Invariance Property of the Brillouin-Wigner Perturbation Series*

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The complete perturbation series for the energy is invariant under the operation of adding a velocity-dependent interaction to the zeroth order Hamiltonian and subtracting the same quantity from the perturbation operator. The same invariance property appear to hold also for an optimum formulation of the terminated energy series generated by the nth order approximation to the wave function. An explicit proof is given for the first- and second-order wave functions and also for the complete energy series. Variational procedures for determining (a) the optimum velocity dependence of the zeroth order Hamiltonian and (b) the optimum uniform displacement of the zeroth order energy spectrum are discussed in relation to the invariant formulations.

1. INTRODUCTION

An effective single-particle potential function can be derived from two-particle interactions by a Hartree-Fock type calculation starting from a zeroth order wave function in the form of a Slater determinant. Calculations with plane wave orbitals and exchange-type two-particle interactions yield a velocity-dependent single-particle potential well.[1-3] The velocity dependence of the well depth can be interpreted as a reduction in the dynamical mass of the nucleon when it moves through nuclear matter. A similar effect occurs in calculations which include configuration interaction by more complete self-consistent procedures.[4]

In a recent note Swiatecki[5] discusses the problem of determining an optimum velocity- (or energy-) dependent term in the zeroth order Hamiltonian in relation to the rate of convergence of the Brillouin-Wigner perturbation series. There is need for further discussion with emphasis on (a) the extremum property of the energy series and (b) the explicit dependence of the third and higher order energy terms on variations in the zeroth order Hamiltonian. These energy terms contain diagonal matrix elements of the perturbation operator and consequently depend explicitly on the assumed velocity-dependent interaction.

To make physical sense it is necessary that the complete perturbation series for the energy be invariant under the operation of adding a velocity-dependent interaction to the zeroth order Hamiltonian and subtracting the same quantity from the perturbation operator. The same invariance property appears to hold also for an optimum formulation of the terminated energy series generated by the nth order approximation to the wave function. An explicit proof is given for the first and second order wave functions and also for the complete formal series.

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2. PERTURBATION METHOD

The analysis is based on the resolution of the given Hamiltonian operator into the sum of a zeroth order operator H_0 and a perturbation operator W. The eigenfunctions and eigenvalues of H_0 are ψ_l and E_l, respectively; also $E_0 \leqq E_l \leqq E_{l+1} \cdots$. Some of the arbitrariness in the assumed resolution is removed by requiring $W_{00}=0$. Wave functions and energy values should be labeled with a complete set of quantum numbers $\beta \equiv \beta_1, \beta_2, \cdots \beta_p$ in addition to the index l. These quantum numbers are derived from the invariance properties common to H_0, W, and H_0+W, and hence can be used to label eigenfunctions of H_0 and also of the complete Hamiltonian H_0+W. The eigenfunctions of H_0 are thought of as grouped according to values of β; the given functions $\psi_0, \cdots \psi_l, \cdots$ belong to one of these groups. Thus E_0 is the lowest eigenvalue for the given β, not necessarily the lowest eigenvalue of H_0. In the same way, Ψ and E refer to exact or approximate eigenfunctions and eigenvalues of H_0+W for the given value of β.

We begin with the approximate wave function

$$\Psi=\frac{1}{N}\Big[\psi_0+G_1\sum{}'\psi_n\frac{W_{n0}}{E-E_n} + \cdots + G_k\sum{}'\psi_r\frac{W_{rq}W_{qp}\cdots W_{m0}}{(E-E_r)(E-E_q)\cdots(E-E_m)}\Big], \quad (1)$$

and setting $G_1=\cdots=G_k=1$ we obtain the implicit formula for the energy:

$$E=E_0+\epsilon_2+\epsilon_3+\cdots+\epsilon_{2k+1}, \quad (2)$$

in which

$$\epsilon_2=\sum{}'\frac{W_{0n}W_{n0}}{E-E_n}, \qquad \epsilon_{2k+1}=\sum{}'\frac{W_{0m}W_{mn}\cdots W_{rs}W_{s0}}{(E-E_m)(E-E_n)\cdots(E-E_s)}. \quad (3)$$

These are the basic formulas of the Brillouin-Wigner perturbation procedure. The lowest root of Eq. (2) lies

higher than the corresponding lowest eigenvalue of H_0+W.

A closer approach to the lowest eigenvalue and the corresponding wave function can be attained by minimizing the expectation value of H_0+W with respect to the parameters G_1, G_2, $\cdots G_k$. The explicit general formulas are then rather complicated but reduce to simple forms in several special cases.[6] In particular, if all the G's except G_1 vanish, then

$$G_1=\frac{1}{1-\epsilon_3/\epsilon_2} \tag{4}$$

and

$$\begin{aligned} E&=E_0+\epsilon_2+\frac{\epsilon_3}{1-\epsilon_3/\epsilon_2} \\ &=E_0+\frac{\epsilon_2}{1-\epsilon_3/\epsilon_2}. \end{aligned} \tag{5}$$

The lowest root of Eq. (5) falls below E_a, the lowest root of $\epsilon_2-\epsilon_3=0$, and also below E_0. It is clear from the explicit forms of ϵ_2 and ϵ_3 that $\epsilon_2-\epsilon_3$ is negative below E_a. Consequently,

$$\epsilon_2+\epsilon_3>\frac{\epsilon_2}{1-\epsilon_3/\epsilon_2}, \tag{6}$$

for a range of values of the energy including the lowest root of Eq. (5).

If only G_1 and G_2 do not vanish, the general variational formula for the energy is[6]

$$\begin{aligned} E=E_0+(2G_1-G_1^2)\epsilon_2+(G_1^2+2G_2-2G_1G_2)\epsilon_3 \\ +(-G_2^2+2G_1G_2)\epsilon_4+G_2^2\epsilon_5. \end{aligned} \tag{7}$$

The stationary value of the right-hand member as a function of G_1 and G_2 is found most simply by a process of completing squares, with the result

$$\begin{aligned} E=E_0+&\frac{\epsilon_2}{1-\epsilon_3/\epsilon_2} \\ &+\frac{[\epsilon_2\epsilon_4-\epsilon_3^2]^2/\epsilon_2}{(1-\epsilon_3/\epsilon_2)[(\epsilon_2-\epsilon_3)(\epsilon_4-\epsilon_5)-(\epsilon_3-\epsilon_4)^2]}. \end{aligned} \tag{8}$$

The stationary form actually is a minimum if the conditions,

$$\epsilon_2-\epsilon_3<0, \quad (\epsilon_2-\epsilon_3)(\epsilon_4-\epsilon_5)-(\epsilon_3-\epsilon_4)^2>0, \tag{9}$$

hold for a range of values of E including the lowest root of Eq. (8). If the odd-order energy terms vanish, E, the lowest root of Eq. (8), falls below E_a, the lowest, root of $\epsilon_2-\epsilon_4=0$, and also $\epsilon_2-\epsilon_4$ is negative below E_a and $0<\epsilon_4/\epsilon_2<1$. Thus Eq. (9) certainly holds if odd-order terms in the energy series vanish.

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3. VELOCITY DEPENDENCE AND INVARIANCE PROPERTY

Consider now the possibility of introducing an explicitly energy-dependent term into the zeroth order Hamiltonian. This is accomplished by adding a term proportional to H_0-E to H_0 and subtracting the same term from W, with the result

$$\begin{aligned} H&=H_0'+W', \\ H_0'&=H_0+(\mu-1)(H_0-E), \\ H_0'-E&=\mu(H_0-E), \\ W'&=W-(\mu-1)(H_0-E) \\ &=W-[(\mu-1)/\mu](H_0'-E). \end{aligned} \tag{10}$$

These definitions and relations now yield

$$E=E_0+\sum_{n=0}^{\infty}\epsilon_{n+2}' \tag{11}$$

in which

$$\begin{aligned} \epsilon_{n+2}'&=\sum{}'\frac{W_{0m}'W_{mn}'\cdots W_{rs}'W_{s0}'}{(E-E_m')(E-E_n')\cdots(E-E_s')} \\ &=\frac{1}{\mu^{n+1}}\sum_{s=0}^{n}\binom{n}{s}(\mu-1)^s\epsilon_{n+2-s}. \end{aligned} \tag{12}$$

The discussion of Eq. (11) may begin with the approximate formula derived from the first-order wave function (with $G_1=1$):

$$\begin{aligned} E&=E_0+\epsilon_2'+\epsilon_3' \\ &=E_0+\frac{2\mu-1}{\mu^2}\epsilon_2+\frac{1}{\mu^2}\epsilon_3. \end{aligned} \tag{13}$$

The minimum value of E occurs for

$$\mu=1-\epsilon_3/\epsilon_2, \tag{14}$$

and is the lowest root of Eq. (5). Equation (14) actually implies $\epsilon_3'=0$; thus the optimum value of μ associated with the conventional first-order wave function is determined by the condition

$$\epsilon_3'=0. \tag{15}$$

This result justifies the initial assumption $G_1=1$.

The diagonal matrix element W_{nn} may be expected to increase algebraicly with increasing E_n; a plausible inference then is that diagonal terms,

$$\sum{}'\frac{|W_{0n}|^2W_{nn}}{(E-E_n)^2},$$

determine the sign and approximate magnitude of ϵ_3. The conclusion,

$$1-\epsilon_3/\epsilon_2>1,$$

then follows; thus $\mu>1$ and $(\mu-1)/\mu>0$ appears to

be a reasonable expectation in the absence of actual numerical values.

In the simple problem of free particles in a box, M/μ is identified with the effective mass of a nucleon in nuclear matter. If an oscillator Hamiltonian,

$$H_0=\tfrac{1}{2}\hbar\omega\sum(p_i^2+q_i^2)+U,$$

is chosen to define the zeroth order description of the physical system, then $\mu\hbar\omega$ is the effective oscillator energy unit.

An alternative procedure starts from

$$G_1=\frac{1}{1-\epsilon_3'/\epsilon_2'} \tag{16}$$

and

$$E=E_0+\frac{\epsilon_2'}{1-\epsilon_3'/\epsilon_2'}. \tag{17}$$

Equation (5) for E then follows independently of the value assigned to μ in consequence of Eq. (12).

Thus G_1 and μ accomplish the same end in a curiously complementary fashion. If E is minimized with respect to G_1, the resulting equation for E does not depend on μ and has the same form as results from minimizing with respect to μ starting from $G_1=1$.

The preceding analysis can be extended readily to the energy formula generated by the second order wave function. In Eqs. (7) and (8), ϵ_n may be replaced by ϵ_n'. If we eliminate the primed quantities with the aid of Eq. (12), all dependence on μ cancels out and the primed form of Eq. (8) reverts back to the original unprimed form.

The preceding results suggest a general statement to the effect that the formula for E obtained by minimizing $E(G_1, G_2, \cdots G_k, \mu)$ with respect to the amplitudes $G_1, G_2, \cdots G_k$ does not depend on μ. The proof of this statement appears to require an elaborate algebraic technique. However the corresponding formal proof for the complete perturbation series with $G_1=\cdots=G_n=\cdots=1$ is quite simple, as shown below:

$$\begin{aligned}\sum_0^\infty \epsilon_{n+2}' &= \sum_0^\infty \frac{1}{\mu^{n+1}} \sum_{s=0}^n \binom{n}{s} (\mu-1)^{n-s}\epsilon_{s+2} \\ &= \sum_{s=0}^\infty \epsilon_{s+2}\mu^{-s-1} \sum_{n=0}^\infty \binom{n}{s}\left(\frac{\mu-1}{\mu}\right)^{n-s} \\ &= \sum_0^\infty \epsilon_{s+2}\mu^{-s-1}\left(1-\frac{\mu-1}{\mu}\right)^{-s-1} \\ &= \sum_0^\infty \epsilon_{s+2},\end{aligned} \tag{18}$$

subject to the restriction $|(\mu-1)/\mu|<1$. If the restriction fails, the proof of invariance can be carried through in n identical steps with n defined by the condition

$$\frac{\mu_n-1}{\mu_n}=\frac{1}{n}\frac{\mu-1}{\mu}, \quad \left|\frac{\mu_n-1}{\mu_n}\right|<1.$$

A general proof of invariance for an optimum formulation of the finite perturbation series may also throw light on the conditions under which the optimum values of $G_1, G_2, \cdots G_n, \cdots$ tend to unity as the order of the perturbation series is increased without limit.

4. UNIFORM DISPLACEMENT OF THE ZEROTH ORDER LEVEL SYSTEM

The condition $W_{00}=0$ enters the preceding discussion only in the qualitative discussion of the sign of $\epsilon_3(W)$. While $W_{00}=0$ fulfills the purpose of making W_{nn} small when $|E-E_n|$ is small, it does not represent the optimum condition in calculations with a limited number of terms in the perturbation series.

To discuss the possibility of an optimum condition, let

$$\begin{aligned}W&=X-X_{00},\\ W'&=W-(U-X_{00}),\\ H_0'&=H_0+U-X_{00},\\ E_n'&=E_n+U-X_{00},\\ N_2'(W)&=\sum{}'\frac{|W_{0n}|^2}{E-E_n'},\\ N_3'(W)&=\sum{}'\frac{W_{0m}W_{mn}W_{n0}}{(E-E_m')(E-E_n')}\left[\frac{1}{E-E_m'}+\frac{1}{E-E_n'}\right],\\ P_2'(W)&=\sum{}'\frac{|W_{0n}|^2}{(E-E_n')^3}.\end{aligned} \tag{19}$$

Consider the invariant energy formula

$$E-E_0=\epsilon_2'(W')^2/[\epsilon_2'(W')-\epsilon_3'(W')], \tag{20}$$

subject to the supplementary condition $\partial E/\partial U=0$. The supplementary condition requires

$$U-X_{00}=\frac{\epsilon_2'N_3'(W)-2N_2'\epsilon_3'(W)}{2[\epsilon_2'P_2'-N_2'^2]}, \tag{21}$$

and this relation in combination with Eq. (20) gives an implicit equation for $E-E_0-U+X_{00}$. The possible numerical values of $E-E_0-U+X_{00}$ inserted in Eqs. (20) and (21) then determine $E-E_0$ and $U-X_{00}$.

The numerator factor in Eq. (21) is expected to be small because of the relation

$$N_3'(W)/2N_2'\sim\epsilon_3'(W)/\epsilon_2', \tag{22}$$

which is suggested by the form of the normalization

and energy quantities. Explicitly,

$$\epsilon_2'N_3'(W)-2\epsilon_3'(W)N_2' \cong\sum'\frac{|W_{0m}|^2|W_{0n}|^2(E_n'-E_m')}{(E-E_m')^2(E-E_n')^2}(E_n'-E_m') \times\left[\frac{W_{nn}}{E-E_n'}-\frac{W_{mm}}{E-E_m'}\right], \quad (23)$$

suggesting a high degree of internal cancellation. Internal cancellation is relatively ineffective in reducing the magnitude of the denominator since it is actually a sum of positive-definite terms:

$$\epsilon_2'P_2'-N_2'^2=\tfrac{1}{2}\sum'\frac{|W_{0m}|^2|W_{0n}|^2}{(E-E_m')^2(E-E_n')^3} \times(E_n'-E_m')^2. \quad (24)$$

Finally, the formal invariance of the complete perturbation series with respect to uniform displacements of the zeroth order energy spectrum can be demonstrated by a calculation closely resembling that of Eq. (18).

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Degeneracy of the n-Dimensional, Isotropic, Harmonic Oscillator

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We show that what has previously been considered the "accidental" degeneracy in the energy levels of the n-dimensional, isotropic, harmonic oscillator is actually a consequence of its symmetry group. The additional symmetry, beyond the n-dimensional rotation group, arises from the symmetry between the coordinates and momenta.

IF the Hamiltonian for a given quantum-mechanical problem is invariant under a group of operations (for example, rotations of the coordinate space), then the eigenfunctions which correspond to each energy eigenvalue form the basis of a representation of this symmetry group. As any representation is a sum of irreducible representations, we see that the degeneracy of an eigenstate is directly related to the dimensionality of the irreducible representations. In many cases we can enlarge the symmetry group so that each energy eigenstate is composed of only one irreducible representation, although all irreducible representations need not appear.[1] In specific cases, however, it is not always easy to find the complete symmetry group. Fock[2] has found the symmetry group for the hydrogen atom and shown that the degeneracy of its energy levels is a necessary consequence of the symmetry properties of its Hamiltonian, but the degeneracy of the n-dimensional, isotropic, harmonic oscillator (hereafter referred to as n-oscillator) has not been understood in terms of the symmetry properties of its Hamiltonian. We shall now show that the degeneracy of its energy levels is a consequence of invariance under the n-dimensional unitary group.

The Hamiltonian operator for the n-oscillator is

$$H=\sum_{k=1}^{n}[(p_k^2/2m)+2\pi^2m\nu^2q_k^2]. \quad (1)$$

If we introduce[3] the non-Hermitian operators a_k, which are defined by the relations

$$a_k=[1/(2mh\nu)^{\frac{1}{2}}](2\pi m\nu q_k+ip_k), \quad (2)$$

we obtain

$$H=h\nu\sum_{k=1}^{n}(a_k^*a_k+\tfrac{1}{2}). \quad (3)$$

The a_k satisfy the commutation relations,

$$a_ka_r-a_ra_k=a_k^*a_r^*-a_r^*a_k^*=0, \quad a_ka_r^*-a_r^*a_k=\delta_{kr}. \quad (4)$$

We shall now show that the quantum mechanical problem of the n-oscillator is invariant under the n-dimensional unitary group. Let us define

$$A_k=\sum_{r=1}^{n}U_{kr}a_r, \quad (5)$$

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