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Lower bounds to bound state eigenvalues

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Whenever the residual potential is repulsive the introduction of Padé approximants into the Brillouin-Wigner perturbation expansion generates lower bounds to the exact eigenvalues. The method is extended to perturbation from a subspace and to singular repulsions.

[NUCLEAR STRUCTURE Padé approximants replace the Brillouin-Wigner (BW) equation by an equation whose solutions are lower bounds to the BW solutions.]

I. INTRODUCTION

Atomic or nuclear systems with a finite number N of degrees of freedom are usually described by a Hamiltonian H which is semibounded from below. Most often, the spectrum of that Hamiltonian is made up of a discrete set of eigenvalues $E_0, E_1 \ldots$ and a continuum above them. The ground state energy E_0 is usually nondegenerate. It is relatively easy to get upper bounds to E_0 through a systematic use of the Rayleigh-Ritz variational principle and it may be stressed that such a systematic use provides, theoretically, convergent approximations towards E_0 from above. It is less easy, however, to obtain lower bounds to E_0 in the same systematic way. When H contains only a kinetic energy and a potential with finite depth, a trivial lower bound to E_0 can be related to that depth. More elaborate lower bounds have been proposed in the literature.[1] The purpose of the present paper is to show how the introduction of Padé approximants into the Brillouin-Wigner (BW) perturbation theory may generate, in a special case of broad interest, a convergent sequence of lower bounds to E_0.

The outline of our argument[2] is as follows. First we split H into an easily diagonalizable Hamiltonian H_0, with at least the accurate knowledge of its ground state $|\phi_0\rangle$ and corresponding eigenvalue ϵ_0 which should be nondegenerate, and assume that the residual operator $V = H - H_0$ is *semipositive definite*. Then we introduce a coupling constant $\lambda \geq 0$ and $H(\lambda) \equiv H_0 + \lambda V$ with the corresponding spectrum $E_0(\lambda), E_1(\lambda) \ldots$. The physical situation corresponds to $\lambda = 1$, obviously. The well-known BW implicit equation reads

$$E = \epsilon_0 + F(E, \lambda), \tag{1}$$

where

$$F(E, \lambda) \equiv \left\langle \phi_0 \middle| \lambda V + \lambda V \frac{Q}{E - H_0 - \lambda QVQ} \lambda V \middle| \phi_0 \right\rangle, \tag{2}$$

with

$$Q \equiv 1 - |\phi_0\rangle\langle\phi_0|. \tag{3}$$

As will be discussed below, it turns out that diagonal ($[M/M]$) Padé approximants of $F(E, \lambda)$ with respect to λ may approximate Eq. (1) by

$$E = \epsilon_0 + F_M(E, \lambda), \tag{4}$$

where $F_M < F$. For any solution $E_n(\lambda)$ of Eq. (1) (for a given, fixed value of λ) there exists a solution $E_n(\lambda)$ of Eq. (4) with the property $E_{nM}(\lambda) < E_n(\lambda)$. Lower bounds will thus be obtained.

Furthermore, as will be discussed also, there are cases in which $F_M \to F$ when $M \to \infty$. Then $E_{nM} \to E_n$, or, in other words, we can expect a converging sequence of increasing lower bounds. Together with the Rayleigh-Ritz principle, this opens the way towards rigorous error bars in calculations of the binding energy.

Section II of this paper contains the proofs of several basic properties of $F(E, \lambda)$ which are needed for a rigorous derivation of our argument. Section III describes a numerical application. Section IV is a generalization including matrix[3] Padé approximants and the Bloch-Horowitz[4] method. The case of singular potentials is considered in Sec. V. A discussion and a conclusion are proposed in Sec. VI.

II. BASIC PROPERTIES

For the sake of simplicity, we assume in what follows that the spectrum of H_0 is made, like that of H, of a discrete set $\epsilon_0, \epsilon_1, \epsilon_2 \ldots$, and a continuum above. When V is semipositive definite, it is safe to claim that the discrete eigenvalues $E_0(\lambda)$, $E_1(\lambda), E_2(\lambda) \ldots$ of $H(\lambda)$ and those $\eta_0(\lambda) = \epsilon_0, \eta_1(\lambda)$, $\eta_2(\lambda) \ldots$ of $H_0 + \lambda QVQ$ are larger than, and converge smoothly towards, $\epsilon_0, \epsilon_1, \epsilon_2 \ldots$, respectively, when $\lambda \to 0$. Furthermore, the positivity of V makes all those eigenvalues $E_n(\lambda), \eta_n(\lambda)$ (except η_0,

of course) monotonically increasing functions of λ. Finally, the thresholds for the continuum cannot be lower for $H(\lambda)$ and $H_0+\lambda QVQ$ than that for H_0. We choose the latter threshold as an origin for the energy scale, and restrict our interest, from now on, to negative eigenvalues and energies. The case of positive energies has been considered in an earlier work,[5] where instead of F we actually studied the distorted-wave K matrix.

A. Behavior of $F(E,\lambda)$ with respect to λ

It is easy to derive from Eq. (2) that the partial derivative

$$\frac{\partial F}{\partial \lambda}=\left\langle \phi_0 \middle| \left(1+\lambda V\,\frac{Q}{E-H_0-\lambda QVQ}\right) V \left(1+\frac{Q}{E-H_0-\lambda QVQ}\,\lambda V\right) \middle| \phi_0 \right\rangle, \tag{5}$$

is a non-negative number, because V is non-negative. Besides, when $E<0$, it is clear from Eq. (2) that the only singularities of F are poles, which occur when λ is such that an eigenvalue $\eta_n(\lambda)$, $n\neq 0$, coincides with E. In particular, as long as $E<\epsilon_1$, it is seen that F is regular, because $\eta_n(\lambda)$, $n\neq 0$, remains larger than ϵ_1 when λ takes on all positive values. Conversely, if $\epsilon_p<E<\epsilon_{p+1}$ and the eigenvalues ϵ are nondegenerate, a first pole of F occurs when $\eta_p(\lambda)$ increases as a function of λ and reaches E, a second one occurs when η_{p-1} reaches E, and so on, until λ is large enough to let η_1 coincide with E. These properties of F are schematically pictured in Fig. 1.

B. Behavior of $F(E,\lambda)$ with respect to E

One obtains trivially from Eq. (2) the partial derivative

$$\frac{\partial F}{\partial E}=-\left\langle \phi_0 \middle| \lambda V\,\frac{Q}{(E-H_0-\lambda QVQ)^2}\,\lambda V \middle| \phi_0 \right\rangle, \tag{6}$$

which is obviously a nonpositive number. When the value of λ is kept fixed, F is regular when E takes on all values between $-\infty$ and η_1. Then poles occur as E coincides with η_1, η_2, and so on. This behavior is schematically pictured in Fig. 2.

C. Phase shift and boundary conditions

Although a monotonically increasing function of λ and decreasing function of E, as established in Secs. II A and II B, the function $F(E,\lambda)$ is not very easy to handle because of its poles. It is here convenient to define the phase shift[6]

$$\Delta(E,\lambda)\equiv \arctan F(E,\lambda), \tag{7}$$

which is still a monotonic increasing function of λ and decreasing function of E, because

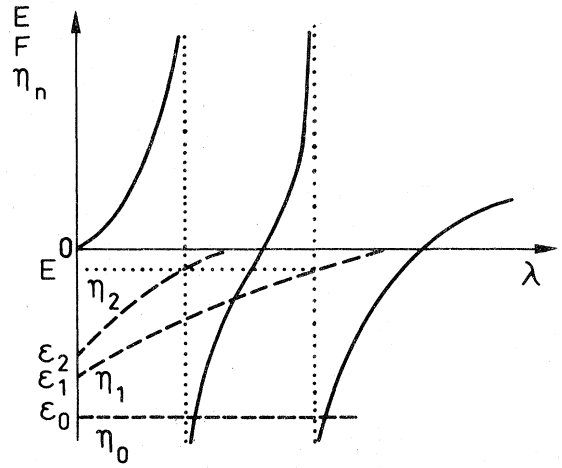

FIG. 1. (Qualitative). The three dashed lines show the behavior of the eigenvalues η_0, η_1, η_2 of $H_0+\lambda QVQ$ as functions of λ. The full line shows F as a function of λ for that fixed value of E shown on the figure. The first vertical dotted line is an asymptote for the full line and corresponds to that value of λ for which $\eta_2=E$. The second vertical dotted line is also an asymptote and corresponds to $\eta_1=E$.

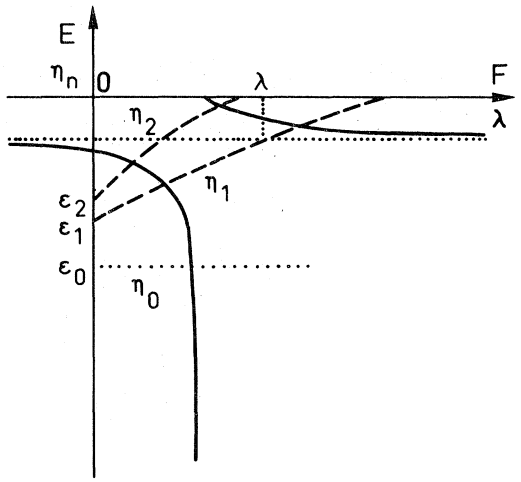

FIG. 2. (Qualitative). The three dashed lines are the same as in Fig. 1. The axis for F is now the same as the λ axis, and the full line shows F as a function of E. The horizontal dotted line is the only asymptote, for only η_1 exists for that value of λ shown on the figure (η_2 has vanished for a smaller value of λ).

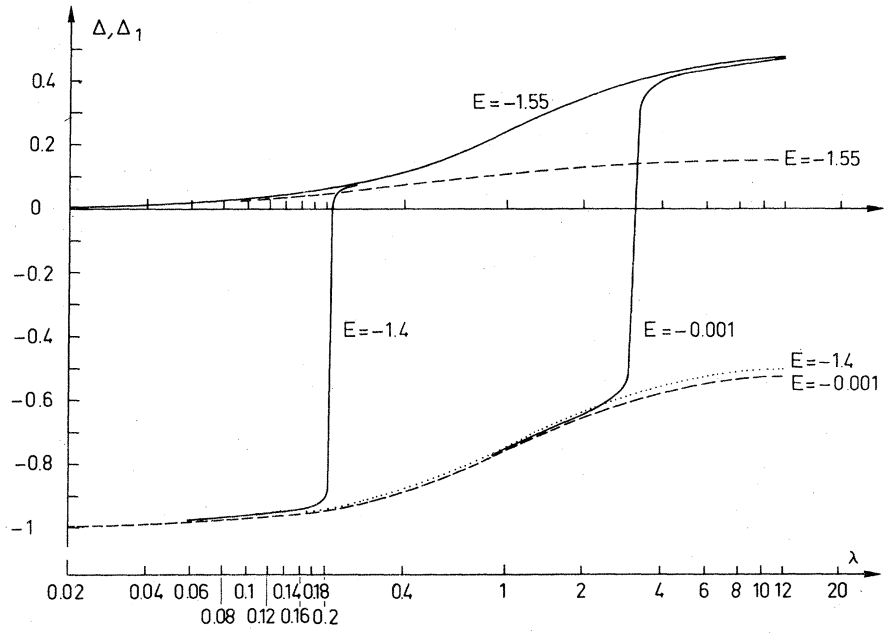

FIG. 3. Δ (full lines) and Δ_1 (dotted or dashed lines) as functions of λ for $E=-1.550$, -1.400, and -0.001. The scale for λ is logarithmic, that for Δ and Δ_1 is in units of π. The full line for $E=-1.4$ is first hardly above that for $E=-0.001$ then jumps near $\lambda=0.206$ and is finally hardly below that for $E=-1.55$. The dotted line for $E=-1.4$ is always below the full line for the same energy, and above the dotted line for $E=-0.001$, which is itself always below the full line for $E=-0.001$.

it is a monotonic increasing function of F. The advantage of Δ is obviously that poles of F are regularized into jumps through $\pi/2$ or some odd number times $\pi/2$.

It is clear from Eq. (2) that $F(E,0)=0$. Thus $\Delta(E,0)$ equals 0 or any integer times π. Besides, we have seen that F is a regular function of λ when $E<\epsilon_1$. It is thus convenient to set $\Delta(E,0)=0$ when

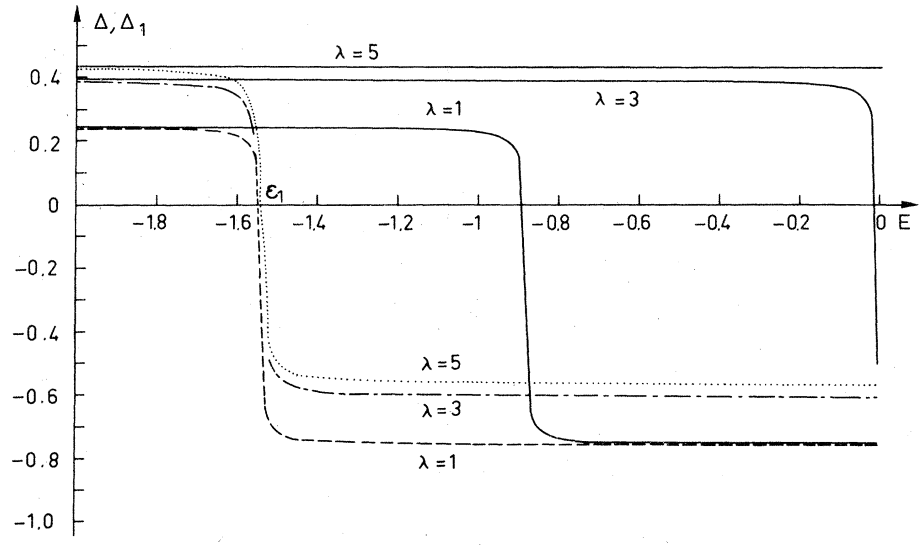

FIG. 4. Δ (full lines) and Δ_1 (dotted or dashed lines) as functions of E for $\lambda=1$, 3, and 5. All curves become practically horizontal when $E<-2$. The scale for Δ and Δ_1 is in units of π. For the sake of simplicity, the curves $\arctan(E-\epsilon_0)$ have not been plotted ($\epsilon_0=-9.184$). Notice how the three curves for Δ_1 cross the E axis at $E=\epsilon_1=-1.544$ and are tangent to one another at that point.

$E < \epsilon_1$. This definition confines $\Delta(E, \lambda)$ to an increase from 0 to $\pi/2$ when λ increases from 0 to $+\infty$. Conversely when $\epsilon_p < E < \epsilon_{p+1}$, we have seen that there are p poles for F as a function of λ. Accordingly, one must set $\Delta(E, 0) = -p\pi$, and Δ increases from $-p\pi$ to $\pi/2$ as λ takes on all values between 0 and $+\infty$.

This choice of boundary conditions makes Δ a smooth function of E and λ (except of course when λ is strictly equal to zero). It can be checked that the plots of Δ versus λ at fixed E, or versus E at fixed λ, fill the whole relevant domain. In other words, there are no "holes" in the plot domain. This situation is illustrated by the numerical example given in Sec. III and by Figs. 3 and 4.

D. Modified implicit equation

Rather than Eq. (1), we now consider the set of equations

$$\text{Arctan}[E - \epsilon_0] - n\pi = \Delta(E, \lambda), \quad n = 0, 1\ldots, \qquad (8)$$

where Arctan here means the principal determination of arctan, namely that confined between $-\pi/2$ and $\pi/2$. The value of λ in Eq. (8) is kept fixed, the left-hand side is an increasing function of E and the right-hand side is a decreasing function of E. For each value of n, there can thus be at most one solution, $E_n(\lambda)$. That solution is also, obviously, a solution of Eq. (1). Therefore the procedure defined by Eq. (8) and that defined by Eq. (1) are equivalent, with the advantage that Eq. (8) contains only regular quantities.

E. Padé approximants to F

Since λV is non-negative, there exists a unique, semipositive-definite square root $(\lambda V)^{1/2}$. Then Eq. (2) also reads

$$F(E, \lambda) = \lambda \left\langle \phi_0 \left| V^{1/2} \left(1 - \lambda V^{1/2} \frac{Q}{E - H_0} V^{1/2}\right)^{-1} \right.\right.$$
$$\left.\left. \times V^{1/2} \right| \phi_0 \right\rangle. \qquad (9)$$

More details on this result, and on the fact that suitable Padé approximants to F can be derived from Eq. (9), can be found for instance in the book of Baker,[7] the work of Bessis *et al.*,[6] or in Ref. 5. The point of interest is that Eq. (9) introduces the operator

$$\mathcal{K} \equiv V^{1/2} \frac{Q}{E - H_0} V^{1/2}, \qquad (10)$$

and that F is nothing but λ times the diagonal matrix element of the resolvent $(1 - \lambda\mathcal{K})^{-1}$ for the vector $|\tilde{\phi}_0\rangle = V^{1/2}|\phi_0\rangle$. A well known result in the theory of Padé approximants is that the $[M - 1/M]$ Padé approximant of such a resolvent matrix element is exactly equal to

$$\langle \tilde{\phi}_0 | (1 - \lambda\mathcal{K}_M)^{-1} | \tilde{\phi}_0 \rangle,$$

where $\mathcal{K}_M$ is the projection of $\mathcal{K}$ on the subspace built upon

$$|\tilde{\phi}_0\rangle, \mathcal{K}|\tilde{\phi}_0\rangle, \ldots \mathcal{K}^{2M-1}|\tilde{\phi}_0\rangle.$$

In other words, that $[M - 1/M]$ approximant to the resolvent matrix element is the *exact* resolvent matrix element of an approximant of $\mathcal{K}$. *In what follows, we consider the* $[M/M]$ *Padé approximants* F_M *of* F *with respect to* λ. Since F derives from the resolvent matrix element

$$\langle \tilde{\phi}_0 | (1 - \lambda\mathcal{K})^{-1} | \tilde{\phi}_0 \rangle$$

by an additional multiplication by λ, it is correct to choose $[M/M]$ approximants of F in order to take advantage of $[M - 1/M]$ approximants for that resolvent matrix element.

As a consequence of these considerations the theory of Padé approximants shows that, whenever $\mathcal{K}$ is positive semidefinite, then $F_{M_1} < F_{M_2}$ if $M_1 < M_2$. This inequality follows because the subspace which defines $\mathcal{K}_{M_2}$ contains the subspace which defines $\mathcal{K}_{M_1}$, and therefore $\mathcal{K}_{M_1} < \mathcal{K}_{M_2}$. Furthermore $\mathcal{K}$ is larger than its projection $\mathcal{K}_M$. Thus $F > F_M$. It is clear that the Padé approximants we have chosen form a convergent and increasing sequence of lower bounds to F. The only condition is that $\mathcal{K}$ be positive semidefinite. It is seen from Eq. (10) that this is true as long as $E < \epsilon_1$.

When $\epsilon_p < E < \epsilon_{p+1}$, one expects from Eq. (10) that the spectrum of $\mathcal{K}$ contains p negative eigenvalues. Because of these negative eigenvalues, inequalities such as $\mathcal{K}_{M_1} < \mathcal{K}_{M_2} < \mathcal{K}$ and $F_{M_1} < F_{M_2} < F$ when $M_1 < M_2$ cannot be claimed any more. We notice by the theory of Padé approximants, however, that the poles of the resolvent matrix elements $\langle \tilde{\phi}_0 | (1 - \lambda\mathcal{K})^{-1} | \tilde{\phi}_0 \rangle$, $\langle \tilde{\phi}_0 | (1 - \lambda\mathcal{K}_M)^{-1} | \tilde{\phi}_0 \rangle$ occur when λ is equal to the inverse of the *positive* eigenvalues of $\mathcal{K}$, respectively to $\mathcal{K}_M$, for we only consider positive values of λ. Furthermore the positive eigenvalues of $\mathcal{K}$ are larger than those of the projection $\mathcal{K}_M$ (in a suitable correspondence between eigenvalues). Accordingly, for each pole of the resolvent of $\mathcal{K}_M$ there exists a pole of the resolvent of $\mathcal{K}$ at a smaller value of λ. (This correspondence does not prevent $\mathcal{K}$ from generating more poles than $\mathcal{K}_M$, at larger values of λ.) In the same way, if $M_1 < M_2$, each of the first M_1 poles generated by $\mathcal{K}_{M_2}$ occurs earlier than the corresponding pole generated by $\mathcal{K}_{M_1}$.

There is a simple way to summarize all these ordering properties. Let us define the phase shift approximants

$$\Delta_M(E,\lambda) \equiv \arctan F_M(E,\lambda), \tag{11}$$

with boundary conditions identical to those described in Sec. II C. Namely, $\Delta_M(E,0) = -p\pi$ if $\epsilon_p < E < \epsilon_{p+1}$. Let us furthermore notice that Δ_M and F_M, like Δ and F, are increasing functions of λ and decreasing functions of E. When $E < \epsilon_1$, we can claim definitely that $\Delta_{M_1} < \Delta_{M_2} < \Delta$ (when $M_1 < M_2$) and that $\Delta_M \to \Delta$ when $M \to \infty$. When $E > \epsilon_1$, we again expect $\Delta_{M_1} < \Delta_{M_2} < \Delta$ (but the numerical example below shows that a fast convergence of Δ_M towards Δ when $M \to \infty$ may be more subtle to predict).

III. PRACTICAL EXAMPLE

A. Technical details

We first show explicitly the [1/1] and [2/2] Padé approximants of F. The Taylor series of F with respect to λ reads

$$F(E,\lambda) = a_1\lambda + a_2\lambda^2 + a_3\lambda^3 + a_4\lambda^4 + \cdots, \tag{12}$$

where the coefficients $a_2, a_3, \ldots$ are functions of E. One readily obtains

$$a_1 = \langle \phi_0 | V | \phi_0 \rangle, \tag{13}$$

$$a_2 = \left\langle \phi_0 \middle| V \frac{Q}{E - H_0} V \middle| \phi_0 \right\rangle, \tag{14}$$

$$a_3 = \left\langle \phi_0 \middle| V \frac{Q}{E - H_0} V \frac{Q}{E - H_0} V \middle| \phi_0 \right\rangle, \tag{15}$$

$$a_4 = \left\langle \phi_0 \middle| V \left(\frac{Q}{E - H_0} V \right)^3 \middle| \phi_0 \right\rangle, \tag{16}$$

and so on. The [1/1] Padé approximant is

$$F_1 = \frac{\lambda a_1^{\,2}}{a_1 - \lambda a_2}. \tag{17}$$

The [2/2] Padé approximant is

$$F_2 = \frac{\lambda b_1 + \lambda^2 b_2}{1 + \lambda c_1 + \lambda^2 c_2}, \tag{18}$$

with

$$b_1 = a_1, \tag{19}$$

$$b_2 = \frac{a_2^{\,3} + a_1^{\,2} a_4 - 2 a_1 a_2 a_3}{a_2^{\,2} - a_1 a_3}, \tag{20}$$

$$c_1 = \frac{a_1 a_4 - a_2 a_3}{a_2^{\,2} - a_1 a_3}, \tag{21}$$

$$c_2 = \frac{a_3^{\,2} - a_2 a_4}{a_2^{\,2} - a_1 a_3}. \tag{22}$$

When ϕ_0 is a Slater determinant and V a two-body interaction, Eqs. (17) and (14) show that the calculation of F_1 demands the computation of two-particle–two-hole diagrams, which is still a calculation of a reasonable size. For F_2, as shown by Eqs. (18) to (22), one needs as much as the three-particle–three-hole diagrams implied by Eq. (16), which is rather unwieldy. It looks difficult to go beyond F_2 at present in a full many-body problem. Actually, we shall even restrict ourselves to F_1 in the simple numerical model below.

Our model is just a one particle problem, with a square well. The unperturbed Hamiltonian H_0 contains a radial kinetic energy operator $-d^2/dr^2$ with a system of units such that $\hbar^2/2m = 1$, and an attractive square well $V_0(r)$ of intensity -12 and range $\pi/2$ in that system. We consider only s waves in ordinary three-dimensional space and radial wave functions $\psi(r)$ which have been multiplied by r, as usual. Therefore $\psi(0) = 0$ when ψ is regular, and the normalization is given by $\int_0^\infty |\psi^2(r)| dr$. It is trivial to check that such a depth and range generate only two bound states, with eigenvalues $\epsilon_0 = -9.184$ and $\epsilon_1 = -1.544$. It is also trivial to express explicitly $\phi_0(r)$ as a sine, then an exponential.

The residual operator V is chosen as a repulsive square well with intensity 1 and the same range $\pi/2$ as V_0. It follows from that choice that the physical values of λ are restricted to $0 < \lambda < 12$.

It is trivial to obtain $a_1 = 0.959$. For the calculation of a_2, Eq. (14), we consider the differential equation

$$\left[E + \frac{d^2}{dr^2} + 12\,\theta\left(\frac{\pi}{2} - r\right) \right] \psi(r) = 0, \tag{23}$$

where θ is the usual step function, and obtain (i) the solution $u(r)$ which is regular at the origin, and (ii) the solution $v(r)$ which decreases exponentially when $r \to \infty$, through straightforward manipulations and matchings of sines, cosines, and exponentials. It is then easy to express $(E - H_0)^{-1}$ by means of the traditional Green's function $u(r<)v(r>)/w$, where w is the suitable Wronskian. The calculation of $(E - H_0)^{-1} Q V | \phi_0 \rangle$ boils down to an integration of that Green's function with $QV|\phi_0\rangle$, an analytical manipulation of sines, cosines, and exponentials again. Finally one tabulates a_2 as a function of E and just inserts the values of λ into the formula for F_1, Eq. (17).

A comparison between F_1 and F, or rather Δ_1 and Δ, is provided by Figs. 3 and 4. For that purpose, we must calculate F. It turns out in the present model that the calculation of F is very analogous to that of a_2. This is because

$$F = \langle \phi_0 | \lambda V | \Psi \rangle, \tag{24}$$

where $|\Psi\rangle$ obeys the equation

$$|\Psi\rangle = |\phi_0\rangle + \frac{Q}{E - H_0} \lambda V |\Psi\rangle, \tag{25}$$

or

$$(E - H_0 - \lambda V)|\Psi\rangle = \mu|\phi_0\rangle , \tag{26}$$

with

$$\mu = E - \epsilon_0 - \langle\phi|\lambda V|\Psi\rangle . \tag{27}$$

Let Ψ_1 be the solution of

$$(E - H_0 - \lambda V)|\Psi_1\rangle = |\phi_0\rangle . \tag{26a}$$

Then $\Psi = \mu\Psi_1$, thus

$$\mu = E - \epsilon_0 - \mu\langle\phi|\lambda V|\Psi_1\rangle , \tag{27a}$$

and finally

$$F = \frac{\lambda\langle\phi_0|V|\Psi_1\rangle(E-\epsilon_0)}{1+\lambda\langle\phi_0|V|\Psi_1\rangle} . \tag{28}$$

To solve Eq. (26a), namely to invert $E - H(\lambda)$, we replace in Eq. (23) the strength 12 by $(12 - \lambda)$, solve for the solutions u and v which are regular at the origin and infinity, respectively, then generate again the Green's function and let it act upon ϕ_0. Calculations are again analytical almost all the way.

B. Dependence on the coupling constants

We have plotted on Fig. 3 the behaviors of Δ and Δ_1 as functions of λ for three values of E, namely -1.550, -1.400, and 0.001. Full lines correspond to Δ, dotted (or dashed) lines to Δ_1. Curves for $-\infty < E < -1.550$ are slightly above those for $E = -1.550$, as expected from Eq. (6), but so close by that they would have been lying on top of each other if they had been plotted. This happens because the Born term $\langle\phi_0|\lambda V|\phi_0\rangle$ is large, for $E < -1.550$, with respect to the contribution to Δ (or Δ_1) of the term with a propagator, such as, e.g.,

$$\langle\phi_0|\lambda V Q(E - H_0 - \lambda QVQ)^{-1}\lambda V|\phi_0\rangle$$

for Δ. When E approaches $\epsilon_1 = -1.544$, Δ and Δ_1 depend much more strongly on the precise value of E. We have checked numerically in great detail that nothing remarkable happens when E approaches $\epsilon_0 = -9.184$. This is not surprising, because the Q projector indeed eliminates the influence of ϵ_0.

For $E = -1.550$, we are still below ϵ_1. No pole for either F or F_1 is expected nor found (actually F_1 has an unphysical pole at a negative value of λ, -0.574) and Δ and Δ_1 increase smoothly between 0 and $\pi/2$. As expected again, $\Delta_1 < \Delta$, and we can claim that further approximants $\Delta_2, \Delta_3 \ldots$ should pile up between Δ_1 and Δ and converge to Δ. Finally, both Δ and Δ_1 do increase when λ increases. For $\lambda = 12$, we find $\Delta = 0.471$ and $\Delta_1 = 0.154$ (in units of π). If we consider the unphysical region $\lambda > 12$, the limits of Δ and Δ_1 when $\lambda \to \infty$ are respectively $\pi/2$ and $\mathrm{Arctan}(-a_1^2/a_2) = \mathrm{Arctan}(0.550)$, with $a_2 = -1.67$ for that value of E.

For $E = -1.400$, which is above ϵ_1, we set $\Delta = \Delta_1 = -\pi$ for $\lambda = 0$, as specified in Sec. II C. Then Δ and Δ_1 increase as functions of λ. A pole for $F(\Delta = -\pi/2)$ occurs for $\lambda = 0.206$, corresponding to a sharp rise of the corresponding curve. Then that curve almost joins (it is actually slightly below) the curve for Δ with $E = -1.550$. While the pole for F occurs at $\lambda = 0.206$, the pole for F_1 occurs, as predicted in Sec. II E, at a larger value of λ (actually much larger), $\lambda = 14.3$. As expected, $\Delta_1 < \Delta$ all the way.

There is nothing abnormal in the fact that for

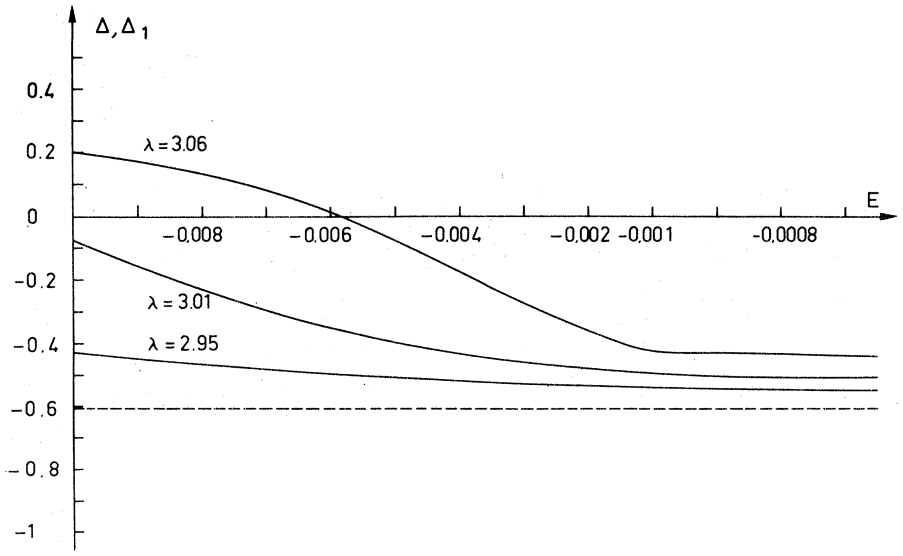

FIG. 5. Δ (full lines) and Δ_1 (dashed line) in units of π near $E = 0$ for $\lambda = 2.96$, 3.01, and 3.06.

$E=-1.400$ the pole of F_1 at $\lambda=14.3$ is beyond the physical range of λ $(0<\lambda<12)$. When E takes on all values between ϵ_1 and -1.400, the position of that pole moves continuously between $\lambda=0$ and $\lambda=14.3$. Simultaneously, the position of the pole of F moves continuously between $\lambda=0$ and $\lambda=0.206$. If for instance $E=-1.450$, the pole for F_1 occurs at $\lambda=9.25$, which is in the physical range, and that for F occurs at $\lambda=0.12$.

For $E=-0.001$, the pole for F occurs at $\lambda=3.01$ and that for F_1 is completely out of the physical range of λ. As ever, $\Delta_1<\Delta$. The fact that E almost vanishes shows that in Figs. 4 and 5, where Δ and Δ_1 are plotted as functions of E with λ as a fixed parameter, no pole for F should be expected when λ exceeds, say, 3.05.

It can be concluded from Fig. 3 that the following properties have been confirmed, namely (i) Δ and Δ_1 are increasing functions of λ and decreasing functions of E, (ii) $\Delta_1<\Delta$, (iii) there are regions for which Δ_1 is a good approximation of Δ, or higher Padé approximants would even converge, and (iv) there are no holes in the domain paved by the Δ curves, nor in that paved by the Δ_1 curves. (It will be noticed, however, that those domains may be quite different. For instance the limiting curve for Δ at $E=\epsilon_1$ is slightly below the curve of Δ for $E=-1.550$, while the limit curve for Δ_1 is just $\Delta_1=0$.)

C. Dependence on the energy

We have plotted on Fig. 3 the dependence of Δ and Δ_1 on E, for three fixed values of λ, namely $\lambda=1$, 3, and 5. When E is smaller than -2, Δ and Δ_1 turn out to depend little on E (in particular, nothing happens at $E=\epsilon_0$) and thus Fig. 4 is restricted to the domain $-2<E<0$. It must be stressed here that the solving of Eq. (8) for $n=0$ [search for the ground state of $H(\lambda)$] consists in taking the intersections of the curves plotted on Fig. 4 with the curve $\mathrm{Arctan}(E-\epsilon_0)$. It turns out that those intersections occur in the region $E<-2$, where Δ_1 is very close to Δ. Indeed, Fig. 4 shows that Δ_1 (dotted lines) deviates from Δ (full lines) only if $E>-1.7$. We can already conclude that the [1/1] Padé approximant provides, in the present special case, a very satisfactory result in the search for $E_0(\lambda)$. Conversely, a poor result can be expected for $E_1(\lambda)$, namely $n=1$ in Eq. (8), for Fig. 4 shows the intersections will occur in a region where Δ_1 and Δ are quite different.

We recall that there exists a critical value of λ, of order 3.05, for which the operator $H_0+\lambda QVQ$ has a vanishing eigenvalue η_1. This is why on Fig. 4 the curves $\lambda=1$ and $\lambda=3.00$ for Δ reach $-\pi/2$, and the last curve $(\lambda=5)$ does not. More details on what happens when E is near zero and λ near 3.05 are found on Fig. 5.

Once again the following properties are confirmed, namely (i) Δ and Δ_1 are decreasing functions of E and increasing functions of λ, (ii) $\Delta_1<\Delta$, (iii) there are regions in which Δ_1 is a good approximation of Δ and where one could expect convergence of higher Padé approximants, and (iv) Δ and Δ_1 are continuous functions of E and λ, except for the limiting curve for $\lambda=0$, where $\Delta=\Delta_1=0$ if $E<\epsilon_1$ and $\Delta=\Delta_1=-\pi$ if $E>\epsilon_1$.

There appears on Fig. 4 a peculiar property of Δ_1, which was not obvious on Fig. 3. Namely, all Δ_1 curves go through zero at $E=\epsilon_1$ and are tangent to one another at that point. Cancellation of F_1, Eq. (17), for $E=\epsilon_1$ occurs because a_2, Eq. (14), diverges at that value of E, while a_1, which is a constant, does not. Let a_2' be the derivative of a_2 with respect to E

$$a_2'=-\left\langle\phi_0\middle|V\frac{Q}{(E-H_0)^2}V\middle|\phi_0\right\rangle\ , \tag{29}$$

and F_1' be the derivative of F_1

$$F_1'=\frac{\lambda^2 a_1^{\,2}a_2'}{(a_1-\lambda a_2)^2}\ . \tag{30}$$

Let $|\phi_1\rangle$ be the eigenstate of H_0 corresponding to ϵ_1 (we have assumed there was no degeneracy, and indeed our model fulfills the condition). The divergence of a_2 at $E=\epsilon_1$ goes like $|\langle\phi_0|V|\phi_1\rangle|^2(E-\epsilon_1)^{-1}$ and that of a_2' like $-\langle\phi_0|V|\phi_1\rangle^2(E-\epsilon_1)^{-2}$. Therefore F_1' has a limit, namely $-a_1^{\,2}\langle\phi_0|V|\phi_1\rangle^{-2}$, *which does not depend on* λ. This is why the Δ_1 curves do not cross one another on Fig. 4 when they all go through zero at the same value of E.

As suggested by the case $\lambda=1$ on Fig. 4 when $E>-0.8$, there are still cases where the first Padé approximant still gives a good result in part of that region $E>\epsilon_1$. It would be interesting to find whether Δ_2 is a much better approximation than Δ_1 and how fast Δ_M would converge.

IV. GENERALIZATION

The undesirable cancellation of F_1 which happens for $E=\epsilon_1$ is obviously prevented for $E=\epsilon_0$ by the projector Q which excludes $|\phi_0\rangle$. It is thus interesting to exclude also $|\phi_1\rangle$ and, more generally, to define the projector

$$Q_L\equiv 1-\sum_{i=0}^{L}|\phi_i\rangle\langle\phi_i|\ , \tag{31}$$

where the $|\phi_i\rangle$'s are the first $L+1$ eigenstates of H_0, and the operator

$$\mathfrak{F}(E,\lambda) \equiv P_L \left(\lambda V + \lambda V \frac{Q_L}{E - H_0 - \lambda Q_L V Q_L} \lambda V \right) P_L , \tag{32}$$

with $P_L \equiv 1 - Q_L$. As long as $E < \epsilon_{L+1}$, no pole can make $\mathfrak{F}$ singular, for $\lambda Q_L V Q_L$ is a non-negative operator.

Let $|\chi\rangle$ be the projection of an eigenstate of $H(\lambda)$ into the subspace spanned by $|\phi_0\rangle, |\phi_1\rangle \cdots |\phi_L\rangle$. Let E be the corresponding eigenvalue of $H(\lambda)$. It is well known[4] that χ obeys the equation

$$E|\chi\rangle = P_L H_0 |\chi\rangle + \mathfrak{F}(E,\lambda)|\chi\rangle , \tag{33}$$

where actually P_L commutes with H_0 and could have been omitted. The point is, E is an eigenvalue of the matrix of dimension $(L+1)$ which represents $H_0 + \mathfrak{F}(E,\lambda)$ (on the basis $|\phi_0\rangle, |\phi_1\rangle, \ldots |\phi_L\rangle$ for instance). When $L = 0$, that matrix reduces to the plain number $\epsilon_0 + F(E,\lambda)$, and we recover Eq. (1).

The Taylor expansion of $\mathfrak{F}$ with respect to λ is

$$\mathfrak{F}(E,\lambda) = \mathfrak{A}_1\lambda + \mathfrak{A}_2\lambda^2 + \mathfrak{A}_3\lambda^3 + \mathfrak{A}_4\lambda^4 + \cdots , \tag{34}$$

where

$$\mathfrak{A}_1 = P_L V P_L , \tag{35}$$

$$\mathfrak{A}_2 = P_L V \frac{Q_L}{E - H_0} V P_L , \tag{36}$$

and more generally

$$\mathfrak{A}_n = P_L V^{1/2} \left(V^{1/2} \frac{Q_L}{E - H_0} V^{1/2} \right)^{n-1} V^{1/2} P_L . \tag{37}$$

Let $\overline{\mathfrak{A}}_n$ be the matrix, of dimension $(L+1)$, which represents $\mathfrak{A}_n$. The [1/1] *matrix Padé approximant*[3] we want to consider is the matrix, again of dimension $(L+1)$,

$$\overline{\mathfrak{F}}_1 = \lambda \overline{\mathfrak{A}}_1 (\overline{\mathfrak{A}}_1 - \lambda \overline{\mathfrak{A}}_2)^{-1} \overline{\mathfrak{A}}_1 , \tag{38}$$

which is clearly a generalization of F_1, Eq. (17). It is as well possible to generalize Eqs. (18) to (22) and define $\overline{\mathfrak{F}}_2$, the [2/2] matrix Padé approximant to $\overline{\mathfrak{F}}$, the matrix which represents exactly $\mathfrak{F}$, and so on for $\overline{\mathfrak{F}}_M$.

For the sake of simplicity, we consider only the region $E < \epsilon_{L+1}$, where no pole for $\overline{\mathfrak{F}}$ or $\overline{\mathfrak{F}}_M$ occurs. It can be shown[3] that the properties of F and F_M studied in Sec. II can be generalized to $\overline{\mathfrak{F}}$ and $\overline{\mathfrak{F}}_M$. In particular, if $M_1 < M_2$, then $\overline{\mathfrak{F}}_{M_1} < \overline{\mathfrak{F}}_{M_2} < \overline{\mathfrak{F}}$. Also $\overline{\mathfrak{F}}_M \to \overline{\mathfrak{F}}$ when $M \to \infty$. (Actually, when $E > \epsilon_{L+1}$, one could also attempt to generalize the use of a phase shift in Sec. II in order to regularize poles, but we do not need this extension here.) The equation

$$\det[(E - \epsilon_i)\delta_{ij} - \overline{\mathfrak{F}}_{M,ij}] = 0 , \tag{39}$$

where det means determinant and $i, j = 0, 1, \ldots L$ refer to the matrix elements of the matrices of dimension $(L+1)$ under consideration, is thus the generalization of Eq. (4). Those out of its solutions which are smaller than ϵ_{L+1} provide lower bounds to the corresponding eigenvalues of $H(\lambda)$.

V. REGULARIZATION OF SINGULAR REPULSIVE POTENTIALS

It happens many times in molecular or nuclear physics that H contains a repulsive two-body interaction which is singular[8] at short distances. Let that singular repulsion be included in V. As in earlier works,[5,6,8] let us cut off V into a regular operator V_ω depending upon a regularization parameter $\omega > 0$ in such a way that (i) $V_\omega \to V$ when $\omega \to +\infty$ and (ii) $dV_\omega/d\omega > 0$. Just to give an example, if V is a local operator, one might take $V_\omega = \theta(\omega - V)$ or, in other words, chop away all parts of V larger than ω. This regularization now defines

$$\mathfrak{F}(E, \lambda, \omega) \equiv P_L \left(\lambda V_\omega + \lambda V_\omega \frac{Q_L}{E - H_0 - \lambda Q_L V_\omega Q_L} \lambda V_\omega \right) P_L , \tag{40}$$

whose derivative with respect to ω is

$$\frac{\partial \mathfrak{F}}{\partial \omega} = P_L \left(1 + \lambda V_\omega \frac{Q_L}{E - H_0 - \lambda Q_L V_\omega Q_L} \right)^{-1} \times \frac{dV_\omega}{d\omega} \left(1 + \frac{Q_L}{E - H_0 - \lambda Q_L V_\omega Q_L} \lambda V_\omega \right)^{-1} P_L , \tag{41}$$

obviously a non-negative operator since $dV_\omega/d\omega$ is a positive operator. Therefore the regularized (ω finite) $\mathfrak{F}$, or the phase shift derived from it, is smaller than its physical limit obtained when $\omega \to \infty$. Again we generate lower bounds, which can be maximized with respect to ω.

VI. DISCUSSION AND CONCLUSION

Throughout Secs. II, IV, and V and with the illustration of Sec. III, we have definitely established an algorithm which provides lower bounds to binding energies. The question is, how practical is that algorithm? Three main difficulties must be faced, namely (i) the complications, and lack of fast convergence, which occur in the "pole region", (ii) the difficulties in obtaining coefficients of the Taylor series of higher order than 2 or 3, at most 4, and (iii) the necessity that the residual Hamiltonian V be non-negative.

The first two difficulties are of a technical nature only. Indeed, as regards the problem of poles, it must be remembered that an *upper* bound E_0^* to E_0 can in principle be obtained through the Rayleigh-Ritz variational principle. It is therefore sufficient

to use the matrix Padé technique with L large enough to ensure $E_0^* < \epsilon_{L+1}$. Then *a fortiori*, $E_0 < \epsilon_{L+1}$, which guarantees that at least the ground state energy is in the no-pole region, where Padé approximants do converge fast to the exact value. As regards the problem of high orders in Taylor coefficients, it must be stressed that the [1/1] matrix Padé approximation becomes exact when $P_L \to 1$. There should be therefore some help in letting L become as large as possible, even larger than needed for the condition $E_0^* < \epsilon_{L+1}$. In case the [1/1] matrix Padé is felt to be insufficient, it is an open problem whether recent methods[9] for the estimation of large orders of the perturbation expansion can be trusted to provide rigorous lower bounds.

The third difficulty is of a physical nature. There can be *a priori* no easy way to split an arbitrary H into an "easy" H_0 and a positive V. Fortunately, such a way exists for an atom, where it is trivial to take for V the repulsion between electrons and for H_0 the sum of the kinetic energy and central attraction. Atomic physics thus appears like a favorable domain for our algorithm.

In nuclear physics, however, it is customary to consider H_0 as the sum of the nucleonic kinetic energy and average Brueckner-Hartree-Fock potential, and V as a residual interaction which contains at least partly attractive two-body forces. The problem is, that sort of nuclear H_0 does not necessarily overbind the nucleus enough to make the residual V a pure repulsion. It can even be noticed that the bare nucleonic two-body interaction has attractive parts, which cannot be overcounted by a centered one-body field when a pair of nucleons cluster far enough from the rest of the nucleus. To avoid this "remote-pair effect" one should restrict all operators to a tricky subspace of many-body wave functions confined near the origin of the centered, one-body average field. This confinement problem might be an interesting line of research. Another would be, in a way completely opposed to tradition, to take as much as possible the nucleonic interaction as H_0 and the kinetic energy as V. Since the nucleonic interaction is believed to be fairly local, short ranged, highly repulsive at short distances, and only attractive at intermediate distances, the structure of $|\phi_0\rangle$ would be glass- or crystal-like. Indeed the α-cluster model has found some success in nuclear physics, at least for light nuclei.[10] Then to use the kinetic energy as a perturbation would be to use $\hbar$ as a coupling constant. Our algorithm would then be related to semiclassical limits.

In a completely different way, one might notice that if V is negative rather than positive, E_0 then becomes smaller than ϵ_0. Thus $(H_0 - E_0)$ is positive, and one can investigate the region $E < \epsilon_0$, where $(H_0 - E)$ is positive. The function

$$F = \left\langle \phi_0 \middle| V - V \frac{Q}{H_0 - E + QVQ} V \middle| \phi_0 \right\rangle \tag{42}$$

also reads

$$F = \left\langle \phi_0 \middle| V - V(H_0 - E)^{-1/2} \frac{Q}{1 + (H_0 - E)^{-1/2} QVQ (H_0 - E)^{-1/2}} (H_0 - E)^{-1/2} V \middle| \phi_0 \right\rangle , \tag{43}$$

a form which is suitable for Padé approximants. It is easy to check, unfortunately, that one obtains easily upper rather than lower bounds.

A last, but not least, open problem is whether the lower bounds which can be extracted from the present application of Padé approximants are saturating bounds, namely proportional to the number N of particles rather than its square or any other power. If those lower bounds turn out to be saturating, it is hoped that the exact eigenvalue carries the same property. It is interesting to note that if one can handle the mathematical difficulties to be expected when using nuclear attraction as H_0 and kinetic energy as V, a glass- or crystal-like structure of ϕ_0 indicates that ϵ_0 is saturating with short range forces (finite number of neighbors involved), provided short range repulsions due to the interaction itself or the Pauli principle prevent that glass or crystal from collapse when N increases. With a (quasi?) local H_0 and a repulsive V, the search of a proof of saturation of nuclear matter is thus (almost?) reduced to a problem of classical mechanics.

It can be concluded that, whether in atomic physics or in nuclear physics, quite a few problems can be investigated from the point of view of the Padé lower bounds to binding energy described in this paper.

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