body Problem

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Exact upper bounds are established for the errors associated with approximate computations of total, kinetic, and potential energies of a few-body system. As a consequence, error bounds are also established for arbitrary coordinate functions. Reduction methods are developed to treat expectations of coordinate functions which are divergent at some spatial point, e.g., the delta function or the inverse square, or at infinity, e.g., the mean-square radius. Positronium is used as a test case to study the relative accuracy of the estimates.

1. INTRODUCTION

ONE is usually compelled to resort to approximation techniques when dealing with the few-body problem, the problem of several particles interacting via a pair potential. There are two approaches which one can follow in quantum mechanics in calculating the expectation value of some physical quantity. A direct approach is to obtain an approximate solution to the Schrödinger equation and use this to evaluate the physical quantity. This method, of course, is inefficient since it yields a great deal more information than desired. A more modest approach is to approximate the physical quantity directly, without considering the accuracy

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of the corresponding wave function. An example is the Rayleigh-Ritz minimum principle for the energy. Here one can arrive at a good value of the energy, but one does not know how accurate other quantities are when calculated with the associated wave function. Indeed, slight changes in the wave function may produce large changes in other expectation values, although the energy may not change by very much. Preuss[1] has discussed this point, and has given an example to demonstrate the necessity of investigating the accuracy of other physical quantities.

One possible remedial measure is to work with a variational principle for the expectation in question. This can be done and will be considered in a future paper. However, variational principles are not, in general, minimum principles, and so one is not really certain of the accuracy of the result. An alternative approach involves calculating an upper bound to the error for the quantity desired—dipole moment, quadrupole moment, Coulomb radius, etc. We shall carry out this approach in the present paper, bearing in mind that since only a necessary, not a sufficient, condition on the accuracy can be obtained, a large upper bound does not necessarily imply a large error. Following Kinoshita,[2] Redei[3] has given such a method of evaluating an exact upper bound to the error in the density of atomic electrons. For a general discussion of upper and lower bounds for errors of expectation values, and for further references in this line, see Bazley and Fox.[4] A rough estimation of the error in the mean-square radius of a model triton has also been made by the authors.[5] In this paper, we shall extend the method of Redei to general interparticle forces, and, more importantly, extend it to quantities such as the mean-square radius, whose asymptotic divergence does not permit error evaluation by merely integrating over particle density.

In Sec. 2, we establish a known basic expression for the error of an expectation. This is tested in several ways in Sec. 3. The errors associated with functions of total, kinetic, and potential energy are established in Sec. 4, and that for an arbitrary pair coordinate function comes as a consequence. In Sec. 5, reduction methods are developed to treat expectations of coordinate functions which are divergent, either at a finite location, or asymptotically at infinity such as the mean-square radius. Finally, positronium is used as a test case in Sec. 6 to study the relative accuracy of the estimates.

2. ERROR BOUNDS ON EXPECTATIONS

We shall be concerned with the properties of the normalized ground state, assumed nondegenerate,

$$H\psi=E_0\psi \tag{2.1}$$

of a few-body system. By "ground state" we refer to the lowest level which is simultaneously an eigenstate of a selected set of constants of motion—these constants will be maintained for all wave functions considered. If an approximation ϕ, assumed normalized, is obtained by some unspecified technique, the energy

$$\mathcal{E}_0\equiv\langle\phi|H|\phi\rangle \tag{2.2}$$

is an upper bound to E_0, and indeed the error may be estimated in a variety of ways. To bound the error of an expectation other than the energy, it is helpful to regard the error in ψ as due to a perturbation of the Hamiltonian. In fact, it is clear—tautologically clear—that

$$(H-W)\phi=\mathcal{E}_0\phi \tag{2.3}$$

for any perturbation W for which

$$W\phi=(H-\mathcal{E}_0)\phi. \tag{2.4}$$

The quantity W may depend only on coordinates, or may involve moments, or even projections; its specific realization will not enter.

Since the true system Hamiltonian is regular, or at least its irregularities are known, we shall carry out the comparison of states by applying the perturbation $-W$, thereby perturbing ψ to ϕ. It is best to separate our strictly normalization changes in expectations from changes in form. For this purpose, we define

$$\hat{\phi}=\phi/\langle\psi|\phi\rangle,$$
$$\text{i.e.,}\qquad \langle\psi|\hat{\phi}\rangle=1, \tag{2.5}$$

which is, incidentally, particularly appropriate to a many-body system, where the condition $\langle\psi|\phi\rangle\to 0$ is difficult to avoid. Now ψ and $\hat{\phi}$ may be related in the spirit of the Wigner-Brillouin perturbation method, i.e., by first defining

$$P\equiv 1-|\psi\rangle\langle\psi|, \tag{2.6}$$

so that for any function f,

$$Pf=f-\langle\psi|f\rangle\psi \tag{2.6'}$$

is the part of f with ψ projected out. Then

$$\psi=(1-P)\hat{\phi}=\hat{\phi}-(P/(H-\mathcal{E}_0))(H-\mathcal{E}_0)\hat{\phi},$$

or

$$\psi=\hat{\phi}-GW\hat{\phi},$$

where

$$G=P/(H-\mathcal{E}_0). \tag{2.7}$$

[In the usual Wigner-Brillouin method, $\hat{\phi}$ would be obtained from ψ by a Neumann expansion of the integral equation for $\hat{\phi}$.]

If A is non-negative, then according to the triangle inequality,

$$|\langle\psi|A|\psi\rangle^{1/2}-\langle\hat{\phi}|A|\hat{\phi}\rangle^{1/2}|\leq\langle\psi-\hat{\phi}|A|\psi-\hat{\phi}\rangle^{1/2}. \tag{2.8}$$

Hence inserting (2.7),

$$|\langle\psi|A|\psi\rangle^{1/2}-\langle\hat{\phi}|A|\hat{\phi}\rangle^{1/2}|\leq\langle\hat{\phi}|W^*GAGW|\hat{\phi}\rangle^{1/2}. \tag{2.9}$$

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[1] H. Preuss, Z. Naturforsch. **16a**, 598 (1961).
[2] T. Kinoshita, Phys. Rev. **115**, 366 (1959).
[3] L. B. Redei, Phys. Rev. **130**, 420 (1963).
[4] N. W. Bazley and D. W. Fox, Rev. Mod. Phys. **35**, 712 (1963).
[5] S. Aranoff and J. K. Percus, Nucl. Phys. **A98**, 263 (1967).

If we introduce the notation

$$\langle\phi|Q|\phi\rangle\equiv\langle Q\rangle \tag{2.10}$$

and define

$$\langle\hat{\phi}|\hat{\phi}\rangle\equiv(1+\gamma)^2, \tag{2.11}$$

then (2.9) yields at once

$$|\langle\psi|A|\psi\rangle^{1/2}-\langle A\rangle^{1/2}| \leq(1+\gamma)\langle W^*GAGW\rangle^{1/2}+\gamma\langle A\rangle^{1/2}. \tag{2.12}$$

This is our basic expression for the error of an expectation, divided into intrinsic and normalization terms.

3. ASSESSMENT OF THE BOUND

The quantity γ of (2.11) is in a sense a uniform measure of the closeness of the approximate wave function ϕ to the exact ψ. From Eqs. (2.5) and (2.11), we see that

$$|\langle\psi|\phi\rangle|=(1+\gamma)^{-1}. \tag{3.1}$$

The overlap $|\langle\psi|\phi\rangle|$ does not exceed 1, becoming 1 only when $\phi=\psi$ (to within phase). Hence $0\leq\gamma\rightarrow 0$ as $\phi\rightarrow\psi$. The uniformity of the measure is also indicated by observing, directly from definition, that

$$\langle\psi-\hat{\phi}|\psi-\hat{\phi}\rangle=\gamma(2+\gamma). \tag{3.2}$$

If the exact ground state E_0 (or a lower bound to it) is known, it is possible to estimate γ in a number of ways. For example, if the first excited energy E_1 (or an upper bound to it) is also known, we have

$$\begin{aligned}E_1-E_0&\leq\langle\psi-\hat{\phi}|H-E_0|\psi-\hat{\phi}\rangle/\langle\psi-\hat{\phi}|\psi-\hat{\phi}\rangle\\&=\langle\hat{\phi}|H-E_0|\hat{\phi}\rangle/\langle\psi-\hat{\phi}|\psi-\hat{\phi}\rangle\\&=(\mathcal{E}_0-E_0)(1+\gamma)^2/[(1+\gamma)^2-1],\end{aligned}$$

so that

$$1+\gamma\leq[(E_1-E_0)/(E_1-\mathcal{E}_0)]^{1/2} \tag{3.3}$$

or the somewhat weaker

$$\gamma\leq\tfrac{1}{2}(\mathcal{E}_0-E_0)/(E_1-\mathcal{E}_0). \tag{3.3'}$$

We can at this point make a simple check of the approximations (inequalities) which have been and will be used. For the normalization, we need only set $A=1$ in Eq. (2.9), obtaining

$$\gamma\leq\langle\hat{\phi}|W^*G^2W|\hat{\phi}\rangle^{1/2}. \tag{3.4}$$

But, assuming that at least $E_1>\mathcal{E}_0$, the lowest eigenvalue of $G=P/(H-\mathcal{E}_0)$ is $1/(E_1-\mathcal{E}_0)$. Hence (3.4) becomes $\gamma\leq 1/(E_1-\mathcal{E}_0)\langle W^*W\rangle^{1/2}(1+\gamma)$, or

$$\frac{\gamma}{1+\gamma}\leq\frac{\langle(H-\mathcal{E}_0)^2\rangle^{1/2}}{E_1-\mathcal{E}_0}. \tag{3.5}$$

Now it is known (Weinstein's[6] method) that

$$\langle(H-\mathcal{E}_0)^2\rangle^{1/2}$$

is indeed an upper bound to $\mathcal{E}_0-E_0$, but that numerically it is very conservative; thus the bound (3.5) will be equally conservative compared to the estimate (3.3').

To further analyze the implication that by using quite general kinematic (Hamiltonian-independent) arguments, we are intrinsically limited as to the tightness of our bound, we may look at the energy expectation itself. Thus let $A=H-E_0$ in (2.9), yielding

$$\mathcal{E}_0-E_0\leq\langle W^*G(H-E_0)GW\rangle. \tag{3.6}$$

Equation (3.6) is, in fact, an equality, as is readily verified, and this is because one arm of the triangle inequality vanishes here. However, if $G(H-E_0)G$ is replaced by its maximum eigenvalue $(E_1-E_0)/(E_1-\mathcal{E}_0)^2$, as before, (3.6) becomes

$$\mathcal{E}_0-E_0\leq\left(\frac{E_1-E_0}{E_1-\mathcal{E}_0}\right)\frac{\langle(H-\mathcal{E}_0)^2\rangle}{E_1-E_0}.$$

This is essentially Temple's[7] bound and is far better in practice than the Weinstein bound, although still a substantial overestimate. We conclude at this stage first that there is a basic irreducible loss of accuracy in the replacement of the Green's function $G=P/(H-\mathcal{E}_0)$ by its maximum eigenvalue. Further, the division of ψ into $\psi-\hat{\phi}$ and $\hat{\phi}$ associated with the triangle inequality introduces an estimate whose conservative character depends markedly upon the specific expectation we desire.

4. PROTOTYPE DEVIATIONS

Recapitulating, the problem of bounding the error in the expectation of an observable A is reduced to that of bounding the deviation

$$D(A)\equiv\langle W^*GAGW\rangle. \tag{4.1}$$

While $D(A)$ is, except for normalization, just the quantity $\langle\psi-\hat{\phi}|A|\psi-\hat{\phi}\rangle$, the explicit form of (4.1) will be essential in what follows. In particular, since all eigenvalues of $G=P/(H-\mathcal{E}_0)$ lie between 0 and $1/(E_1-\mathcal{E}_0)$, a computationally effective bound would result if this pair of factors could be removed. If A, assumed non-negative, commutes with the Hamiltonian, we have indeed $D(A)=\langle W^*A^{1/2}G^2A^{1/2}W\rangle$, so that

$$\text{if}\quad D(A)\leq\langle W^*AW\rangle/(E_1-\mathcal{E}_0)^2 \qquad [A,H]=0,\quad A\geq 0. \tag{4.2}$$

Our major task will be to relate deviations of observables to others in which a process like (4.2) can be carried out. The basic observables of the latter type are, of course, functions of the energy and for these in fact (4.2) can be improved somewhat. From

$$D((H-E_0)^s)=\langle\psi-\hat{\phi}|(H-E_0)^s|\psi-\hat{\phi}\rangle/\langle\hat{\phi}|\hat{\phi}\rangle,$$

[6] D. H. Weinstein, Phys. Rev. **40**, 797 (1932).

[7] G. Temple, Proc. Roy. Soc. (London) **119**, 276 (1928).

noting that $(H-E_0)\psi=0$, we have

$$D((H-E_0)^s)=\langle(H-E_0)^s\rangle \quad \text{for} \quad s>0, \tag{4.3}$$

while for $s=0$,

$$D(1)=\langle\psi-\hat{\phi}|\psi-\hat{\phi}\rangle/\langle\hat{\phi}|\hat{\phi}\rangle,$$

or

$$D(1)=1-1/(1-\gamma)^2. \tag{4.4}$$

Next, we explicitly separate the energy into kinetic and potential parts:

$$H=T+V, \quad T=\sum_1^N \frac{p_i^2}{2m}, \quad V=\tfrac{1}{2}\sum_{i,j=1}^{N}{}' v(\mathbf{r}_i-\mathbf{r}_j), \tag{4.5}$$

where

$$\sum{}' v_{ij}=\sum_{i\neq j} v_{ij},$$

and try to build up the potential energy deviation by itself. One method of doing this is to note that

$$\begin{aligned}1/|\mathbf{r}_{ij}-\mathbf{x}| &=\tfrac{1}{2}\nabla_i\cdot(\mathbf{r}_{ij}-\mathbf{x})/|\mathbf{r}_{ij}-\mathbf{x}| \\ &=(i/2\hbar)[\mathbf{p}_i\cdot,(\mathbf{r}_{ij}-\mathbf{x})/|\mathbf{r}_{ij}-\mathbf{x}|],\end{aligned} \tag{4.6}$$

so that from Schwartz's inequality,

$$D(1/|\mathbf{r}_{ij}-\mathbf{x}|)\leq D(p_i^2)^{1/2}D(1)^{1/2}/\hbar.$$

Hence

$$D(\textstyle\sum_{i,j}{}' 1/|\mathbf{r}_{ij}-\mathbf{x}|)\leq KD(T)^{1/2},$$

where

$$K=N(N-1)(2mD(1)/N\hbar^2)^{1/2}. \tag{4.7}$$

As a consequence of (4.7), we can write for any potential u

$$|D(\textstyle\sum'_{i,j} u(\mathbf{r}_{ij}))|\leq K_u D(T)^{1/2}, \tag{4.8}$$

where K_u may be determined in a variety of ways. Perhaps the simplest way is to note that

$$\begin{aligned}u(\mathbf{r}) &= \int u(\mathbf{x})\delta(\mathbf{r}-\mathbf{x})d\mathbf{x} \\ &= -\int u(\mathbf{x})\nabla^2 1/|\mathbf{r}-\mathbf{x}|\,d\mathbf{x}/4\pi \\ &= -\int 1/|\mathbf{r}-\mathbf{x}|\,\nabla^2 u(\mathbf{x})d\mathbf{x}/4\pi,\end{aligned}$$

so that

$$K_u\leq\frac{K}{4\pi}\int|\nabla^2 u(\mathbf{x})|\,d\mathbf{x}. \tag{4.9}$$

Alternatively, and generally the superior method, if $|u(\mathbf{x})|\leq c/|\mathbf{x}|$, then certainly $|D(u(\mathbf{r}))|\leq cD(1/r)$; hence

$$K_u\leq K\max|xu(\mathbf{x})|. \tag{4.10}$$

For example, for a Gaussian potential $u(\mathbf{x})=\exp-\frac{1}{2}x^2$, (4.9) yields $K_u\leq 2K(3/e)^{3/2}$, while from (4.10),

$$K_u\leq Ke^{-1/2}.$$

The relation between V, T, and H now permits us to close the circle and obtain the separate deviations. From Eq. (4.8),

$$D(V)\leq\tfrac{1}{2}K_v D(T)^{1/2}. \tag{4.11}$$

This can be extended by noting that

$$D(|v(r_{ij})|^s)\leq K_{|v|^s}D(T)^{1/2}/N(N-1),$$

so that from Minkowski's inequality[8] ($A_\alpha\geq 0$)

$$\langle(\textstyle\sum A_\alpha)^s\rangle^{1/s}\leq\sum\langle A_\alpha{}^s\rangle^{1/s}, \tag{4.12}$$

we find

$$D(V^s)\leq\tfrac{1}{2}[N(N-1)/2]^{s-1}K_{|v|^s}D(T)^{1/2}. \tag{4.13}$$

Combining the sequences (4.3), (4.4), and (4.13), we can therefore isolate kinetic and potential terms. To start with,

$$D(T)=D(H)-D(V)\leq D(H)+\tfrac{1}{2}K_v D(T)^{1/2},$$

whence

$$D(T)^{1/2}\leq D(H)^{1/2}+\tfrac{1}{2}K_v. \tag{4.14}$$

Next, $D(T^2)^{1/2}=D((H-V)^2)^{1/2}$, so from the triangle inequality

$$D(T^2)^{1/2}\leq D(H^2)^{1/2}+D(V^2)^{1/2}. \tag{4.15}$$

Proceeding further,

$$D(T^4)^{1/2}=D[((H-V)^2)^2]^{1/2}\leq D[(2(H^2+V^2))^2]^{1/2},$$

or

$$D(T^4)^{1/2}\leq 2D(H^4)^{1/2}+2D(V^4)^{1/2}, \tag{4.16}$$

and so forth. Thus we have available bounds on the deviations of powers of the total, kinetic, or potential energies, and by virtue of (4.8), on any potential sum.

5. SHORT- AND LONG-RANGE REDUCTION

If an observable $u(\mathbf{r}_{ij})$ is too singular at some point in space, the bounding techniques of (4.9) and (4.10) are unavailable. In this case, however, one can trade inverse coordinates for moments. The reduction technique is in fact precisely that used in (4.6) and (4.7), which we now write more generally as

$$\begin{aligned}D(\hbar/i\nabla\cdot\mathbf{F}) &= D(\mathbf{p}\cdot\mathbf{F}-\mathbf{F}\cdot\mathbf{p}) \\ &= D(\mathbf{p}\cdot r^{-s}r^s\mathbf{F})-D(r^s\mathbf{F}\cdot r^{-s}\mathbf{p})\end{aligned}$$

for suitable s. Thus

$$|D(\hbar\nabla\cdot\mathbf{F})|\leq 2D(\mathbf{p}\cdot r^{-s}\mathbf{p})^{1/2}D(r^s\mathbf{F}\cdot r^{-s}r^s\mathbf{F})^{1/2},$$

or

$$|D(\nabla\cdot\mathbf{F})|\leq(2/\hbar)D(\mathbf{p}\cdot r^{-s}\mathbf{p})^{1/2}D(\mathbf{F}\cdot\mathbf{r}^s\mathbf{F})^{1/2} \tag{5.1}$$

for any coordinate functions $\mathbf{r}$ and $\mathbf{F}$. For example, to handle $|\mathbf{r}_{ij}-\mathbf{x}|^{-2}$, we choose

$$\mathbf{F}=(\mathbf{r}_{ij}-\mathbf{x})|\mathbf{r}_{ij}-\mathbf{x}|^{-2}, \quad r=|\mathbf{r}_{ij}-\mathbf{x}|, \quad s=0, \quad \mathbf{p}=\tfrac{1}{2}(\mathbf{p}_i-\mathbf{p}_j),$$

[8] G. H. Hardy, J. E. Littlewood, and G. Polya, *Inequalities* (Cambridge University Press, New York, 1934), p. 30.

obtaining at once

$$D(|\mathbf{r}_{ij}-\mathbf{x}|^{-2})\leq(1/\hbar)D((\mathbf{p}_i-\mathbf{p}_j)^2)^{1/2}D(|\mathbf{r}_{ij}-\mathbf{x}|^{-2})^{1/2},$$

so that

$$D(|\mathbf{r}_{ij}-\mathbf{x}|^{-2})\leq(1/\hbar^2)D((\mathbf{p}_i-\mathbf{p}_j)^2).$$

But for a translationally invariant system at zero total momentum,

$$\begin{aligned}4mND(T)&=\textstyle\sum_{i,j}D(p_i^2+p_j^2)\\&=D[\textstyle\sum_{i,j}(p_i^2+p_j^2)-2\sum_j\mathbf{p}_j^2]\\&=N(N-1)D((\mathbf{p}_i-\mathbf{p}_j)^2).\end{aligned}$$

Hence

$$D(|\mathbf{r}_{ij}-\mathbf{x}|^{-2})\leq[4m/(N-1)\hbar^2]D(T). \quad (5.2)$$

On the other hand, for the stronger singularity $\delta(\mathbf{r}_{ij}-\mathbf{x})$, we of course select

$$\mathbf{F}=(1/4\pi)(\mathbf{r}_{ij}-\mathbf{x})\,|\mathbf{r}_{ij}-\mathbf{x}|^{-3},$$

but $s=2$, yielding now

$$\begin{aligned}D(\delta(\mathbf{r}_{ij}-\mathbf{x}))\leq(\tfrac{1}{4}\pi\hbar)&D(\mathbf{p}_i-\mathbf{p}_j)\cdot|\mathbf{r}_{ij}-\mathbf{x}|^{-2}\\&\times(\mathbf{p}_i-\mathbf{p}_j))^{1/2}D(|\mathbf{r}_{ij}-\mathbf{x}|^{-2})^{1/2}.\end{aligned}$$

By virtue of Eq. (5.2), we also have

$$\begin{aligned}&D((\mathbf{p}_i-\mathbf{p}_j)\cdot|\mathbf{r}_{ij}-\mathbf{x}|^{-2}(\mathbf{p}_i-\mathbf{p}_j))\\&\quad\leq 4m/(N-1)\hbar^2D((\mathbf{p}_i-\mathbf{p}_j)\cdot T(\mathbf{p}_i-\mathbf{p}_j))\\&\quad=[4m/(N-1)\hbar]^2D(T^2),\end{aligned}$$

and so

$$D(\delta(\mathbf{r}_{ij}-\mathbf{x}))\leq\frac{1}{4\pi}\left(\frac{4m}{(N-1)\hbar^2}\right)^{3/2}D(T^2)^{1/2}D(T)^{1/2}. \quad (5.3)$$

Equation (5.3) may now be used in an alternative expression for K_u of (4.8), yielding on integration with the weight $u(\mathbf{x})$

$$K_u\leq\frac{N(N-1)}{4\pi}\left(\frac{4m}{(N-1)\hbar^2}\right)^{3/2}D(T^2)^{1/2}\int|u(\mathbf{x})|\,d\mathbf{x}. \quad (5.4)$$

This is valid, although not necessarily optimal, for singular but integrable potentials as well.

For observabales which do not decrease rapidly enough at infinity, Eqs. (4.9), (4.10), and (5.4) are inadequate. For example, if $u(x)=x^2$, they diverge, respectively, as x^3, x^3, and x^5. Under these conditions, a different reduction technique is appropriate, one which effectively replaces coordinates by momenta. Suppose that H has even parity, but that B is an observable of odd parity. (This assumption is readily removed, e.g., by replacing an even parity B by $\hat{r}B$, but irrelevant complications are thereby introduced.) Then

$$\begin{aligned}B(H-\mathcal{E}_0)^{-1}PW\phi=&PB(H-\mathcal{E}_0)^{-1}W\phi\\&+\psi\langle\psi|B(H-\mathcal{E}_0)^{-1}W|\phi\rangle, \quad (5.5)\end{aligned}$$

the term on the right must vanish. We now couple this with the observation that

$$\begin{aligned}B(H-\mathcal{E}_0)^{-1}=&(H-\mathcal{E}_0)^{-1}B\\&+(H-\mathcal{E}_0)^{-1}[H,B](H-\mathcal{E}_0)^{-1}, \quad (5.6)\end{aligned}$$

and conclude that (note that $PW\phi=W\phi$)

$$BGW\phi=GBW\phi+G[H,B]GW\phi. \quad (5.7)$$

Hence applying the triangle inequality,

$$\begin{aligned}\langle W^*GB^*BGW\rangle^{1/2}\leq&\langle W^*B^*G^2BW\rangle^{1/2}\\&+\langle W^*G[B^*,H]G^2[H,B]GW\rangle^{1/2}, \quad (5.8)\end{aligned}$$

and removing G^2 as in (4.2), we see that

$$\begin{aligned}D(B^*B)^{1/2}\leq&(E_1-\mathcal{E}_0)^{-1}\langle W^*B^*BW\rangle^{1/2}\\&+(E_1-\mathcal{E}_0)^{-1}D([B^*,H][H,B])^{1/2}. \quad (5.9)\end{aligned}$$

The first term on the right of (5.9) is what would have been expected from direct removal of G^2 as in (4.2), while in the residue, B has been replaced by $[H,B]$, essentially an $\mathbf{r}\rightarrow\mathbf{p}$ replacement for a pure coordinate function.

As prototype for the reduction (5.9), we may consider the mean-square radius about the center of mass (c.m.):

$$R^2=\sum_1^N\left(\mathbf{r}_i-\frac{1}{N}\sum_1^N\mathbf{r}_j\right)^2\Big/N$$

or

$$R^2=\frac{1}{2N^2}\sum(\mathbf{r}_i-\mathbf{r}_j)^2. \quad (5.10)$$

Then from (5.9), with $[H,\mathbf{r}_i-\mathbf{r}_j]=(\hbar/im)(\mathbf{p}_i-\mathbf{p}_j)$, and using the argument preceding (5.2),

$$\begin{aligned}D(R^2)^{1/2}\leq&(E_1-\mathcal{E}_0)^{-1}\langle WR^2W\rangle^{1/2}\\&+\frac{(2\hbar^2/mN)^{1/2}}{E_1-\mathcal{E}_0}D(T)^{1/2}, \quad (5.11)\end{aligned}$$

which can be explicitly evaluated.

6. EXAMPLE AND APPLICATION

As we have indicated many times, the bounds obtained are quite conservative. It is instructive to see the relative accuracy of the estimates made, and for this purpose let us consider a positronium atom, with Hamiltonian

$$\begin{aligned}H&=(1/2m)[p_1^2+p_2^2]-e^2/r_{12}\\&=p_{12}^2/m-e^2/r_{12}+P^2/4m. \quad (6.1)\end{aligned}$$

[$P=p_1+p_2$, $p_{12}=\frac{1}{2}(p_1-p_2)$.] The ground state, normalized to unit volume for the c.m.,

$$\psi(\mathbf{r}_{12})=(\alpha^3/\pi)^{1/2}e^{-\alpha r_{12}},\quad E_0=-(\hbar^2/m)\alpha^2$$

where

$$\alpha=me^2/2\hbar^2. \quad (6.2)$$

We may fabricate an approximate wave function by

changing the scale:

$$\phi(\mathbf{r}_{12})=(\beta^3/\pi)^{1/2}e^{-\beta r_{12}},\quad \mathcal{E}_0=-(\hbar^2/m)\beta(2\alpha-\beta). \quad (6.3)$$

It then follows that

$$\langle\psi|\phi\rangle=[2\alpha^{1/2}\beta^{1/2}/(\alpha+\beta)]^3,$$
$$\gamma=[\tfrac{1}{2}(\alpha/\beta)^{1/2}+\tfrac{1}{2}(\beta/\alpha)^{1/2}]^3-1. \quad (6.4)$$

For the sake of comparison, let us choose the mean-square radius $R^2=\frac{1}{4}r_{12}^2$, for which we find

$$\langle R^2\rangle=3/4\beta^2,\quad \langle\psi|R^2|\psi\rangle=3/4\alpha^2. \quad (6.5)$$

There is little point in assessing higher than second order terms in the difference of α and β. Hence with

$$\beta=(1-\delta)\alpha, \quad (6.6)$$

we desire a comparison of bounds with the known

$$\gamma=\tfrac{3}{8}\delta^2,$$
$$|\langle\psi|R^2|\psi\rangle^{1/2}-\langle R^2\rangle^{1/2}|=(\tfrac{3}{4})^{1/2}(1/\alpha)(\delta+\delta^2). \quad (6.7)$$

From (3.3), using the known value of E_0, Eq. (6.3),

$$\gamma\leq\tfrac{1}{2}(\mathcal{E}_0-E_0)/(E_1-E_0)=\tfrac{2}{3}\delta^2, \quad (6.8)$$

off by a factor of almost 2. If we replace E_0 by E_L, the lower bound found from Temple's method, we find $\gamma\leq(32/9)\delta^2$, a factor of 5 worse than (6.8), which uses the exact E_0. It appears that large errors may arise from the uncertainty of the energy eigenvalue. Indeed, in atomic-physics problems, E_0 is considerably closer to $\mathcal{E}_0$ than to E_L ,and Schmid *et al.*[9] show that the same is true for a deuteron bound by a Gaussian potential.

Noting that

$$\langle W^*GR^2GW\rangle=\langle R^2\rangle-[2/(1+\gamma)]\langle\psi|R^2|\psi\rangle$$
$$+[1/(1+\gamma)^2]\langle\psi|R^2|\psi\rangle, \quad (6.9)$$

we readily find that

$$D(R^2)=\langle W^*GR^2GW\rangle=3(3\delta/4\alpha)^2. \quad (6.10)$$

Thus, in Eq. (2.12), using $\gamma=\frac{3}{8}\delta^2$, we have

$$|\langle\psi R^2|\psi\rangle^{1/2}-\langle R^2\rangle^{1/2}|\leq 2(\tfrac{3}{4})^{3/2}\delta/\alpha+(9/32\alpha)\delta^2. \quad (6.11)$$

[9] E. W. Schmid, Y. C. Tang, and R. C. Herndon, Nucl. Phys. 42, 95 (1963).

The exact value is $(\frac{3}{4})^{1/2}\delta/\alpha$, showing that the triangle inequality is already responsible for a conservative factor of 1.5.

Finally, let us check our estimate of $D(R^2)$. Since

$$W\phi=\beta^{3/2}\pi^{-1/2}e^{-\beta r_{12}}(\hbar^2/m)2\delta\alpha(\beta-1/r_{12}), \quad (6.12)$$

we obtain

$$\langle W^*R^2W\rangle=(\hbar^2/m)^2\delta^2\alpha^2, \quad (6.13)$$

and from Eq. (4.14) [together with (4.3), (4.4), and (4.7)],

$$D(T)^{1/2}\leq\tfrac{1}{2}\alpha\delta(\hbar^2/m)^{1/2}(1+\sqrt{3}). \quad (6.14)$$

Hence Eq. (5.11) yields

$$D(R^2)^{1/2}\leq\tfrac{2}{3}\sqrt{3}(1+\sqrt{3})\delta/\alpha. \quad (6.15)$$

Comparing this with the exact value, Eq. (6.10), we see that we have another conservative factor of about 2.4, attributable primarily to the $D(T)^{1/2}$ evaluation, and here mainly to the size of K_v.

In practice, the crucial value of γ may have to be determined in the absence of firm knowledge of the ground state E_0. The exact energy would then have to be replaced by a lower bound involving the energy dispersion $\langle(H-\mathcal{E}_0)^2\rangle$. For atomic systems, where the energy dispersion in available computations can be quite small, the technique described should give usable bounds on, e.g., the mean-square radius. However, for model nuclei such as the model triton previously studied by the authors,[5] the energy dispersion is sizable, and an upper-bound estimate for the mean-square radius turns out to be several times the radius. This conclusion is unaltered even when the parameters of the wave function in this model are varied to minimize the above upper bound. Furthermore, the overlap, $(1+\gamma)^{-1}$, decreases exponentially with the number of particles, so that the estimate becomes especially poor for a large many-body system. For systems of the above types, exact error bounds are luxuries, and one must be content with approximate techniques for improving expectations. We shall describe in a future paper one such technique which has proven highly effective.