# Further Refinements on the Brillouin-Wigner Perturbation Procedure*

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(Received October 4, 1956)

The first-order correction to the wave function in the Brillouin-Wigner perturbation procedure is generalized by associating independent amplitude coefficients $G_x$ with each physically distinct type of interaction $W^{(x)}$ occurring in the interaction operator. The modified formulas for wave function and energy can be evaluated by using only quantities which occur in the original formulation of the perturbation procedure (characterized by $G_x=1$). The energy formula is invariant under a transformation which changes the scale of all energy denominators by a constant factor. A uniform displacement of the zeroth-order energy spectrum provides an additional variational parameter.

A simple example is worked out to show how the computed energy improves as the amplitude parameters are displaced from $G_x=1$ to optimum values. An incidental result is the observation that the statistical weight of the first order correction to the wave function depends strongly on the amplitude parameters.

Finally, results for degenerate and nondegenerate zeroth order states are embodied in an effective interaction operator which determines the energy and the correct zeroth-order linear combination.

## I. INTRODUCTION

In a recent paper[1] we described a method for improving the Brillouin-Wigner (B-W) perturbation procedure in accuracy and rapidity of convergence by a simple modification of the approximate wave functions used in that procedure. The modified formulas for wave functions and energies can be evaluated by using only quantities which occur in the original formulation of the perturbation procedure.

An additional refinement is possible in problems where the perturbation operator $W$ appears as a linear combination of distinct types. This is, in fact, the usual situation. For example, in a nuclear problem, $W$ may contain short-range radial repulsive terms, radial exchange interactions, tensor operators, and harmonic oscillator potentials.

We write

$$W=\sum_x W^{(x)}-U, \tag{1}$$

the index $x$ distinguishing the different types, and, in the simplest possible formulation of the proposed refinement, use the approximate wave function[2]

$$\psi=\left[\psi_0+\sum_x G_x \sum_n{}' \psi_n \frac{W_{n0}{}^{(x)}}{E-E_n}\right]N^{-1} \tag{2}$$

to estimate the energy $E$ of the state generated by the zeroth-order function $\psi_0$. We proceed in Sec. II to develop formulas for computing $E$ when no degeneracy exists in the zeroth order description of the state. The problem of degeneracy is treated in Sec. III. An example to illustrate the use of the method is worked out in Sec. IV.

* Supported in part by the U. S. Atomic Energy Commission, the Office of Naval Research, and the Office of Scientific Research.
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[1] P. Goldhammer and E. Feenberg, Phys. Rev. **101**, 1233 (1956); also B. A. Lippmann, Phys. Rev. **103**, 1149 (1956).
[2] In the total Hamiltonian $H_0+W$, $H_0$ possesses a complete set of normalized orthogonal eigenfunctions $\psi_n$ and associated eigenvalues $E_n (E_0\leqq E_1\leqq E_2\leqq\cdots)$. The constant $-U$ in $W$ compensates for a uniform displacement of the zeroth-order energy spectrum by the amount $+U$.

## II. NONDEGENERATE ZEROTH ORDER

The variational formula for the energy,

$$E=(\psi|H_0+W|\psi)/(\psi,\psi), \tag{3}$$

now yields

$$E=E_0+W_{00}+\sum_x(\bar{G}_x\epsilon_{2x}+G_x\bar{\epsilon}_{2x}) -\sum_{x,y}\bar{G}_xG_y(\epsilon_{2xy}-\epsilon_{3xy}), \tag{4}$$

in which

$$\epsilon_{2xy}=\sum_m{}'\frac{W_{0m}{}^{(x)}W_{m0}{}^{(y)}}{E-E_m}, \qquad \epsilon_{2x}=\sum_y\epsilon_{2xy}, \tag{5}$$

$$\epsilon_{3xy}=\sum_{m,n}{}'\frac{W_{0m}{}^{(x)}W_{mn}W_{n0}{}^{(y)}}{(E-E_m)(E-E_n)}, \qquad \epsilon_{3x}=\sum_y\epsilon_{3xy}.$$

Also

$$\epsilon_2=\sum_{x,y}\epsilon_{2xy}, \qquad \epsilon_3=\sum_{x,y}\epsilon_{3xy}. \tag{6}$$

The condition $G_x=1$ characterizes the original formulation of the B-W procedure in the first order approximation to the wave function. The modified procedure described in reference 1 involves replacement of $G_x$ by $G$ (independent of $x$) and application of the extremum condition $dE/dG=0$ to obtain

$$G=(1-\epsilon_3/\epsilon_2)^{-1}, \qquad E=E_0+W_{00}+\epsilon_2/(1-\epsilon_3/\epsilon_2). \tag{7}$$

The trivial, but useful, generalization which we now consider, is just to treat the set of amplitudes $G_x$ as independent variational parameters. Applying the condition

$$\partial E/\partial\bar{G}_x=\partial E/\partial G_x=0 \tag{8}$$

to the right-hand member of Eq. (4), we get

$$\sum_y(\epsilon_{2xy}-\epsilon_{3xy})G_y=\epsilon_{2x}, \tag{9}$$

and

$$E=E_0+W_{00}+\tfrac{1}{2}\sum_x(\bar{G}_x\epsilon_{2x}+G_x\bar{\epsilon}_{2x}). \tag{10}$$

Equation (9) determines $G_x$; with these amplitudes Eq. (10) becomes a definite implicit equation for $E$.

If all third-order energy terms $\epsilon_{3xy}$ vanish (or are neglected), Eq. (9) yields $G_x=1$ and Eq. (10) reduces to $E=E_0+W_{00}+\epsilon_2$. In general however $\epsilon_{3xy}\not\equiv 0$ and $G_x$ is not as a rule independent of $x$. To facilitate the applications, we give explicit formulas for $G_x$ and $E$. The notation

$$q_{xy}=\epsilon_{2xy}-\epsilon_{3xy} \tag{11}$$

is convenient here.

$x=a,\ b.$—

$$G_a=\frac{q_{bb}\epsilon_{2a}-q_{ab}\epsilon_{2b}}{q_{aa}q_{bb}-|q_{ab}|^2}=1+\frac{q_{bb}\epsilon_{3a}-q_{ab}\epsilon_{3b}}{q_{aa}q_{bb}-|q_{ab}|^2},$$

$$G_b=\frac{q_{aa}\epsilon_{2b}-q_{ba}\epsilon_{2a}}{q_{aa}q_{bb}-|q_{ab}|^2}=1+\frac{q_{aa}\epsilon_{3b}-q_{ba}\epsilon_{3a}}{q_{aa}q_{bb}-|q_{ab}|^2}, \tag{12}$$

$$E=E_0+W_{00}+\frac{q_{aa}|\epsilon_{2b}|^2+q_{bb}|\epsilon_{2a}|^2-q_{ab}\epsilon_{2a}\bar{\epsilon}_{2b}-q_{ba}\bar{\epsilon}_{2a}\epsilon_{2b}}{q_{aa}q_{bb}-|q_{ab}|^2}. \tag{13}$$

In this case the conditions $q_{aa}<0$, $q_{bb}<0$, $q_{aa}q_{bb}-|q_{ab}|^2>0$, insure that the extreme value of the energy determined by Eq. (12) is actually a minimum.

$x=a,\ b,\ c,\ \cdots;\ q_{ax}=q_{bx}=0,\ x\neq a\ or\ b,\ q_{xx}<0.$—

Equation (12) is supplemented by the statement

$$G_x=\epsilon_{2x}/q_{xx},\quad x\neq a \text{ or } b, \tag{14}$$

and a term

$$\Delta E=\sum_{x\neq a,b}|\epsilon_{2x}|^2/q_{xx} \tag{15}$$

is added to the right-hand member of Eq. (13).

When two or more nondiagonal $q$'s with shared indices differ from zero, the exact formulas are somewhat cumbersome. A series expansion in powers of $q_{xy}(x\neq y)$ may sometimes converge fast enough to be useful. Applying an obvious iteration procedure to Eq. (9), one finds

$$G_x=\epsilon_{2x}/q_{xx}-\sum_{y\neq x}q_{xy}\epsilon_{2y}/q_{xx}q_{yy}+\cdots, \tag{16}$$

$$E=E_0+W_{00}+\sum_x|\epsilon_{2x}|^2/q_{xx}-\sum_x\sum_{y\neq x}\bar{\epsilon}_{2x}q_{xy}\epsilon_{2y}/q_{xx}q_{yy}+\cdots. \tag{17}$$

The displacement parameter $U$ is still available for adjustment to minimize the computed energy. We observe that $\epsilon_{2xy}$ is a function of $E-U$ only while $\epsilon_{3xy}$ depends also linearly on $U$ through the diagonal matrix elements $W_{nn}$. In some problems the simple condition[3] $W_{00}=0$ may determine $U$ close to the optimum value given by the correct supplementary condition

$$\partial E/\partial U=0. \tag{18}$$

When the implicit equation for $E$ is not too complicated, the supplementary condition can be developed into a semiexplicit equation for $U$. Equation (5) has been treated in this manner in an earlier publication.[4] The general implicit functional relations for $U$ and $E$ have the form

$$\begin{aligned}U&=f(E-U),\\ E-E_0-W_{00}&=g(E-U,\,U)\\ &=g(E-U,\,f(E-U)).\end{aligned} \tag{19}$$

These relations yield an implicit equation for a single unknown:

$$E-U=E_0+W_{00}+g(E-U,\,f(E-U))-f(E-U). \tag{20}$$

A root of Eq. (20) introduced into Eq. (19) determines the associated values of $E$ and $U$.

A simple graphical procedure is available as a practical last resort when semianalytical techniques become too complicated. The function $g(E-U,\,U)$ is first evaluated as a function of $E-U$. The dependence on $U$ is then easily determined since $U$ enters linearly in $\epsilon_{3xy}$ and no where else. Plots of $E-E_0-W_{00}$ and $g(E-U,\,U)$ against $E-U$ yield a lowest root $E(U)$. A series of such plots determines the minimum value of $E$ as a function of $U$.

A parenthetical remark is in order here. The role of displacement parameter $U$ in the general B-W energy series,

$$E=E_0+W_{00}+\sum_{l=2}^{2n+1}\epsilon_l, \tag{21}$$

deserves careful study particularly in connection with the dependence of $E$ on the number of particles $A$ and on the order $2n+1$ of the perturbation series. Let $E(A,n,U)$ denote the lowest root of Eq. (21). This root is given as a function of the number of particles $A$, the order of the energy perturbation series $2n+1$, and the displacement of the zeroth order spectrum $U$. A formal proof that $E(A,\infty,U)$ does not depend on $U$ is easily supplied.[4] For finite $n$, the supplementary condition $\partial E/\partial U=0$ determines $U$ as a function of $A$ and $n$. We are interested in the behavior of $E(A,n,U(A,n))$ as a function of $A$ and $n$, especially the limiting behavior as $A$ becomes infinite for fixed $n$. Brueckner's discussion[5] of the "linked cluster approximation" bears on this problem, but his conclusions are not immediately applicable to $E(A,n,U(A,n))$.

The possibility of introducing an energy-dependent term into the zeroth-order Hamiltonian provides additional variational parameters.[6] However, Eq. (10) for

[3] M. Bolsterli and E. Feenberg, Phys. Rev. **101**, 1349 (1956).

[4] E. Feenberg, Phys. Rev. **103**, 1116 (1956).

[5] K. A. Brueckner, Phys. Rev. **100**, 36 (1955).

[6] W. G. Swiatecki, Phys. Rev. **101**, 1321 (1956)

the energy is invariant under the simplest transformation of this type[4]‡:

$$\begin{aligned} H_0+W&=H_0'+W',\\ H_0'&=H_0+(\mu-1)(H_0-E),\\ W'&=W-(\mu-1)(H_0-E)\\ &=W-\frac{\mu-1}{\mu}(H_0'-E). \end{aligned} \tag{22}$$

The proof of invariance follows immediately from the formulas

$$\begin{aligned} \epsilon_{2xy}'&=\frac{1}{\mu}\epsilon_{2xy},\\ \epsilon_{3xy}'&=\frac{1}{\mu^2}\epsilon_{3xy}+\frac{\mu-1}{\mu^2}\epsilon_{2xy}. \end{aligned} \tag{23}$$

These yield

$$\epsilon_{2xy}'-\epsilon_{3xy}'=\frac{1}{\mu^2}(\epsilon_{2xy}-\epsilon_{3xy}) \tag{24}$$

as in the more limited context of reference 3. Equation (9) now requires $G_x'=\mu G_x$; consequently,

$$\begin{aligned} \sum \bar{G}_x'\epsilon_{2x}'&=\sum \bar{G}_x\epsilon_{2x},\\ \sum_{x,y} \bar{G}_x'G_y'(\epsilon_{2xy}'-\epsilon_{3xy}')&=\sum_{x,y} \bar{G}_xG_y(\epsilon_{2xy}-\epsilon_{3xy}). \end{aligned} \tag{25}$$

### III. DEGENERATE CASE

The zeroth-order wave function $\psi_0$ is given by

$$\psi_0=\sum C_p\psi_{0p}/[\sum \bar{C}_qC_q]^{\frac{1}{2}}, \tag{26}$$

a linear combination of the complete set of normalized orthogonal functions $\psi_{0p}$ belonging to the function space defined by $E_n=E_0$. Now we introduce the notation

$$\begin{aligned} \epsilon_{2xypq}&=\sum_n{}' \frac{(W^{(x)})_{0p,n}(W^{(y)})_{n,0q}}{E-E_n},\\ \epsilon_{2xy}&=\sum_{p,q} \bar{C}_pC_q\epsilon_{2xypq}/\sum_r \bar{C}_rC_r, \end{aligned} \tag{27}$$

in which the prime on the summation symbol means absence of terms with $E_n=E_0$. Equation (4) for the energy becomes

$$E=E_0+\sum_{p,q} \bar{C}_pC_q[W_{0p,0q}+\sum_x(\bar{G}_x\epsilon_{2xpq}+G_x\bar{\epsilon}_{2xqp}) -\sum_{x,y} \bar{G}_xG_y(\epsilon_{2xypq}-\epsilon_{3xypq})]/\sum \bar{C}_rC_r. \tag{28}$$

Equations (9), (10), and (18) are still valid, but must be supplemented by

$$\sum_q C_q[W_{0p;0q}+\sum_x(\bar{G}_x\epsilon_{2xpq}+G_x\bar{\epsilon}_{2xqp}) -\sum_{x,y} G_xG_y(\epsilon_{2xypq}-\epsilon_{3xypq})-(E-E_0)\delta_{pq}]=0. \tag{29}$$

Equations (9), (18), and (29) determine the energy and the variational parameters $G_x$, $C_p$, and $U$.§

In applications, the simplified formulation having $G_x=G=(1-\epsilon_3/\epsilon_2)^{-1}$ may provide a convenient starting point for a procedure of successive approximations. Equation (29) simplifies to

$$\sum C_q\left[W_{0p;0q}+\frac{2\epsilon_{2pq}}{1-\epsilon_3/\epsilon_2}-\frac{\epsilon_{2pq}-\epsilon_{3pq}}{(1-\epsilon_3/\epsilon_2)^2} -(E-E_0)\delta_{pq}\right]=0. \tag{30}$$

Also, in this formulation, Eq. (18) can be reduced to the quasi-explicit form

$$U=\frac{N_3{}^0\epsilon_2-2N_2\epsilon_3{}^0}{2[P_2\epsilon_2-N_2{}^2]}, \tag{31}$$

in which

$$\begin{aligned} N_2&=\sum_n{}' \frac{W_{0n}W_{n0}}{(E-E_n)^2},\\ P_2&=\sum_n{}' \frac{W_{0n}W_{n0}}{(E-E_n)^3},\\ \epsilon_3{}^0&=\sum_{mn}{}' \frac{W_{0m}(W_{mn}+U\delta_{mn})W_{n0}}{(E-E_m)(E-E_n)},\\ N_3{}^0&=\sum_{mn}{}' \frac{W_{0m}(W_{mn}+U\delta_{mn})W_{n0}}{(E-E_m)(E-E_n)}\left[\frac{1}{E-E_m}+\frac{1}{E-E_n}\right]. \end{aligned} \tag{32}$$

A relation equivalent to Eq. (31) is discussed in reference 4.

An even simpler and less accurate starting point is given by the approximation of neglecting third-order energy quantities in conjunction with

$$W_{00}\equiv X_{00}-U=0, \tag{33}$$

‡ *Note added in proof.*—The transformation

$$\begin{aligned} H_0'&=H_0+\mu(H_0-E)^q,\\ W'&=W-\mu(H_0-E)^q, \end{aligned}$$

yields

$$H_0'=E=\mu(H_0-E)(H_0-E+1/\mu).$$

All infinite sums occurring in the energy formula can be transformed into forms suitable for numerical evaluation by the method of reference 3 with the help of the identity

$$\frac{1}{H_0'-E}=\frac{1}{H_0-E}-\frac{1}{H_0-E+1/\mu}.$$

§ *Note added in proof.*—Compare with Van Vleck's treatment of degenerate problems [E. C. Kemble, *The Principles of Quantum Mechanics*, p. 394 (1937)] based on the Schroedinger form for the energy denominators.

as in reference 3. Equation (29) is replaced by

$$\sum C_q\{(1+N_2)X_{0p,0q}+\epsilon_{2pq} - [E+(1+N_2)X_{00}-E_0]\delta_{pq}\}=0. \quad (34)$$

In nuclear problems, characterized by the presence of a strong tensor component in $W$, Eqs. (29), (30), and (34) yield mathematical formulations of Feingold's[7,8] "reduced tensor coupling" model.

## IV. NUMERICAL EXAMPLES

The example of the deuteron may be used to illustrate the theory even though other methods are more suitable for an accurate treatment of the deuteron problem. Following the procedure described in reference 3, we choose for the zeroth-order Hamiltonian

$$H_0=\tfrac{1}{2}\hbar\omega(p^2+q^2)+U, \quad (35)$$

in which

$$\mathbf{q}=(M\omega/2\hbar)^{\frac{1}{2}}\mathbf{r}, \quad \mathbf{r}=\mathbf{r}_{12}, \quad (36)$$
$$\mathbf{p}=-i(2\hbar/M\omega)^{\frac{1}{2}}\nabla_r=-i\nabla_q.$$

The perturbation operator is

$$W=V(q)-\tfrac{1}{2}\hbar\omega q^2-U = V(q)-M-U. \quad (37)$$

A Gaussian radial dependence of the potential function simplifies the calculation of the needed matrix elements. We choose

$$V=A\exp(-a^2r_{12}^2)+B\exp(-b^2r_{12}^2), \quad (38)$$

with

$$1/b=2.18\times10^{-13}\text{ cm}, \quad a^2=8b^2, \quad B<0 \text{ (attractive potential well)}, \quad A>0 \text{ (repulsive core)}. \quad (39)$$

In terms of the dimensionless coordinate $q$, the potential becomes

$$V=A\exp(-\alpha^2q^2)+B\exp(-\beta^2q^2), \quad (40)$$

with

$$\beta^2=(2\hbar/M\omega)b^2, \quad \alpha^2=8\beta^2. \quad (41)$$

Numerical values are required for suitable $xy$ components of the quantities

$$\epsilon_2\equiv\sum_n{}'\frac{|W_{n0}|^2}{E-E_n}=\sum_n\frac{|V_{n0}|^2}{E-E_n}-\frac{V_{00}^2}{E-E_0}+\frac{1}{E-E_2}[(M^2)_{00}-M_{00}^2-2(MV)_{00}+2M_{00}V_{00}],$$

$$N_2\equiv\sum_n{}'\frac{|W_{n0}|^2}{(E-E_n)^2}=-\frac{\partial\epsilon_2}{\partial E},$$

$$\begin{aligned}\epsilon_3+N_2U=&\left[\sum_{m,n}\frac{V_{0m}V_{mn}V_{n0}}{(E-E_m)(E-E_n)}-\frac{2V_{00}}{E-E_0}\sum_n\frac{|V_{n0}|^2}{E-E_n}+\frac{V_{00}^3}{(E-E_0)^2}\right]\\&-\left[\sum_{m,n}\frac{V_{0m}M_{mn}V_{n0}}{(E-E_m)(E-E_n)}-2\frac{V_{00}}{E-E_0}\frac{(MV)_{00}-V_{00}M_{00}}{E-E_2}-\frac{V_{00}^2M_{00}}{(E-E_0)^2}\right]\\&-\frac{2}{E-E_2}\left[\sum_m\frac{V_{0m}(VM)_{m0}}{E-E_m}-M_{00}\sum_m\frac{V_{0m}V_{m0}}{E-E_m}-\frac{V_{00}}{E-E_0}((VM)_{00}-V_{00}M_{00})\right]\\&+\frac{2}{E-E_2}\left[\sum_m\frac{(M^2)_{0m}V_{m0}}{E-E_m}-\frac{(M^2)_{00}V_{00}}{E-E_0}-M_{00}\frac{(MV)_{00}-M_{00}V_{00}}{E-E_2}\right]\\&+\frac{1}{(E-E_2)^2}[(MVM)_{00}-2M_{00}(VM)_{00}+M_{00}^2V_{00}]-\frac{1}{(E-E_2)^2}[(M^3)_{00}-2M_{00}(M^2)_{00}+M_{00}^3].\end{aligned} \quad (42)$$

The separate $xy$ components in the quantities listed above,

$$\sum_m\frac{(W^x)_{0m}(W^y)_{m0}}{E-E_m}=-\int_0^\infty e^{\lambda E}(W^xe^{-\lambda H_0}W^y)_{00}d\lambda,$$
$$\sum_{m,n}\frac{(W^x)_{0m}(V-M)_{mn}(W^y)_{n0}}{(E-E_m)(E-E_n)}=\int_0^\infty\int_0^\infty e^{(\lambda+\lambda')E}(W^xe^{-\lambda H_0}(V-M)e^{-\lambda H_0}W^y)_{00}d\lambda d\lambda', \quad (43)$$

are evaluated with the help of the harmonic oscillator transformation[3] and the notation

$$H_{0s}=H_0-U, \quad \mu=\tfrac{1}{2}\lambda\hbar\omega, \quad \mu'=\tfrac{1}{2}\lambda'\hbar\omega, \quad g=\tanh2\mu, \quad k=1/\cosh2\mu, \quad g'=\tanh2\mu', \quad k'=1/\cosh2\mu'. \quad (44)$$

[7] A. M. Feingold and E. P. Wigner (unpublished calculations, 1950).
[8] A. M. Feingold, Phys. Rev. (to be published).

Results are

$$(\exp(-\alpha^2q^2)\exp(-\lambda H_{0s})M^2)_{00}=\frac{15}{16}(\hbar\omega)^2\left(\frac{k}{2g}\right)^{3/2}\left(\frac{1}{2}+\frac{1}{2g}+\alpha^2\right)^2\left[\left(\frac{1}{2}+\frac{1}{2g}\right)\left(\frac{1}{2}+\frac{1}{2g}+\alpha^2\right)-\frac{k^2}{4g^2}\right]^{-7/2},$$

$$(\exp(-\alpha^2q^2)\exp(-\lambda H_{0s})\exp(-\beta^2q^2))_{00}=\left(\frac{k}{2g}\right)^{3/2}\left[\left(\frac{1}{2}+\frac{1}{2g}+\alpha^2\right)\left(\frac{1}{2}+\frac{1}{2g}+\beta^2\right)-\frac{k^2}{4g^2}\right]^{-3/2},$$

$$(\exp(-\beta^2q^2)\exp(-\lambda H_{0s})\exp(-\alpha^2q^2)M)_{00}=\frac{3}{4}\hbar\omega\left(\frac{k}{2g}\right)^{3/2}\left(\frac{1}{2}+\frac{1}{2g}+\beta^2\right)\left[\left(\frac{1}{2}+\frac{1}{2g}+\beta^2\right)\left(\frac{1}{2}+\frac{1}{2g}+\alpha^2\right)-\frac{k^2}{4g^2}\right]^{-5/2},$$

$$(\exp(-\beta^2q^2)\exp(-\lambda' H_{0s})M\exp(-\lambda H_{0s})\exp(-\alpha^2q^2))_{00}$$

$$=\frac{3}{4}\hbar\omega\left(\frac{k}{2g}\frac{k'}{2g'}\right)^{3/2}\left(\frac{1}{2}+\frac{1}{2g}+\alpha^2\right)\left(\frac{1}{2}+\frac{1}{2g'}+\beta^2\right)\left[\frac{1}{2}\left(\frac{1}{g}+\frac{1}{g'}\right)\left(\frac{1}{2}+\frac{1}{2g}+\alpha^2\right)\left(\frac{1}{2}+\frac{1}{2g'}+\beta^2\right)\right.$$
$$\left.-\left(\frac{k}{2g}\right)^2\left(\frac{1}{2}+\frac{1}{2g}+\alpha^2\right)-\left(\frac{k'}{2g'}\right)^2\left(\frac{1}{2}+\frac{1}{2g'}+\beta^2\right)\right]^{-5/2}, \quad (45)$$

$$(\exp(-\alpha_1^2q^2)\exp(-\lambda' H_{0s})\exp(-\alpha_2^2q^2)\exp(-\lambda H_{0s})\exp(-\alpha_3^2q^2))_{00}$$

$$=\left(\frac{k}{2g}\frac{k'}{2g'}\right)^{3/2}\left[\left(\frac{1}{2g}+\frac{1}{2g'}+\alpha_2^2\right)\left(\frac{1}{2}+\frac{1}{2g'}+\alpha_1^2\right)\left(\frac{1}{2}+\frac{1}{2g}+\alpha_3^2\right)\right.$$
$$\left.-\left(\frac{k}{2g}\right)^2\left(\frac{1}{2}+\frac{1}{2g'}+\alpha_1^2\right)-\left(\frac{k'}{2g'}\right)^2\left(\frac{1}{2}+\frac{1}{2g}+\alpha_3^2\right)\right]^{-3/2}.$$

The final integration with respect to $\lambda$ and $\lambda'$ (or $\mu$ and $\mu'$) can now be carried out by a procedure which restores the original form of the infinite sums, but with all matrix elements replaced by explicit formulas.[3] An alternative representation of the integrals as power series in $(E-U-\frac{3}{2}\hbar\omega)/\hbar\omega$ is also useful.

Tables I, II, and III exhibit numerical results for two sets of force parameters chosen arbitrarily to give eigenvalues between $-2$ and $-3$ Mev. In Table I the interaction is purely attractive ($A=0$) and $U$ is determined by the condition $W_{00}=0$. The sixth column shows the remarkable increase in configuration mixing as refinements are introduced into the first order wave function. The physical parameters of Table I are retained in Table II, but the former supplementary condition $W_{00}=0$ is replaced by $\partial E/\partial U=0$. This change almost doubles the required value of $U$. Now the second-order energy is much larger than before, the third-order energy is greatly reduced, and the optimum value of $G$ is close to 1. Results from varying both $G$ and $U$ are not significantly different from varying $G$ or $U$ alone.

A substantial amount of short-range repulsive potential is included in a second example (Table III). The amplitude parameters $G_A$ and $G_B$ are associated with $A\exp(-8\alpha^2q^2)$ and $B\exp(-\alpha^2q^2)-\frac{1}{2}\hbar\omega q^2$, respectively. Consideration of the expected behavior of the wavefunction near the origin provides a simple interpretation of the result $G_A<1$. The term

$$\sum_n{}'\psi_n\frac{(A\exp(-\alpha^2q^2))_{n0}}{E-E_n}$$

TABLE I. Energy eigenvalues for $B=-41.1$ Mev, $A=0(W_{00}=0)$. All energies are in Mev.

| Method | $E$ | $E_0$ | $\epsilon_2$ | $\epsilon_3$ | $N^2-1$ | $\hbar\omega$ | Remarks |
|---|---|---|---|---|---|---|---|
| $E=E_0$ | $-1.69$ | $-1.69$ | ... | ... | ... | 13.3 | ... |
| $E=E_0+\epsilon_2$ | $-2.21$ | $-1.68$ | $-0.63$ | ... | 0.010 | 12.4 | ... |
| $E=E_0+\epsilon_2+\epsilon_3$ | $-2.41$ | $-1.69$ | $-0.52$ | $-0.20$ | 0.010 | 12.6 | ... |
| $E=E_0+\epsilon_2(1-\epsilon_3/\epsilon_2)^{-1}$ | $-2.53$ | $-1.69$ | $-0.52$ | $-0.20$ | 0.028 | 12.6 | $G=1.64$ |
| $E=E_0+G_B\epsilon_{2B}+G_M\epsilon_{2M}$[a] | $-2.85$ | $-1.69$ | | ... | 0.051 | 12.6 | $G_B=2.21$, $G_M=1.26$[a] |
| Correct value[b] | $-3.0$ | | | | | | |

[a] Here $G_B$ denotes variational coefficient of $B\exp(-\beta^2q^2)$, while $G_M$ is the variational coefficient of $M$.
[b] Estimated from Table III, H. A. Bethe and R. F. Bacher, Revs. Modern Phys. 8, 83 (1936).

TABLE II. Energy eigenvalues for $B=-41.1$ Mev, $A=0$; adjusting $U$ to minimize the energy. All energies are in Mev.

| Method | $E$ | $E_0$ | $\epsilon_2$ | $\epsilon_3$ | $N^2-1$ | $\hbar\omega$ | Remarks |
|---|---|---|---|---|---|---|---|
| $E=E_0+\epsilon_2+\epsilon_3$ | $-2.55$ | $-1.69$ | $-0.85$ | $-0.01$ | 0.029 | 12.6 | $U_{00}=1.95(V_{00}-M_{00})=-40.1$ Mev |
| $E=E_0+\epsilon_2(1-\epsilon_3/\epsilon_2)^{-1}$ | $-2.56$ | $-1.69$ | $-0.82$ | $-0.03$ | 0.029 | 12.6 | $G=1.035$, $U_{00}=1.92(V_{00}-M_{00})=-39.5$ Mev |

TABLE III. Energy eigenvalues for $B=-49.9$ Mev, $A=105$ Mev ($W_{00}=0$). All energies are in Mev.

| Method | $E$ | $E_0$ | $\epsilon_2$ | $\epsilon_3$ | $N^2-1$ | $\hbar\omega$ | Remarks |
|---|---|---|---|---|---|---|---|
| $E=E_0$ | $-1.65$ | $-1.65$ | ... | ... | ... | 10.8 | ... |
| $E=E_0+\epsilon_2$ | $-2.00$ | $-1.64$ | $-0.36$ | ... | 0.009 | 10.3 | ... |
| $E=E_0+\epsilon_2+\epsilon_3$ | $-2.14$ | $-1.64$ | $-0.36$ | $-0.14$ | 0.009 | 10.3 | ... |
| $E=E_0+\epsilon_2(1-\epsilon_3/\epsilon_2)^{-1}$ | $-2.26$ | $-1.64$ | $-0.36$ | $-0.14$ | 0.026 | 10.3 | $G=1.74$ |
| $E=E_0+G_A\epsilon_{2A}+G_B\epsilon_{2B}$[a] | $-2.57$ | $-1.64$ | ... | | 0.029 | 10.3 | $G_A=0.63$, $G_B=1.40$ |
| Correct value | $-2.7\pm0.1$ | | | | | | |

[a] $G_A$ is the variational coefficient of $A\exp(-\alpha^2q^2)$, while $G_B$ is the variational coefficient of both $B\exp(-\alpha^2q^2)$ and $M$.

in Eq. (2) is surely too large. This statement is proved by the observation that the sign of $\psi$ near the origin (with $G_A=1$) can be reversed by making $A$ sufficiently large. The correct wave function approaches zero at the origin as $A$ is increased indefinitely, but never reverses sign. Thus the factor $G_A<1$ is required to compensate for the incorrect behavior at the origin of the wave function generated by the conventional first order procedure.[9]

## V. CONCLUDING REMARKS

An "effective" interaction operator $\tilde{W}$ appears in Eqs. (4) and (29). This operator is defined by the equations

$$\tilde{W}_{0p;0q}=W_{0p;0q}+\sum_x[\bar{G}_x\epsilon_{2xpq}+G_x\bar{\epsilon}_{2xqp}]-\sum_{xy}G_xG_y[\epsilon_{2xypq}-\epsilon_{3xypq}]. \quad (46)$$

The usefulness of the concept of an effective interaction operator depends strongly on the sensitivity of the amplitude parameters $G_x$ to special features of particular problems. The possibility that a fixed or slowly varying set of amplitude parameters may be satisfactory in the $1s$ and $2p$ shells provides a powerful motivation for working out the properties and consequences of this operator as fully as possible. Among other properties we are interested in (a) the relative importance of two- and many-particle terms in $\tilde{W}$ when $W$ contains only 2-particle operators, (b) the magnitude of spin-orbit type components generated by iteration of the tensor interaction,[8] and (c) the relative magnitudes of tensor-type components in $W$ and $\tilde{W}$.[8]

A detailed comparison of the refined B-W procedure with the Brueckner method[10] of computing stationary state properties would have great value. However, numerical results for such comparisons are not yet available. The great power and elegance of Brueckner's method, as evidenced in applications to the infinite nuclear medium, has motivated recent attempts to adapt it to the description of finite nuclei.[11,12] These attempts seem promising, but it is hardly possible to be certain, at present, that the resulting formalism is superior in accuracy or simplicity to the refined B-W procedure in applications to low states of light nuclei (especially in the range $N+Z\leqq16$).

The "absence of clustering" advanced by Eden[11] as a necessary condition for the accuracy of a practical formulation of the Brueckner scheme may also be used to support the neglect of fourth and higher order energy terms as in the present discussion. A recent note on the perturbation treatment of the nuclear many-body problem bears closely on these controversial questions.[13]

## ACKNOWLEDGMENTS

We wish to thank Mr. Joseph Dreitlein for assistance in the numerical work.

[9] A special form of the repulsive potential, $J_A(r)=A$, $\alpha r\leqq1$ and $J_A(r)=0$, $\alpha r>1$, may be used to discuss the limiting situation $A\to\infty$. In this case $AG_A$ approaches a finite limit and all other $G_x$'s approach limiting values. The energy formula also approaches a definite limiting form. These results may be contrasted with the failure of the energy formula $E=E_0+W_{00}+\epsilon_2+\epsilon_3\sim O(A^3)$ in the same limiting situation.

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