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Kinetic energy as a perturbation

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The potential energy V is taken as the unperturbed Hamiltonian and the kinetic energy K is used as the perturbation. As K is a semipositive definite operator, one may use standard Padé approximants to reconstruct the Brillouin-Wigner functional. It is shown that, while the bare projector $(E-V)^{-1}$ is plagued in the complex E plane by the cut which results for the continuous spectrum of V, one may nonetheless solve the Brillouin-Wigner equation in a limit from the complex plane to the real axis. The theory is illustrated by a numerical example.

[NUCLEAR STRUCTURE Brillouin-Wigner perturbation theory, strong coupling, Padé approximants.]

I. INTRODUCTION

The Brillouin-Wigner (BW) theory is usually introduced as follows. Let H_0, λH_1, and $H \equiv H_0+\lambda H_1$ be the unperturbed Hamiltonian, the perturbation, and the total Hamiltonian, respectively. One assumes that H_0 has a square integrable ground state Φ_0, with eigenvalue $\epsilon_0<0$, and that for all real negative values of E one can easily calculate the propagator $Q(E-H_0)^{-1}$, where $Q\equiv 1-|\Phi_0\rangle\langle\Phi_0|$. If Ψ is a square integrable eigenstate of H and E is the corresponding eigenvalue, the BW theory then relies on the two equations

$$\Psi=\Phi_0+\frac{Q}{E-H_0}\lambda H_1\Psi \tag{1.1}$$

and

$$E-\epsilon_0=F(E)\ , \tag{1.2}$$

where

$$F(E)\equiv\langle\Phi_0|\,\lambda H_1+\lambda H_1\frac{Q}{E-H_0-\lambda QH_1Q}\lambda H_1\,|\Phi_0\rangle\ . \tag{1.3}$$

In practice one calculates an approximation of $F(E)$ by a perturbation expansion of Eq. (1.3) with respect to λH_1 and then solves for E with this approximation the implicit Eq. (1.2).

The situation where H_1 is a semipositive definite operator has been analyzed in some detail,[1] for it can be shown that diagonal Padé approximants (DPA) $F_M(E)$ of $F(E)$ with respect to the positive coupling constant λ generate, when inserted in Eq. (1.2), a monotonic sequence of lower bounds to the exact eigenvalues of H. The purpose of this paper is to investigate whether the kinetic energy K, which is the most natural positive operator one may think of in this problem, can be used as H_1.

Besides the benefits expected from the positivity of H_1 a second motivation of this work is also obvious. The coupling λ is nothing but the square of Planck's constant $\hbar$, and the theory would then provide interesting semiclassical approximations. Actually, it has already been shown[2] that the introduction of DPA in the BW theory provides convergent algorithms with respect to $\hbar$, while direct expansions of energies with respect to $\hbar$ are known[3] to be asymptotic rather than convergent.

Two serious difficulties arise at once, however, when one takes as H_0 the nuclear interaction V, which will be assumed to be a local potential in the following. [Local potentials are in order so that $(E-V)^{-1}$ can be easily calculated.] The first difficulty is that V has a continuous spectrum so that Φ_0, the ground state, is a δ function at the bottom of V. Hence Φ_0 is not square integrable and the projector Q is ill defined. The second difficulty

stems from the fact that E, although it is looked for as a discrete eigenvalue of H, lies in the continuum of V; see Fig. 1. Hence $(E-V)^{-1}$ is singular. Because of these two difficulties, one loses Eq. (1.1).

Section II of this paper shows how a minor modification of V generates a square integrable Φ_0. Section III then shows how Eq. (1.1) can be reinstated, provided E is made complex, and how Eq. (1.2) can be solved. Then Sec. IV introduces the DPA to $F(E)$ and Sec. IV contains a numerical application. Section VI contains a discussion and a conclusion.

II. HOW TO PEEL OFF DISCRETE STATES FROM CONTINUUM

Let $\vec{x}\equiv(\vec{x}_1\ldots\vec{x}_A)$ be the set of nucleon coordinates for the A-nucleon system and $V(\vec{x})$ be the internucleon total interaction. It is now assumed that V has a nondegenerate minimum $V_m<0$ at some point $\vec{\bar{x}}$. Now let $\chi(\vec{x})$ be *any* square integrable wave function. For obvious physical reasons, however, it is desirable that χ be a wave packet localized around $\vec{\bar{x}}$. From now on the unperturbed Hamiltonian will be taken as

$$H_0\equiv V-\mu\,|\chi\rangle\langle\chi|\ , \tag{2.1}$$

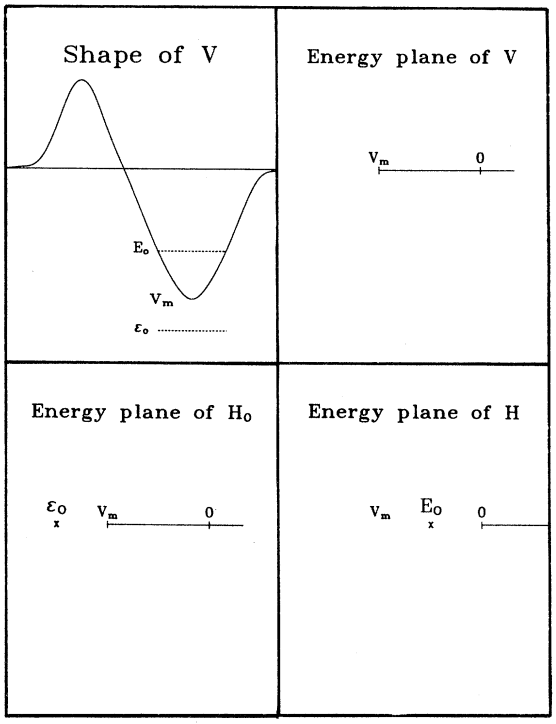

FIG. 1. Spectra of V, H_0, and H. The continuum of V and H_0 is usually at least twofold degenerate.

with μ a positive constant.

There now exists a square integrable eigenstate Φ_0 of H_0. Indeed if

$$[V(\vec{x})-\epsilon_0]\Phi_0(\vec{x})=\mu\chi(\vec{x})\nu\ , \tag{2.2}$$

with

$$\nu\equiv\int d\vec{x}\,\chi^*(\vec{x})\Phi_0(\vec{x})\ , \tag{2.3}$$

then, provided that $\epsilon_0<V_m$, the wave function

$$\Phi_0(\vec{x})=\mu\nu\frac{\chi(\vec{x})}{V(\vec{x})-\epsilon_0} \tag{2.4}$$

is square integrable since the denominator does not vanish either at finite distance or at infinity (again see Fig. 1). The normalization ν is not found by inserting Eq. (2.3) into Eq. (2.4),

$$\nu=\mu\nu\int d\vec{x}\frac{|\chi(\vec{x})|^2}{V(\vec{x})-\epsilon_0} \tag{2.5}$$

for Eq. (2.2) is homogeneous. Rather, Eq. (2.5) is an equation for ϵ_0. Indeed let $I(\epsilon_0)$ be that integral which appears in the right hand side (rhs) of Eq. (2.5). It is trivial that $I(\epsilon_0)$ increases monotonically from 0 to $+\infty$ when ϵ_0 increases from $-\infty$ to V_m. Hence $I(\epsilon_0)$ crosses the value $1/\mu$ once and only once. That value $\epsilon_0(\mu)$ for which $I(\epsilon_0)=\mu^{-1}$ is also obviously a decreasing function of μ. This is confirmed by inspection of Eq. (2.1), where the modification brought to V is obviously attractive. The ground state Φ_0 must then sink when the coefficient μ increases.

If it were necessary to peel off several bound states rather than one, it is trivial to show that the rhs of Eq. (2.1) could be modified by an operator $\sum_i\mu_i\,|\chi_i\rangle\langle\chi_i|$ of rank larger than one. It is also trivial to show that, whatever the modification of *finite* rank, the spectrum of H_0 and that of V retain the same continuum.

These mathematical properties are left as an exercise to the reader and, for practical purposes, the calculation of the Green's function is rather investigated now. In the complex E plane the equation

$$(E-H_0)\,|\xi\rangle=|\phi\rangle\ , \tag{2.6}$$

where ϕ is given and square integrable and ξ is unknown, generates a square integrable ξ except, of course, when E is in the spectrum of H_0. Away from these singularities, the solution of Eq. (2.6) proceeds from

$$[E-V(\vec{x})]\xi(\vec{x})=\phi(\vec{x})-\mu\chi(\vec{x})\nu\ , \tag{2.7}$$

where now

$$\nu \equiv \int d\vec{x}\, \chi^*(\vec{x})\xi(\vec{x}) \,. \tag{2.8}$$

From Eq. (2.7) one obtains

$$\xi(\vec{x}) = \frac{\phi(\vec{x}) - \mu\chi(\vec{x})\nu}{E - V(\vec{x})} \,, \tag{2.9}$$

hence from Eq. (2.8)

$$\nu = \frac{J'(E)}{1+\mu J(E)} \,, \tag{2.10}$$

with

$$J(E) \equiv \int d\vec{x} \frac{\chi^*(\vec{x})\chi(\vec{x})}{E - V(\vec{x})} \,, \tag{2.11}$$

and

$$J'(E) \equiv \int d\vec{x} \frac{\chi^*(\vec{x})\phi(\vec{x})}{E - V(\vec{x})} \,. \tag{2.12}$$

The number ν is finite, for $E \neq \epsilon_0$ where $J(\epsilon_0) = -\mu^{-1}$, and also E is given an imaginary part if ReE in the spectrum of V. A trivial inspection of Eq. (2.9) then shows that ξ is square integrable.

As a result which will be needed in Sec. V, the matrix element $\langle \phi \,|\, (E - H_0)^{-1} \,|\, \phi \rangle$ can then be calculated easily as

$$\langle \phi \,|\, \xi \rangle = J''(E) - \mu \frac{J'(E,\chi^*,\phi)J'(E,\phi^*,\chi)}{1+\mu J(E)} \,, \tag{2.13}$$

where

$$J''(E) = \int d\vec{x} \frac{\phi^*(\vec{x})\phi(\vec{x})}{E - V(\vec{x})} \,. \tag{2.14}$$

To summarize this Section it has been shown that the modification of V, Eq. (2.1), provides two results, (i) a square integrable bound state Φ_0 and (ii) an easily calculable Green's function. Accordingly in the following the perturbation will be

$$H_1 \equiv K + \mu \,|\, \chi \rangle\langle \chi \,| \,, \tag{2.15}$$

a positive and Hermitian operator.

III. BRILLOUIN-WIGNER EQUATION IN THE COMPLEX PLANE

In the usual derivation of the BW theory, Eqs. (1.2) and (1.3) are consequences of Eq. (1.1). One starts from E as an eigenvalue of H and then continues along the real axis. In the present situation where $(E - H_0)^{-1}$ is singular, however, it is suitable to give to E a nonzero imaginary part, disregard Eq. (1.1), and define from the outset $F(E)$ from Eq. (1.3). Then $F(E)$ reads

$$F(E) = \langle \Phi_0 \,|\, \lambda H_1 \,|\, \Psi \rangle \,, \tag{3.1}$$

provided Ψ is defined, as a function of complex E, by

$$|\, \Psi \rangle \equiv \left[1 + \frac{Q}{E - H_0 - \lambda Q H_1 Q} \lambda H_1 \right] \left| \Phi_0 \right\rangle \,. \tag{3.2}$$

The spectrum of $H_0 + \lambda Q H_1 Q$ being real defines Ψ as a square integrable vector as long as Im$E \neq 0$ and $H_1\Phi_0$ is square integrable. A suitable choice of χ, which is a parameter function of the theory, can ensure that $H_1\Phi_0$ be square integrable like Φ_0.

From Eq. (3.2) Ψ obeys

$$(E - H_0 - \lambda H_1)\Psi - \lambda(PH_1P - H_1P - PH_1)\Psi = (E - \epsilon_0 - \lambda PH_1 + \lambda H_1)\Phi_0 \,, \tag{3.3}$$

where $P \equiv |\, \Phi_0 \rangle\langle \Phi_0 \,|$. From Eq. (3.2) one knows that $P\Psi = \Phi_0$, hence Eq. (3.3) boils down to

$$(E - H)\Psi = [E - \epsilon_0 - F(E)]\Phi_0 \,. \tag{3.4}$$

Let E_n be a discrete, isolated eigenvalue of H and let E approach E_n, the vanishing difference $dE = E - E_n$ always retaining an imaginary part. From Eq. (3.4) and a spectral decomposition of H one finds

$$\langle \Phi_0 \,|\, \Psi \rangle = [E - \epsilon_0 - F(E)] \left[\frac{|\langle \Phi_0 \,|\, \Psi_n \rangle|^2}{dE} + \sum_{m \neq n} \frac{|\langle \Phi_0 \,|\, \Psi_m \rangle|^2}{E - E_m} + \int d\epsilon \frac{|\langle \Phi_0 \,|\, \Psi_\epsilon \rangle|^2}{E - \epsilon} \right] \,, \tag{3.5}$$

where one recognizes components on the discrete eigenstate Ψ_n, the other discrete eigenstates Ψ_m, and the continuum eigenstates Ψ_ϵ, respectively. Let ΔE be the distance between E_n and the nearest eigenvalue E_m or ϵ. The sum of the last two terms of Eq. (3.5) can be easily bounded

$$\left| \left\langle \Phi_0 \right| \frac{1 - |\, \Psi_n \rangle\langle \Psi_n \,|}{E - H} \left| \Phi_0 \right\rangle \right| < \frac{1 - |\langle \Phi_0 \,|\, \Psi_n \rangle|^2}{\Delta E - |\, dE \,|} \,, \tag{3.6}$$

hence

$$\lim_{dE\to 0}\frac{E-\epsilon_0-F(E)}{dE}=\frac{1}{|\langle\Phi_0|\Psi_n\rangle|^2}\ , \tag{3.7}$$

where one has taken advantage of the normalization condition $\langle\Phi_0|\Psi\rangle=1$ contained in Eq. (3.2). Hence the quantity $[E-\epsilon_0-F(E)]$ vanishes when E approaches E_n. This result, Eq. (3.7), is of course valid only if $\langle\Phi_0|\Psi_n\rangle\neq 0$, an obvious condition for a perturbation expansion of Ψ_n from Φ_0.

This result, Eq. (3.7), is a justification *ab initio* of the BW equation (1.2). It shows that $F(E)$ can be calculated with nonzero imaginary parts of E, which allows a perturbation expansion of Eq. (1.3)

$$F(E)=\sum_{p=0}^{\infty}\left\langle\Phi_0\left|\lambda H_1\left[\frac{Q}{E-H_0}\lambda H_1\right]^p\right|\Phi_0\right\rangle\ . \tag{3.8}$$

The real solutions of Eq. (1.2) can then be approached from either the upper or the lower energy plane, and one need not use directly the unperturbed propagator $(E-H_0)^{-1}$ on its singularity cut.

To summarize this section, it has been shown that the BW equation can be interpreted in the complex plane, where the individual terms of the perturbation expansion of $F(E)$ are regular. Although the desired solutions E_n of the BW equation are real, they can be conveniently approximated along complex paths.

Further generalizations of the BW equation are possible, because, obviously, $F(E^*)=F^*(E)$. Hence one could consider

$$E-\epsilon_0=F(E^*)\ , \tag{3.9}$$

$$E-\epsilon_0=\mathrm{Re}F(E)\ , \tag{3.10}$$

$$E-\epsilon_0=\alpha F(E)+(1-\alpha)F(E^*)\ , \tag{3.11}$$

or

$$E-\epsilon_0=[F(E)]^{\alpha}[F(E^*)]^{1-\alpha}\ , \tag{3.12}$$

with α an arbitrary constant, and any further combinations of F and F^* which become equivalent to F when E tends towards the real axis. All these equations are equivalent, but they lend to different approximations as will be seen in Sec. IV.

IV. PADÉ APPROXIMANTS TO $F(E)$

As an expansion in powers of the coupling constant λ, the formula, Eq. (3.8), is well known[4,5] to generate convenient Padé approximants. Of special interest are the diagonal ones (DPA), $[N/N]$. For Eq. (3.8) also reads

$$F(E)=\sum_p\left\langle\Phi_0\left|\lambda H_1^{1/2}\left[\lambda H_1^{1/2}\frac{Q}{E-H_0}H_1^{1/2}\right]^p H_1^{1/2}\right|\Phi_0\right\rangle\ , \tag{4.1}$$

where the positivity of H_1 allows the definition of its unique, positive, and Hermitian square root $H_1^{1/2}$. Then, the expansion, Eq. (4.1), sums into

$$F(E)=\left\langle\Phi_0\left|\lambda H_1^{1/2}\left[1-\lambda H_1^{1/2}\frac{Q}{E-H_0}H_1^{1/2}\right]^{-1}H_1^{1/2}\right|\Phi_0\right\rangle\ , \tag{4.2}$$

and appears like a diagonal matrix element of the resolvent of the operator

$$\mathscr{H}\equiv H_1^{1/2}\frac{Q}{E-H_0}H_1^{1/2}\ . \tag{4.3}$$

The $[N/N]$ Padé approximant $F_N(E)$ of $F(E)$ with respect to λ then turns out to be the exact resolvent[4,5] matrix element of the projected operator $\mathscr{H}_N\equiv\mathscr{P}_N\mathscr{H}\mathscr{P}_N$, where $\mathscr{P}_N$ is the projector on the subspace spanned by the vectors $H_1^{1/2}\Phi_0$, $\mathscr{H}H_1^{1/2}\Phi_0,\ldots,\mathscr{H}^{N-1}H^{1/2}\Phi_0$. Again a suitable choice of χ, hence of Φ_0, can ensure that $H_1^{1/2}\Phi_0$ be in the Hilbert space. If $\mathscr{H}$ is a bounded operator, then all vectors $\mathscr{H}^pH_1^{1/2}\Phi_0$ would also be square integrable. Alternately, one would have to further restrict the choice of Φ_0 through χ so that all these vectors remain in the Hilbert space when $p\to\infty$.

This raises the question of the convergence of $\mathscr{P}_N$ towards the identity when $N\to\infty$ and, more important, the question of the convergence of $F_N(E)$ towards $F(E)$. It is known that this convergence occurs when F is a Stieltjes function. In particular, convergence is established when E is real and smaller than V_m. A generalization might also be possible when E is real and lies in the discrete spectrum region of QHQ. Convergence can only be conjectured when E is complex, on the basis of the following argument.

Let the kinetic energy be regularized into a positive bounded range operator as, for instance,

$$K_\eta \equiv \exp(-\eta x^2) K \exp(-\eta x^2) , \tag{4.4}$$

where the parameter η can be taken as small a positive constant as wanted. This modifies H, H_1, and $\mathscr{H}$ into H_η, $H_{1\eta}$, and $\mathscr{H}_\eta$, respectively. It is obvious that this modification yields operator inequalities such as $K_\eta < K$, $H_\eta < H$, and $H_{1\eta} < H_1$. It is also obvious that there is at least a certain amount of weak convergence of the regularized operators towards their original values when $\eta \to 0$. More important, it can be felt that the ground state energy $E_{0\eta}$ of H_η, for instance, converges as a monotonically increasing lower bound towards the ground state energy E_0 of H. As a matter of fact,

$$0 < E_0 - E_{0\eta} < \langle \psi_{0\eta} | (H - H_\eta) | \psi_{0\eta} \rangle , \tag{4.5}$$

from the Rayleigh-Ritz principle applied to H and the normalized ground state $\psi_{0\eta}$ of H_η. Except under pathological conditions, the rhs of inequality (4.5) should vanish when $\eta \to 0$. Indeed, as long as bound states are concerned, the regularization, Eq. (4.4), occurs only at long distances, where only decaying tails are involved. It seems therefore legitimate to apply the theory of Secs. II and III to the search for $E_{0\eta}$, for now $\mathscr{H}_\eta$ is a bounded operator. Indeed $H_{1\eta} = K_\eta + \mu |\chi\rangle\langle\chi|$ is bounded, as a sum of bounded operators. The square root $H_{1\eta}^{1/2}$ is also bounded. Then $\mathscr{H}_\eta$, a product of three bounded operators, is also bounded. The resolvent $(1 - \lambda \mathscr{H}_\eta)^{-1}$ then has a radius of convergence. This is a very favorable feature for the convergence of the DPA.

The regularization can even be sufficient to turn the symmetric (but not Hermitian) operator $\mathscr{H}_\eta$ into a Hilbert-Schmidt operator. For this, the criterion

$$\begin{aligned} \mathrm{Tr} \mathscr{H}_\eta^\dagger \mathscr{H}_\eta = \mu^2 \left| \left\langle \chi \left| \frac{Q}{E - H_0} \right| \chi \right\rangle \right|^2 \\ + 2\mu \, \mathrm{Re} \left\langle \chi \left| \frac{Q}{E - H_0} K_\eta \frac{Q}{E - H_0} \right| \chi \right\rangle \\ + \mathrm{Tr} K_\eta \frac{Q}{E^* - H_0} K_\eta \frac{Q}{E - H_0} < \infty \end{aligned} \tag{4.6}$$

only demands that the last term in the rhs be finite. This is compatible with the finite range induced in K_η by the regularizing factors $\exp(-\eta x^2)$ and any other suitable cutoff in coordinate and momentum space, for instance.

In practice, the regularization is of little importance for low orders of the perturbation expansion such as

$$B_1 \equiv \langle \Phi_0 | H_{1\eta} | \Phi_0 \rangle , \tag{4.7}$$

$$B_2 \equiv \langle \Phi_0 | H_{1\eta} \frac{Q}{E - H_0} H_{1\eta} | \Phi_0 \rangle , \tag{4.8}$$

for only the tail of Φ_0 is concerned by η. A slight influence of η is possible in the next term

$$B_3 \equiv \langle \Phi_0 | H_{1\eta} \frac{Q}{E - H_0} H_{1\eta} \frac{Q}{E - H_0} H_{1\eta} | \Phi_0 \rangle , \tag{4.9}$$

if the propagators $(E - H_0)^{-1}$ are sufficiently nonlocal to carry the short range part of $H_{1\eta}\Phi_0$ into the tail region. Only B_1 and B_2 are needed, however, in the practical example contained in Sec. V, where only the [1/1] Padé approximant is considered.

This first DPA reads

$$F_1(E) = \frac{\lambda B_1^2}{B_1 - \lambda B_2} , \tag{4.10}$$

and it will be noticed that F_1 as a function of E has a cut on the real axis starting from $E = V_m$. Indeed if E is on that cut and one adds or subtracts an infinitesimal imaginary part dE, then B_2 has a cut

$$B_2 = \langle \Phi_0 | H_1 Q \left[\frac{\mathscr{P}}{E - H_0} \pm i\pi \delta(E - H_0) \right] H_1 | \Phi_0 \rangle , \tag{4.11}$$

where $\mathscr{P}$ is the principal part symbol. Except for B_1, a constant, all expansion terms have cuts generated by $(E - H_0)^{-1}$. Hence all the higher DPA, $F_N(E)$, will also have cuts. The point is, $F(E)$ has no cut in this region of the E plane and shows only poles at the discrete eigenvalues of QHQ, as seen from Eq. (1.3). It can be concluded that convergence of $F_N(E)$ towards $F(E)$ when $N \to \infty$ can be checked by the disappearance of the discontinuity of F_N across the cut.

Since F_1 is complex on the real axis, the approximate BW equation

$$E - \epsilon_0 = F_1(E) \tag{4.12}$$

yields, as expected, complex approximations E_{n1} to the real eigenvalues E_n. There is no point in artificially forcing the approximations to be real, from an equation such as

$$E - \epsilon_0 = \mathrm{Re} F_1(E) , \tag{4.13}$$

for one may rather use the Padé approximant to Eq. (3.10). Indeed

$$\mathrm{Re}F(E)=\lambda B_1+\lambda^2\mathrm{Re}B_1+\lambda^3\mathrm{Re}B_3+\cdots\ , \tag{4.14}$$

hence the DPA of order 1 to Eq. (3.10) for E real

$$E-\epsilon_0=\frac{\lambda {B_1}^2}{B_1-\lambda\langle\Phi_0|H_1\mathscr{P}\dfrac{Q}{E-H_0}H_1|\Phi_0\rangle}\ . \tag{4.15}$$

It can be stressed that Eq. (4.15) is more natural than, and differs from, Eq. (4.13). It will also be noticed that, while Eq. (3.10) removes from B_2 the $\delta(E-H_0)$ term, it leaves part of such δ terms (even powers) in B_3, B_4, etc. Hence the DPA of higher order than 1 to Eq. (3.10) depend on more than just $\mathscr{P}/(E-H_0)$.

To summarize this section, there are convenient Padé approximants $F_N(E)$ to $F(E)$ which can be obtained from the perturbation expansion of F with respect to H_1. Convergence is not proved, but likely is $N\to\infty$. These DPA show cut singularities, but nevertheless permit systematic approximations to the BW equation.

V. A NUMERICAL EXAMPLE

One of the simplest cases one may think of is the one-dimensional harmonic oscillator, with $V=x^2$, $K=-(d^2/dx^2)$, and thus spectrum 1, 3, 5, 7, ... The ground state Φ_0 of H_0 is now selected as

$$|\Phi_0\rangle=\frac{1}{\sqrt{2}}(|1\rangle+|0\rangle)\ , \tag{5.1}$$

where $|0\rangle$ and $|1\rangle$ are the first two eigenstates of H. The parameter state χ is adjusted to Φ_0 as $\chi=(V-\epsilon_0)\Phi_0$, hence

$$\chi(x)=(x^2-\epsilon_0)\pi^{-1/4}2^{-1/2}\times(1+2^{1/2}x)\exp\left[-\frac{x^2}{2}\right]\ , \tag{5.2}$$

and $\epsilon_0<0$ is left arbitrary for the time being. One takes μ according to the condition

$$\mu^{-1}=\langle\chi|\Phi_0\rangle=\langle\Phi_0|(V-\epsilon_0)|\Phi_0\rangle=1-\epsilon_0\ , \tag{5.3}$$

hence

$$\mu|\chi\rangle\langle\chi|\Phi_0\rangle=(V-\epsilon_0)|\Phi_0\rangle\ . \tag{5.4}$$

This identifies Φ_0 as the eigenstate of H_0 at eigenvalue ϵ_0. The BW equation also reads

$$E=\left\langle\Phi_0\middle|\left[H+H\frac{Q}{E-QHQ}H\right]\middle|\Phi_0\right\rangle\ , \tag{5.5}$$

and it is trivial to show that QHQ has the same spectrum 5, 7, ... and eigenvectors $|2\rangle$, $|3\rangle$, ... as H, except for the first two eigenvalues, namely (i) 0 for Φ_0 and (ii) 2 for the linear combination orthogonal to Φ_0

$$|\Phi_1\rangle=\frac{1}{\sqrt{2}}(|1\rangle-|0\rangle)\ . \tag{5.6}$$

It is convenient to define

$$|\phi\rangle\equiv H|\Phi_0\rangle$$

$$=\frac{1}{\sqrt{2}}(3|1\rangle+|0\rangle)=2|\Phi_0\rangle+|\Phi_1\rangle\ , \tag{5.7}$$

hence Eq. (5.5) becomes

$$E=2+\frac{1}{E-2} \tag{5.8}$$

with roots $E_0=1$ and $E_1=3$ as expected.

In order to generate the DPA, $F_1(E)$, one first finds the Born term

$$B_1=\langle\Phi_0|K|\Phi_0\rangle+\mu\langle\Phi_0|\chi\rangle\langle\Phi_0|(V-\epsilon_0)|\Phi_0\rangle$$

$$=2-\epsilon_0\ . \tag{5.9}$$

Then the term B_2 also reads

$$B_2=\langle\Phi_0|H\frac{Q}{E-H_0}H|\Phi_0\rangle$$

$$=\langle\phi|(E-H_0)^{-1}|\phi\rangle-\frac{4}{E-\epsilon_0}$$

and one takes advantage of Eq. (2.13) to obtain

$$B=J''-\frac{J'^2}{1-\epsilon_0+J}-\frac{4}{E-\epsilon_0}\ , \tag{5.10}$$

where it is noticed that the wave functions are real, which simplifies J'. It is convenient here to define

$$D_p=\int dx\frac{x^p}{E-x^2}\exp(-x^2)\ , \tag{5.11}$$

which obviously vanishes if p is odd and to notice that

$$\phi(x)=\pi^{-1/4}2^{-1/2}(1+2^{1/2}\cdot 3x)\exp\left[-\frac{x^2}{2}\right]\ . \tag{5.12}$$

From the choice of Φ_0, χ, and according to Eqs. (2.11)–(2.13), J, J', and J'' become

$$J=\langle\Phi_0|(V-E+E-\epsilon_0)(E-V)^{-1}(V-E+E-\epsilon_0)|\Phi_0\rangle=2\epsilon_0-E-1+(E-\epsilon_0)^2\langle\Phi_0|(E-V)^{-1}|\Phi_0\rangle$$
$$=2\epsilon_0-E-1+(E-\epsilon_0)^2\pi^{-1/2}2^{-1}(D_0+2D_2)\,, \tag{5.13}$$
$$J'=\langle\Phi_0|(V-E+E-\epsilon_0)(E-V)^{-1}|\phi\rangle=-2+(E-\epsilon_0)\langle\Phi_0|(E-V)^{-1}|\phi\rangle$$
$$=-2+(E-\epsilon_0)\pi^{-1/2}2^{-1}(D_0+6D_2)\,, \tag{5.14}$$
$$J''=\langle\phi|(E-V)^{-1}|\phi\rangle=\pi^{-1/2}2^{-1}(D_0+18D_2)\,. \tag{5.15}$$

A straightforward, but slightly tedious argument shows that

$$D_0=E^{-1/2}\exp(-E)\times\left[2\pi^{1/2}\int_0^{E^{1/2}}\exp(t^2)dt\mp i\pi\right], \tag{5.16}$$

where the $\mp$ sign is the opposite of that of ImE. It can be checked numerically that a brute force integration of Eq. (5.11) coincides with Eq. (5.16) with a 10^{-3} accuracy if a 1000-point Simson method is used, as long as $\mathrm{Im}E\gg10^{-2}$. A few values of D_0 are listed in Table I. Then one finds

$$D_2=ED_0-\sqrt{\pi}\,. \tag{5.17}$$

Numerical results show that $\mathrm{Im}F_1(E)<0$ when $\mathrm{Im}E>0$. Hence Eq. (4.12) has no solution. It may be replaced, however, by

$$E^*=\epsilon_0+F_1(E)\,, \tag{5.18}$$

in connection with Eq. (3.9). Alternately, an investigation of Eq. (4.15) and of the less justified Eq. (4.13) is in order. The results of these two equations (4.15) (upper curve in the figure) and (4.13) (lower curve) are displayed in Fig. 2. Both equations yield the same approximate root $E_{01}\cong2.65$, and it can be checked numerically that this result is not sensitive to the value of ϵ_0, which was varied from -0.2 to -0.8 in this example. It is interesting to note that Eq. (5.18) has a root in the complex plane, $E'_{01}\cong2.55+0.35i$, the real part of which is in qualitative agreement with E_{01}. It must be noticed, however, that one might have expected a better approximation to the ground state energy $E_0=1$ and that the highly singular nature of the perturbation theory investigated in the present work may have led E_{01} and E'_{01} to approximate the next eigenvalue $E_1=3$ rather than E_0. The question can be solved if one either finds another set of approximate roots E_{11}, E'_{11}, or from the use of the next Padé approximant F_2 and its results E_{02}, E'_{02}. The numerical accuracy of the present example does not provide this information, however.

TABLE I. Numerical values of $D_0(E)$. Imaginary parts are listed below the real parts.

ImE	ReE	0.6	0.9	1.2	1.5	1.8
10^{-5}		2.42	2.02	1.71	1.45	1.25
		−2.23	−1.35	−0.86	−0.57	−0.39
0.05		2.21	1.92	1.64	1.41	1.22
		−2.29	−1.40	−0.91	−0.61	−0.42

A preliminary conclusion provided by the numerical example is therefore that the various approximations deduced from the DPA to the BW equation are coherent, but that the expected convergence, if it exists, is rather slow.

VI. DISCUSSION AND CONCLUSION

There are two main parts in the present work. The first part, Secs. II and III, establishes that the

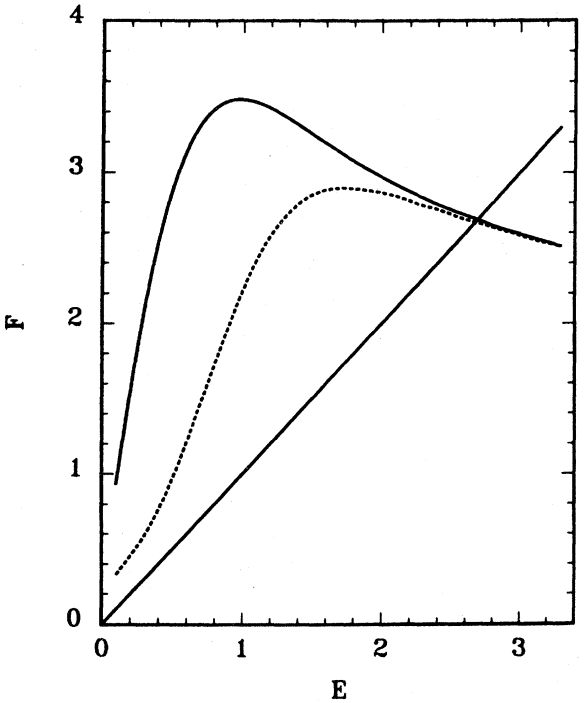

FIG. 2. Solutions of $E=\epsilon_0+[\mathrm{Re}F(E)]_1$ (upper curve) and $E=\epsilon_0+\mathrm{Re}F_1(E)$ (lower curve).

BW equation (i) can be written and (ii) can be solved, even though the bound state energies of H lie in the continuum of H_0. This generalization is achieved by the creation of a normalizable eigenstate of H_0 and by a detour in the complex energy plane. The second part, Secs. IV and V, shows how the positivity of the kinetic energy operator and of the resulting perturbation H_1 allows, at least formally, a reconstruction of the BW functional $F(E)$ by Padé approximants. It was found, however, that this reconstruction could fail to converge rapidly and a further investigation of this reconstruction is needed.

The theory contains a parameter function χ and thus three directions are available for an investigation. Firstly, one may look at whether a variational principle is possible, namely whether the BW roots, or a related functional, are stationary with respect to an optimal choice of χ. Secondly, one should consider higher rank Padé approximants, at least numerically, in order to test the convergence of the DPA reconstruction of $F(E)$. It is known that Padé approximants show variational properties with respect to trial functions, and a connection with an optimal choice of χ may also be in order. Thirdly, if it turns out that the DPA reconstruction fails to converge fast enough, one should attempt to replace $|\chi\rangle\langle\chi|$ by an operator of rank higher than 1, which introduces a parameter subspace in the theory. The outlook for generalizations thus appears to be reasonably wide.

As regards its applicability to the many-body problem, rather than just one particle on one axis, the theory seems to suggest the following line of approach. Because of translation and rotation invariance, the many-body nuclear potential $V(\vec{x})$ has a degenerate minimum V_m and the physical ground state Ψ_0 is also degenerate. But nothing prevents the addition to the physical Hamiltonian of a deformed harmonic oscillator potential

$$V_D=\sum_{i=1}^{A}\sum_{\alpha}\omega_\alpha{}^2 x_{i\alpha}{}^2,\quad \alpha=1,2,3\ , \tag{6.1}$$

which removes the translation and rotation degeneracies and thus makes V_m unique. The total center of mass is then factorized into a deformed Gaussian wave packet, the energy of which is known and can be taken into account at the end.

Then the theory demands multidimensional matrix elements of $(E-V-V_D)^{-1}$, with E complex, which allows Monte Carlo methods without too much of a loss of accuracy.

It is clear, however, that a suitable algorithm must first be found for the reconstruction of $F(E)$, prior to the consideration of the many-body problem. This question is under investigation presently.

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APPENDIX

The purpose of this appendix is to show that, although the nuclear potential looks complicated, the calculations demanded by the theory are straightforward. Three problems arise, namely (i) to find explicitly the ground state of H_0, then (ii) to give an explicit representation of the Green's function $Q(E-H_0)^{-1}$, and (iii) to discuss the influence of the uncertainties which still plague the knowledge of the nuclear interaction.

As a preliminary remark it must be noted that the only calculations which are needed in order to obtain Padé approximants are matrix elements of the form

$$B_p=\langle\Phi_0|H_1[(E-H_0)^{-1}QH_1]^p|\Phi_0\rangle\ . \tag{A1}$$

Furthermore, it is clear that the multiplication of any wave function by QH_1 is a trivial operation, provided this multiplication is numerically carried on with care. Hence the only nontrivial problem of the formalism is to obtain a numerically convenient representation of $(E-H_0)^{-1}$.

For that purpose, as it will now be shown, there is no need to calculate the eigenstates of H_0 if for any given, square integrable $|\phi\rangle$, the equation

$$(E-V-\mu|\chi\rangle\langle\chi|)|\xi\rangle=|\phi\rangle\ , \tag{A2}$$

can be directly solved for $|\xi\rangle$. Indeed, consider for instance the three-body problem for the sake of definiteness, with the potential

$$V(\vec{x})=V_{12}(\vec{x}_{12})S_{12}+V_{23}(\vec{x}_{23})S_{23}+V_{31}(\vec{x}_{31})S_{31}\ , \tag{A3}$$

where, in an obvious notation, $\vec{x}_{ij}$ refers to the relative coordinate of the nucleon pair (ij) and S_{ij} is any relevant "discrete degree of freedom" operator such as the product of spins $\vec{S}_i \cdot \vec{S}_j$ and/or isospins $\vec{T}_i \cdot \vec{T}_j$. Then an expansion of $|\xi\rangle$ and $|\phi\rangle$ into spin and/or isospin channels $|\sigma_1\sigma_2\sigma_3\rangle$ converts Eq. (A2) into the finite set of coupled equations

$$\sum_{\sigma_1'\sigma_2'\sigma_3'} (\sigma_1\sigma_2\sigma_3 | (E-H_0) | \sigma_1'\sigma_2'\sigma_3') \xi_{\sigma_1'\sigma_2'\sigma_3'}(\vec{x}) = \phi_{\sigma_1\sigma_2\sigma_3}(\vec{x}) . \quad \text{(A4)}$$

Each spin-isospin label σ_i takes a finite number of values (2 or 4 for nucleons). With the condensed notation $\sigma \equiv (\sigma_1\sigma_2\sigma_3)$ each matrix element $(\sigma | (E-H_0) | \sigma')$ is a straightforward matrix element, in spin-isospin space only, of $(E-V-\mu | \chi\rangle\langle\chi |)$ and thus becomes of the form

$$\delta_{\sigma\sigma'}[E-V_\sigma(\vec{x})] - W_{\sigma\sigma'}(\vec{x}) - \mu | \chi_\sigma\rangle\langle\chi_{\sigma'} | .$$

Hence Eq. (A4) reads

$$[E-V_\sigma(\vec{x})]\xi_\sigma(\vec{x}) - \sum_{\sigma'} W_{\sigma\sigma'}(\vec{x})\xi_{\sigma'}(\vec{x}) = \phi_\sigma(\vec{x}) + \mu\chi_\sigma(\vec{x})\langle\chi | \xi\rangle . \quad \text{(A5)}$$

For each value of $\nu \equiv \langle\chi | \xi\rangle$, and each value of $\vec{x}$, Eq. (A5) is a set of linear equations for $\xi_\sigma(\vec{x})$, to be solved by standard algorithms. Actually, the left-hand side of Eq. (A5) does not depend on ν and this equation needs only to be solved twice, once with $\phi_\sigma(\vec{x})$ and once with $\chi_\sigma(\vec{x})$ as right-hand sides, respectively. The value of ν can then be adjusted trivially, in the same way as it was with Eq. (2.10).

To summarize this argument, the complications brought by spin and isospin dependence of an otherwise local nuclear interaction do not prevent the Green's function $(E-H_0)^{-1}$ to boil down to numerical inversion of finite matrices. This takes care of problem (ii) listed at the beginning of the Appendix.

As far as problem (iii) is concerned, it is trivial to realize from Eq. (A5), and the very definition of the Green's function $1/(E-H_0)$, that the potential is in the *denominator* of numerical operations. The regions where V suffers some uncertainty are usually regions where V is quite large. It thus makes little difference whether the wave function is a little more or a little less cut by V in these regions, as long as only low orders of the perturbation expansion are concerned.

There remains problem (i), the understanding of eigenstates of H_0. As discussed earlier, only the ground state Φ_0 is actually necessary for the theory and it has been seen in Sec. V after Eq. (5.1) that Φ_0 can be chosen arbitrarily, provided χ is then selected as $\chi = (V-\epsilon_0)\Phi_0$. This allows us to take for Φ_0 an optimized approximation, such as the Hartree-Fock ground state of H, for instance, in order to fasten the convergence of the theory.

If χ were chosen arbitrarily, one could obtain Φ_0 numerically in the following way. Again expanding χ and Φ_0 in "spin-isospin channels," one finds for the Schrödinger equation of H_0:

$$[V_\sigma(\vec{x})-\epsilon_0]\Phi_{0\sigma}(\vec{x}) + \sum_{\sigma'} W_{\sigma\sigma'}(\vec{x})\Phi_{0\sigma'}(\vec{x}) = \mu\chi_\sigma(\vec{x})\nu , \quad \text{(A6)}$$

with again $\nu = \langle\chi | \Phi_0\rangle$. For each value of $\vec{x}$ let $\mathscr{R}_{\sigma\sigma'}(\vec{x})$ be the matrix elements of the inverse of the matrix

$$\mathscr{Y}_{\sigma\sigma'}(\vec{x}) = [V_\sigma(\vec{x})-\epsilon_0]\delta_{\sigma\sigma'} + W_{\sigma\sigma'}(\vec{x}) . \quad \text{(A7)}$$

One obviously finds

$$\Phi_{0\sigma}(\vec{x}) = \mu\nu \sum_{\sigma'} \mathscr{R}_{\sigma\sigma'}(\vec{x})\chi_{\sigma'}(\vec{x}) \quad \text{(A8)}$$

and the eigenvalue ϵ_0 is provided by the condition

$$\nu = \mu\nu \int d\vec{x} \sum_{\sigma\sigma'} \chi^*_\sigma(\vec{x})\mathscr{R}_{\sigma\sigma'}(\vec{x})\chi_{\sigma'}(\vec{x}) . \quad \text{(A9)}$$

Of academic interest are the other eigenstates of H_0, which actually belong to a continuum. It is here convenient to use an eigenchannel representation, namely, for each value of $\vec{x}$ one diagonalizes the (Hermitian) matrix $\mathscr{Y}_{\sigma\sigma'}(\vec{x})$,

$$\sum_{\sigma'} \mathscr{Y}_{\sigma\sigma'}(\vec{x}) y^\tau_{\sigma'}(\vec{x}) = \tau(\vec{x}) y^\tau_\sigma(\vec{x}) . \quad \text{(A10)}$$

The wave functions are now expanded in this representation, for instance

$$\chi(\vec{x}) = \sum_\tau \chi_\tau(\vec{x}) \sum_\sigma y^\tau_\sigma(\vec{x}) | \sigma) . \quad \text{(A11)}$$

The potential is then locally diagonalized and the Schrödinger equation for H_0 reads

$$[\tau(\vec{x})+\epsilon_0-\epsilon]\Phi_\tau(\vec{x}) = \mu\chi_\tau(\vec{x})\nu , \quad \text{(A12)}$$

where the eigencomponents Φ_τ of an eigenstate at energy ϵ are completely decoupled. There is at least one point $\vec{x}_0$ and one eigenchannel τ_0 for which $\epsilon - \epsilon_0 = \tau_0(\vec{x}_0)$, hence

$$\Phi_{\tau_0}(\vec{x})=\delta(\vec{x}-\vec{x}_0)+\frac{\mathscr{P}}{\tau_0(\vec{x})+\epsilon_0-\epsilon}\mu\nu\chi_{\tau_0}(\vec{x}) \tag{A13}$$

in that eigenchannel. In other, "closed" channels, one finds

$$\Phi_{\tau}(x)=\frac{\mu\nu\chi_{\tau}(\vec{x})}{\tau(\vec{x})+\epsilon_0-\epsilon}\ , \tag{A14}$$

and a whole zoology of continuum eigenstates can be developed with a transposition to coordinate representation of the methods traditional in momentum representation for the coupled-channel Lippman-Schwinger equation.

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