Effective forces and rigorous variational principles

B. G. Giraud
Service de Physique Théorique, Commissariat à l'Energie Atomique,
Centre d'Etudes Nucléaires de Saclay, Boîte Postale No. 2, F-91191 Gif-sur-Yvette Cédex, France

G. Y. Vichniac
Laboratory for Computer Science, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
(Received 16 October 1984)

The Rayleigh-Ritz variational principle can be modified to generate upper bounds to the exact ground-state energy even when the local repulsive core of a two-body interaction V is replaced by the corresponding T or G matrix calculated for a negative energy $(-\omega)$. One obtains this result by adding a suitable counterterm to the resulting regularized Hamiltonian and selecting ω as an additional variational parameter.

I. INTRODUCTION

The strong repulsion which most often occurs when two nucleons, nuclei, atoms, or ions meet inside their "core" region ($r>a$) can make realistic calculations in nuclear and molecular physics unpractical. Such a strong repulsion is in most cases expressed in terms of a *local* two-body potential $V(r)$ which is singular[1] when the distance r between the two particles vanishes. Out of the core region, the interaction V is usually considered as (bounded) regular and can be either attractive, repulsive, or both. In this paper, we shall concentrate on the repulsive core region (keeping in mind the potential contains enough attraction to generate bound states).

One way to handle the divergent matrix elements due to the singularity of V in the neighborhood of $r=0$ is to use a cutoff procedure in which V is converted into a regularized and still local potential depending on a parameter $\varepsilon>0$ in such a way that $V_\varepsilon \to V$, in some sense, when $\varepsilon \to 0$. One must then study how physical quantities depend on ε, and hopefully converge[2,3] when $\varepsilon \to 0$. It has been shown[4,5] in particular that, when $V(r)$ is a monotonically decreasing function near the origin $r=0$ and V_ε is defined as

$$V_\varepsilon(r)=V(r)\Theta(\varepsilon^{-1}-V(r))+\varepsilon^{-1}\Theta(V(r)-\varepsilon^{-1}) ,$$

where Θ is the usual step function, then the energy $E(\varepsilon)$ of a bound state ψ_ε corresponding to V_ε lies below the energy E of the associated bound state ψ governed by V and that the difference between E and $E(\varepsilon)$ is smaller than proportional to $\varepsilon^{1/2}$. Such a convergence property can obviously be used to reduce a large class of unpractical calculations with repulsively singular, local potentials to easier calculations with finite, local potentials.

There is an important class of problems for which the regularized interaction V_ε of interest is not a local potential deduced from V by a straight cutoff in coordinate space, but is rather related to the *nonlocal* T matrix calculated from V. The regularizing parameter is then the negative energy $-\omega=-\varepsilon^{-1}$ at which that T matrix is calculated. The Brueckner method,[6] where the now traditional G matrix plays the central role of an effective interaction, is probably the best example of that class of problems where the short-range repulsion between particles has been regularized into a nonlocal interaction. Except for the presence of a Pauli operator and an average field in the integral equation which defines the G matrix, there is little difference between the behaviors of $G(-\omega)$ and $T(-\omega)$, which both restore the bare V when $\omega \to \infty$. The purpose of the present paper is to study the corresponding behavior of binding energies as functions of ω.

This work attempts to generalize the results, obtained earlier[4,5] for local potentials, to the case of nonlocal regularizations. We evaluate the derivative of the binding energy, taken as a function of the regularization parameter with respect to that parameter. Furthermore, we suggest that a solution might be available for two traditional problems of the Brueckner method.

(i) By defining the best choice of the regularization parameters or, in other words, by eliminating the ambiguities in the selection of starting energies.

(ii) By relating the method to a rigorous variational principle yielding an upper bound to the ground-state energy. Such a variational principle is in demand. Indeed, whereas Hartree-Fock theory follows from the Rayleigh-Ritz principle, standard Brueckner-Hartree-Fock calculations do not rely on any variational basis, and they have been suspected[7] to induce overbinding.

Preliminary definitions and two basic theorems, one which corresponds to a variational principle, are given in Sec. II. A reduction of the "nonlocal" regularization to a problem with an alternative local potential follows in Sec. III, where the counterterm involved in the variational principle derived in Sec. II is replaced by a simpler, though cruder counterterm. Section IV contains a rigorous upper bound to the counterterm for a two-body bound state, and its generalization for a many-body bound state. These results are discussed in Sec. V with a numerical application, followed by a conclusion in Sec. VI.

II. DEFINITIONS AND BASIC RESULTS

It will first be shown that the T and G matrices, when calculated for a real, negative energy, are operators which decrease monotonically when that energy increases. This statement is actually a special case of a more general result valid for homographic transforms of operators. Let A, B, and Q be, respectively, two Hermitian operators semibounded from below and a projector which commutes with A.

Let $(-\alpha)$ be the smallest of the eigenvalues of AQ and $Q(A+B)Q$. Assuming $-\alpha \leq 0$, if one chooses $\omega > \alpha$, the operators $(\omega+A)Q$ and $(\omega+A+QB)Q$ are positive semidefinite and can be inverted in the subspace conserved by Q. The implicit equation

$$C(-\omega)=B-B(\omega+A)^{-1}QC(-\omega) \tag{1}$$

reduces to

$$C(-\omega)=B-B(\omega+A+QBQ)^{-1}QB\ . \tag{2}$$

A simple differentiation of Eq. (2) with respect to $(-\omega)$ yields

$$\frac{dC(-\omega)}{d(-\omega)}=-B(\omega+A+QBQ)^{-2}QB\ . \tag{3}$$

The right-hand side being a negative semidefinite operator, we have the following.

Theorem I:

$$\frac{dC(-\omega)}{d(-\omega)}<0\ ,$$

which means that C decreases monotonically when $-\omega$ increases from $-\infty$ to $-\alpha$.

For the two-body problem, C is readily identified with the T matrix when Q, A, and B are 1, t_r, and V, respectively the unit and the relative kinetic and potential energy operators. If Q excludes occupied single-particle states, if furthermore $A=t_i+t_j+U_i+U_j$ consists of the total kinetic energy and one-body average potentials, and if $B=V_{ij}$ is the interaction of the particle pair (ij), then C becomes the G matrix for that pair [see below, Eqs. (1′) and (2′)]. (In the following the potentials U_i are understood to be energy independent.)

Theorem I extends to many-body operators whenever they are defined by equations analogous to Eqs. (1) and (2). [Effective operators in the Bloch-Horowitz[8] theory fall into this category. In that case, theorem I expresses the fact that an effective Hamiltonian defined for the ground-state energy is more attractive (in the operator sense) than the Hamiltonian defined for an excited state, provided that no pole of the relevant propagator has been passed in the meantime.] Theorem I applies to our main concern here, the system of N particles governed by the "effective" Hamiltonian

$$H(\boldsymbol{\omega})=\sum_{i=1}^{N}t_i+\sum_{\substack{i,j=1\\ i>j}}^{N}G_{ij}(-\omega_{ij})\ , \tag{4}$$

which contains the usual single-particle kinetic energy operators t_i and an effective two-body interaction made out of G matrices, which are denoted here

$$G_{ij}(-\omega_{ij})=V_{ij}-V_{ij}(\omega_{ij}+t_i+t_j+U_i+U_j)^{-1}QG_{ij}(-\omega_{ij}), \tag{1′}$$

or

$$G_{ij}(-\omega_{ij})=V_{ij}-V_{ij}(\omega_{ij}+t_i+t_j+U_i+U_j+QV_{ij}Q)^{-1}QV_{ij}\ . \tag{2′}$$

The energies $(-\boldsymbol{\omega})\equiv\{-\omega_{ij}\}$ at which the G matrices are calculated may or may not depend on the pairs under consideration. If one chooses N single-particle parameters ω_i and defines $\omega_{ij}=\omega_i+\omega_j$, then $H(\boldsymbol{\omega})$ depends on N parameters rather than $N(N-1)/2$. Whatever the number of independent parameters ω, it is clear from theorem I that $H(\boldsymbol{\omega})$, as an operator, is a monotonic function of each of them. Any discrete eigenvalue $E(\boldsymbol{\omega})$ of $H(\boldsymbol{\omega})$ is therefore also a monotonic function. The limit of $H(\boldsymbol{\omega})$ when all parameters ω_{ij} tend towards $+\infty$ is the "bare" Hamiltonian

$$H=\sum_{i=1}^{N}t_i+\sum_{\substack{i,j=1\\ i>j}}^{N}V_{ij}\ . \tag{5}$$

For the sake of simplicity we will now assume that the N particles described by $H(\boldsymbol{\omega})$ are distinct. (The case of identical fermions will be discussed later.) As a further simplification, it will be assumed in the following that $\omega_{ij}=\Omega_{ij}\varepsilon^{-1}$, where the set of parameters $\Omega_{ij}>0$ has been chosen in advance and only one variable parameter $\varepsilon>0$ is left. As discussed in more detail in Appendix A, the values allowed to ε are restricted to a finite domain, $0<\varepsilon<\varepsilon_M$. The first condition which defines that domain is that each parameter ω_{ij} must be larger than the positive number α_{ij} which was associated, at the beginning of the present section, to the lowest eigenvalue of $Q(t_i+t_j+U_i+U_j+V_{ij})Q$. Additional conditions will be formulated below.

Henceforth, we will write $H(\boldsymbol{\omega})$ as $H(\varepsilon)$, an operator depending only on one variable parameter ε. A trivial use of theorem I shows that $H(\varepsilon)$ and any of its discrete eigenvalues $E(\varepsilon)$ decrease when ε increases from 0 to ε_M. If one follows the behavior of an eigenstate ψ_ε of $H(\varepsilon)$, the corresponding eigenvalue $E(\varepsilon)$ can be expected to converge smoothly[2,3] when $\varepsilon\to 0$, towards the corresponding eigenvalue E of the limit Hamiltonian H defined by Eq. (5). This statement reads

$$E=E(\varepsilon)+\int_0^\varepsilon d\varepsilon'\left[-\frac{dE(\varepsilon')}{d\varepsilon'}\right]\ , \tag{6}$$

where it can be noticed that the derivative $dE/d\varepsilon$ is negative.

Let $M(\varepsilon)$ be an integrable upper bound of $(-dE/d\varepsilon)$ and define the integral

$$F(\varepsilon)=\int_0^\varepsilon d\varepsilon' M(\varepsilon')\ . \tag{7}$$

It is clear that $F(\varepsilon)$ is larger than the integral in the right-hand side of Eq. (6), and thus

$$E<E(\varepsilon)+F(\varepsilon)\ . \tag{8}$$

Since $F(\varepsilon)$ vanishes when $\varepsilon\to 0$, one obtains E as a lower limit

$$E=\inf_{\varepsilon}\{E(\varepsilon)+F(\varepsilon)\} . \tag{9}$$

As discussed in a previous work,[4] such a lower-limit property, Eq. (9), is very convenient, for $E(\varepsilon)$ is also a lower limit when ψ_ε is the ground state. Indeed, if ϕ is an arbitrary trial function normalized to unity, $\langle\phi\,|\,\phi\rangle=1$, the Rayleigh-Ritz variational principle reads, for the ground-state energy,

$$E(\varepsilon)=\inf_{\phi}\{\langle\phi\,|\,H(\varepsilon)\,|\,\phi\rangle\} \tag{10}$$

which gives, upon insertion of Eq. (10) into Eq. (9), the following.

Theorem II:

$$E=\inf_{\varepsilon,\phi}\{\langle\phi\,|\,H(\varepsilon)\,|\,\phi\rangle+F(\varepsilon)\} . \tag{11}$$

This result, Eq. (11), means that ε, or the energies ω_{ij}, can be treated as variational parameters as well as the trial function, provided a suitable counterterm is added to the Hamiltonian. One must minimize with respect to both ε and ϕ the sum of the expectation value of $H(\varepsilon)$ and that counterterm $F(\varepsilon)$. It is obvious from Eq. (11) that this variational principle yields an upper bound to the exact eigenvalue. No overbinding need be feared.

If furthermore $M(\varepsilon)$ were exactly equal to $(-dE/d\varepsilon)$ and if ϕ is restricted to products of single-particle wave functions, one might claim that the energies ω_{ij} for which the lowest minimum of the right-hand side of Eq. (11) is reached are thus uniquely defined and are the proper parameters to be used in a Brueckner-Hartree theory.

Actually, as shown in the following sections, the derivative $(-dE/d\varepsilon)$ is not easily estimated. Practical numerical results depend, hopefully slightly, on the details of the chosen $M(\varepsilon)$. Theorem II remains valid, nonetheless.

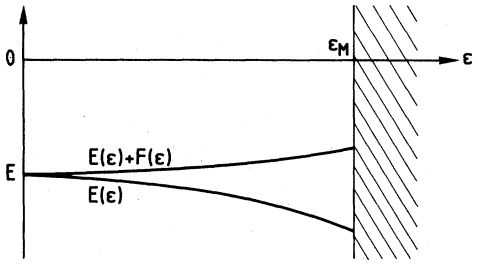

FIG. 1. Variations with respect to the regularization parameter ε of the energy $E(\varepsilon)$ and of energy augmented by the counterterm $E(\varepsilon)+F(\varepsilon)$. Parameter ε varies between zero (where the exact eigenvalue E is reached) and a maximum allowed value ε_M (see Appendix A).

Figure 1 illustrates this variational principle.

Finally, one may stress that both theorems I and II are valid for a large class of potentials V_{ij}. Except for the restriction that those potentials must be semibounded from below ($V_{ij}>-\beta_{ij}$, $\forall ij$, with β_{ij} a sufficiently large positive number to allow for bound states) they can be regular or irregular, as well as local or nonlocal.

III. AN ALTERNATIVE POTENTIAL

The main quantity under study in this paper is the *rate* of convergence of $E(\varepsilon)$ (convergence itself has been proved[2,3]). Stipulating that the normalization of any discrete eigenstate is kept fixed when ε varies, $\langle\psi_\varepsilon\,|\,\psi_\varepsilon\rangle=1$, one obtains that rate from Eqs. (3) and (4) with the parametrization $\omega_{ij}=\Omega_{ij}\varepsilon^{-1}$

$$-\frac{dE}{d\varepsilon}=\sum_{\substack{i,j=1\\ i>j}}^{N}\Omega_{ij}\langle\psi_\varepsilon\,|\,V_{ij}[\Omega_{ij}+\varepsilon(t_i+t_j+U_i+U_j+QV_{ij}Q)]^{-2}QV_{ij}\,|\,\psi_\varepsilon\rangle . \tag{12}$$

Since the presence of (squared) nonlocal propagators and projectors makes the task of finding an upper bound for the right-hand side of Eq. (12) difficult, let us consider a simpler Hamiltonian where neither the differential operator t nor Q appear in a propagator

$$\mathscr{H}(\varepsilon)=\sum_{i=1}^{N}t_i+\sum_{\substack{i,j=1\\ i>j}}^{N}\omega_{ij}(\varepsilon) . \tag{13}$$

To be acceptable, $\mathscr{H}(\varepsilon)$ must fulfill the following three conditions: (i) $\mathscr{H}(\varepsilon)$ must reduce to H when $\varepsilon\to 0$, (ii) the matrix elements generated by $d\omega_{ij}/d\varepsilon$ must be easier to calculate than those found in Eq. (12), and (iii) the discrete eigenvalues $\mathscr{E}(\varepsilon)$ of $\mathscr{H}(\varepsilon)$ when ε varies in its domain $0<\varepsilon<\varepsilon_M$ must be smaller than the corresponding eigenvalues $E(\varepsilon)$.

Condition (i) may be expressed by

$$E=\mathscr{E}(\varepsilon)-\int_0^{\varepsilon}d\varepsilon'\frac{d\mathscr{E}(\varepsilon')}{d\varepsilon'} . \tag{6'}$$

Condition (ii) means that an upper bound $\mathscr{M}(\varepsilon)$ for the modulus of the derivative $d\mathscr{E}/d\varepsilon$ can be easily found, hence a counterterm

$$\mathscr{F}(\varepsilon)=\int_0^{\varepsilon}d\varepsilon'\mathscr{M}(\varepsilon') . \tag{7'}$$

In the same way as Eq. (8) one obtains

$$E<\mathscr{E}(\varepsilon)+\mathscr{F}(\varepsilon) , \tag{8'}$$

which becomes, under condition (iii), the following.

Theorem III:

$$E<E(\varepsilon)+\mathscr{F}(\varepsilon) . \tag{8''}$$

The alternative Hamiltonian $\mathscr{H}(\varepsilon)$ which fulfills the above three conditions provides us with counterterm $\mathscr{F}(\varepsilon)$ which can replace the previous counterterm $F(\varepsilon)$. This result is illustrated in Fig. 2.

In order to construct a projector-free ω, let us introduce a variable "pseudoprojector"

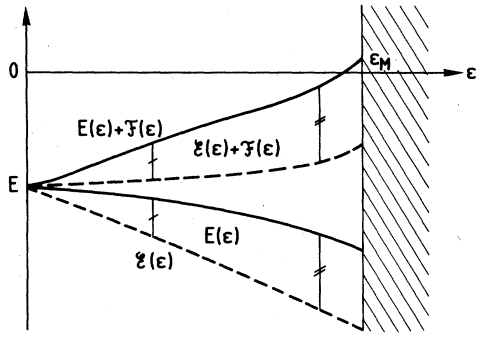

FIG. 2. Same as Fig. 1. Script letters indicate quantities calculated with the alternative potential ω.

$$Q(\lambda)=Q+\lambda(1-Q),\quad 0\leq\lambda\leq 1\ . \tag{14}$$

When $\lambda\to 0$, $Q(\lambda)$ reduces to Q and when $\lambda\to 1$, Q obviously becomes the unit operator. Except for those limiting cases, $Q(\lambda)$ is not a projector, but still remains a positive-definite operator. Actually, $Q(\lambda)$ suppresses the Pauli blocking in a progressive way in

$$\mathcal{G}_{ij}(-\Omega_{ij}\varepsilon^{-1},\lambda)=V_{ij}-V_{ij}(\Omega_{ij}\varepsilon^{-1}+t_i+t_j+U_i+U_j)^{-1}\times Q(\lambda)\mathcal{G}_{ij}(-\Omega_{ij}\varepsilon^{-1},\lambda)\ . \tag{1''}$$

In order to prove that $\mathcal{G}_{ij}$ is a decreasing function of λ, let us notice that $Q(\lambda)$ commutes, whatever the value of λ, with the propagator of Eq. (1''), which is assumed to commute with $Q=Q(0)$. In order to avoid difficulties with new propagator poles, it is then convenient to limit the domain of ε, so that all the operators

$$\{\Omega_{ij}\varepsilon^{-1}+t_i+t_j+U_i+U_j+[Q(\lambda)]^{1/2}V_{ij}[Q(\lambda)]^{1/2}\}$$

remain positive definite when λ varies from 0 to 1. The solution of Eq. (1'') is then

$$\mathcal{G}_{ij}(-\Omega_{ij}\varepsilon^{-1},\lambda)=V_{ij}-V_{ij}[Q(\lambda)]^{1/2}\{\Omega_{ij}\varepsilon^{-1}+t_i+t_j+U_i+U_j+[Q(\lambda)]^{1/2}V_{ij}[Q(\lambda)]^{1/2}\}^{-1}\times[Q(\lambda)]^{1/2}V_{ij}\ . \tag{2''}$$

A straightforward manipulation of Eq. (1'') gives

$$\frac{d\mathcal{G}_{ij}}{d\lambda}=-\mathcal{G}_{ij}(1-Q)^{1/2}(\Omega_{ij}\varepsilon^{-1}+t_i+t_j+U_i+U_j)^{-1}\times(1-Q)^{1/2}\mathcal{G}_{ij}\ , \tag{15}$$

where the right-hand side is a negative semidefinite operator for an appropriate domain of ε (see Appendix A). The operator $\mathcal{G}_{ij}$ which is obtained for $\lambda=1$ thus defines an effective interaction W_{ij} which is a smaller operator than that obtained for $\lambda=0$, namely G_{ij} itself. Now W_{ij} is obviously simpler. It reads

$$W_{ij}(\varepsilon)=V_{ij}-V_{ij}(\Omega_{ij}\varepsilon^{-1}+t_i+t_j+U_i+U_j+V_{ij})^{-1}V_{ij}\ . \tag{16}$$

The potential W_{ij} is projector-free, but still nonlocal, because of the presence of the derivative operator t_i+t_j in the propagator of Eq. (16). But, for an appropriate domain of ε (see Appendix A), the operator $(\Omega_{ij}\varepsilon^{-1}-\gamma_i-\gamma_j+V_{ij})$ is positive and smaller than the operator $(\Omega_{ij}\varepsilon^{-1}+t_i+t_j+U_i+U_j+V_{ij})$ where $(-\gamma_k)$ denotes the lowest eigenvalue of the single-particle Hamiltonian T_k+U_k (usually $\gamma_k>0$). Thus the operator

$$\omega_{ij}(\varepsilon)=V_{ij}-V_{ij}(\Omega_{ij}\varepsilon^{-1}-\gamma_i-\gamma_j+V_{ij})^{-1}V_{ij} \tag{17}$$

is smaller than W_{ij}, and *a fortiori* smaller than G_{ij}. The preceding equation can also be written, with $\gamma=\gamma_i+\gamma_j$,

$$\omega(\varepsilon,r)=\frac{V(r)}{1+\eta V(r)}\quad\text{with}\ \eta=\frac{\varepsilon}{\Omega-\varepsilon\gamma}\ , \tag{17'}$$

where η is small, not very different from $\omega^{-1}=\Omega^{-1}\varepsilon$. As mentioned above, a major advantage of the potential $\omega_{ij}(\varepsilon)$ defined by Eq. (17) is that it is local whenever V_{ij} is local, which is the most frequent practical case. It is easy to check that the three conditions which were required from $\mathcal{H}(\varepsilon)$ defined by Eq. (13) are now satisfied. Indeed (i) when $\varepsilon\to 0$, then $\omega_{ij}(\varepsilon)\to V_{ij}$ and thus $\mathcal{H}(\varepsilon)\to H$, (ii) the derivative of $\omega_{ij}(\varepsilon)$ with respect to ε is

$$\frac{d\omega_{ij}}{d\varepsilon}=-\frac{\Omega_{ij}}{(\Omega_{ij}-\varepsilon\gamma_i-\varepsilon\gamma_j)^2}[\omega_{ij}(\varepsilon)]^2\ , \tag{18}$$

which is simple enough since it is proportional to the square of that potential, and finally, (iii) since $\omega_{ij}(\varepsilon)$ is smaller than $W_{ij}(\varepsilon)$ which is itself smaller than $G_{ij}(-\Omega_{ij}\epsilon^{-1})$, then $\mathcal{H}(\epsilon)$ is smaller than $H(\varepsilon)$. For any discrete eigenvalue $E(\varepsilon)$ labeling a bound state of $H(\varepsilon)$ there exists therefore a smaller eigenvalue $\mathcal{E}(\varepsilon)$ and a corresponding bound state of $\mathcal{H}(\varepsilon)$ and both $\mathcal{E}(\varepsilon)$ and $E(\varepsilon)$ have the same limit E when $\varepsilon\to 0$. For the sake of simplicity it may be assumed that degeneracies in the spectra of $\mathcal{H}(\varepsilon)$ and $H(\varepsilon)$ may be discarded.

In summary, it has thus been shown that the counterterm demanded by the variational principle established in Sec. II can be derived from the simpler effective potential defined by Eq. (17). The purpose of Sec. IV is to give an estimate of the matrix elements deduced from Eq. (18). Since in most cases V_{ij} is local, while neither $G_{ij}(\varepsilon)$ nor $W_{ij}(\varepsilon)$ are, it must be stressed again that $\omega_{ij}(\varepsilon)$ is local. The search for a counterterm has thus been reduced to a problem with local potentials.

IV. AN UPPER BOUND FOR THE COUNTERTERM

Let us introduce the numbers (see Fig. 3)

$$0<a''<a'<a$$

which define four regions for ω. The value of a'' is chosen so that for the innermost region ($r<a''$) ω is smoothed whereas for $a''<r<a'$ ω varies like V. Then, a' is defined such that $V(a')$ has a "moderate" value (40 MeV for nucleons), and a is the innermost point where V vanishes. Let Ξ_ε be the eigenstate of $\mathcal{H}(\varepsilon)$ corresponding to $\mathcal{E}(\varepsilon)$. If the normalization of Ξ_ε is always kept equal to 1, the derivative of $\mathcal{E}(\varepsilon)$ is

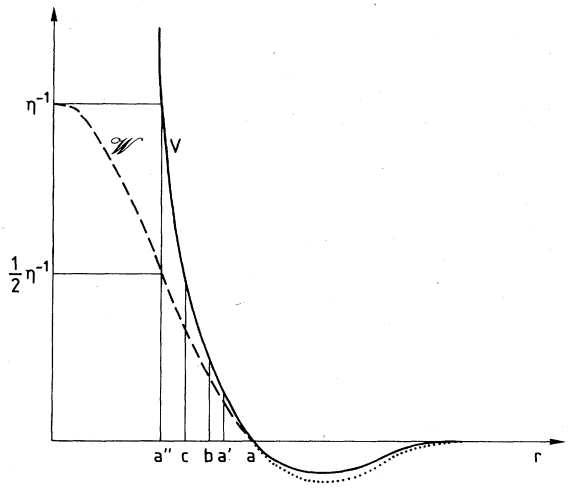

FIG. 3. Behavior of the exact (V) and regularized (ω) potentials. In Sec. V, a potential built from ω for $r<a'$ and from V for $r>a'$ is used.

$$\frac{d\mathscr{E}(\varepsilon)}{d\varepsilon}=-\sum_{\substack{i,j=1\\ i>j}}^{N}\frac{\Omega_{ij}}{(\Omega_{ij}-\varepsilon\gamma_i-\varepsilon\gamma_j)^2}\langle\Xi_\varepsilon|[\omega_{ij}(\varepsilon)]^2|\Xi_\varepsilon\rangle\ . \tag{12'}$$

To derive an upper bound to the counterterm as well as to the expectation value $\langle\omega^2\rangle$ in Eq. (12') one can use the fact that $|\omega|$ is bounded for $r>a$ and that $|\Xi_\varepsilon|$ is bounded in a specific way for $r<a$. [The reader who is not interested in mathematical details can skip to the paragraph following Eq. (42).] If we restrict ourselves to local potentials V_{ij} the contribution of the outer region ($r>a$) is easy to control, since in most practical cases, as that shown by Fig. 3, the modulus of V_{ij} in the outer region is smaller than the maximum depth β_{ij} of the attractive part. It is then simple to adjust the domain available for ε in such a way that the modulus of $\omega_{ij}(\varepsilon)$ remains smaller, in the outer region, than $\mu\beta_{ij}$, where μ is a suitable coefficient larger than 1. [See condition (iv) in Appendix A.] The contribution of the outer region to the matrix element $\langle\omega_{ij}^2\rangle$ will then always be smaller than $\mu^2\beta_{ij}^2$.

In order to study the contribution of the core region, one may first consider the two-body problem with spinless particles in a relative s wave. In a system of units where $\hbar^2/2m=1$, with m as the relative mass, the radial Schrödinger equation reads

$$\xi_\varepsilon''(r)=[\omega(\varepsilon,r)-\mathscr{E}(\varepsilon)]\xi_\varepsilon(r)\ , \tag{19}$$

where ξ_ε is defined, as usual, by a multiplication of Ξ_ε by r. What follows now consists in finding an upper bound for $\xi_\varepsilon^2(r)$ in the core region.

As shown by Fig. 3, there are two parts in ω in the core region ($r<a'$), namely (i) a smoothed part ($0<r<a''$), corresponding to the case when $V(r)>\eta^{-1}$, hence $\frac{1}{2}\eta^{-1}<\omega(\varepsilon,r)<\eta^{-1}$, and (ii) a steep part ($a''<r<a'$) corresponding to the case when $V(r)<\eta^{-1}$ and where $\omega(\varepsilon,r)$ is only a little smaller than $V(r)$.

Since $V(r)$ is assumed to be positive in the core region, $\omega(\varepsilon,r)$ is also positive there, and *a fortiori* $[\omega(\varepsilon,r)-\mathscr{E}(\varepsilon)]$ is positive when $\mathscr{E}(\varepsilon)$ is negative. One may thus choose $\xi_\varepsilon(r)$ as real and positive in the core region because its second derivative $\xi_\varepsilon''(r)$, as shown by Eq. (19), will also be real and positive and will correspond to a curvature which serves to increase $\xi_\varepsilon(r)$ when r increases inside that region.

It is now necessary to assume that $V(r)$ is a continuous decreasing function of r in the core region. This is true in all practical cases and does not reduce the interest of the argument. It follows that both $\omega(\varepsilon,r)$ and the "wave number" $k(r)=[\omega(\varepsilon,r)]^{1/2}$ are also decreasing functions of r in the core region. Let now b and c be two numbers with the condition $0<c<b<a$. As proved in Appendix B and illustrated in Fig. 4, the following inequality holds when $0<r<c$:

$$\xi_\varepsilon(r)<\xi_\varepsilon(c)\chi(r)\ , \tag{20}$$

where the function χ is given by

$$\chi(r)=\{\sinh[ck(c)]\}^{-1}\sinh[rk(c)]\ , \tag{21}$$

and is defined as the regular solution of the differential equation

$$\chi''(r)=\omega(\varepsilon,c)\chi(r)\ , \tag{22}$$

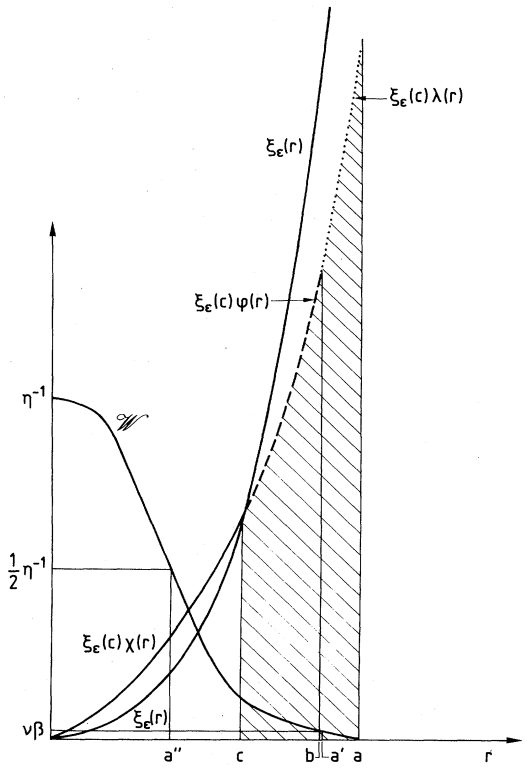

FIG. 4. Behavior in the repulsive region of the radial wave function ξ_ε. Its comparison with hyperbolic sine approximation $\xi_\varepsilon(c)\chi(r)$, intermediate estimate $\xi_\varepsilon(c)\varphi(r)$, and linear extrapolation $\xi_\varepsilon(c)\lambda(r)$. Hatched area corresponds to less than unity.

with the boundary condition $\chi(c)=1$. As proved in Appendix C and also shown in Fig. 4, the following inequality holds when $c<r<b$:

$$\xi_\varepsilon(r)>\xi_\varepsilon(c)\varphi(r)\ , \tag{23}$$

where the function φ is defined as the solution of the differential equation

$$\varphi''(r)=\omega^2(\varepsilon,b)\varphi(r)\ , \tag{24}$$

with the boundary conditions (i) $\varphi(c)=\chi(c)=1$ and (ii) $\varphi'(c)=\chi'(c)$. Finally, because of the curvature of $\xi_\varepsilon(r)$, it is clear that, when $b<r<a$, an additional inequality holds,

$$\xi_\varepsilon(r)>\xi_\varepsilon(c)\lambda(r)\ , \tag{25}$$

where $\lambda(r)$ is just the linear extrapolation of $\varphi(r)$ from $r=b$ towards $r=a$. Inequalities (23) and (25) will give the basis for an upper bound on ξ_ε.

From the definitions of φ and λ one obtains

$$\varphi(r)=\cosh[(r-c)k(b)]+D\sinh[(r-c)k(b)]\ , \tag{26}$$

where

$$D=[k(b)]^{-1}k(c)\coth[ck(c)]\ , \tag{27}$$

and

$$\lambda(r)=[1+(r-b)Dk(b)]\cosh[(b-c)k(b)] +[D+(r-b)k(b)]\sinh[(b-c)k(b)]\ , \tag{28}$$

It will be recalled that φ and λ are positive in their respective domains of interest. Since, according to inequalities (23) and (25), $\xi_\varepsilon(r)$ is larger than $\xi_\varepsilon(c)$ times $\varphi(r)$ or $\lambda(r)$ in the domains $c<r<b$ or $b<r<a$, respectively, and since furthermore the normalization of ξ_ε is kept equal to unity, one finds the relation

$$1=\int_0^\infty dr\,\xi_\varepsilon^2(r)>\xi_\varepsilon^2(c)n(\varepsilon,c,b)\ , \tag{29}$$

where

$$n(\varepsilon,c,b)=\int_c^b dr\,\varphi^2(r)+\int_b^a dr\,\lambda^2(r)\ . \tag{30}$$

An upper bound for the wave function ξ_ε results at once from Eq. (29) and reads

$$\xi_\varepsilon^2(c)<[n(\varepsilon,c,b)]^{-1}\ . \tag{31}$$

It is useful here to stress that b is arbitrary except for the condition $c<b<a$. Thus b can be used as a variational parameter, hence

$$\xi_\varepsilon^2(c)<\inf_b\{[n(\varepsilon,c,b)]^{-1}\},\quad c<b<a\ . \tag{32}$$

The upper bound given by inequality (31) cannot be used when c, and thus b, are nearly equal to a, because the integral $n(\varepsilon,c,b)$ defined by Eq. (30) vanishes when $c\to a$. Remembering that the contribution of the outer region to the matrix element $\langle\omega^2\rangle$ has been bounded by $\mu^2\beta^2$, one can define $a'<a$ as suggested in the beginning of this section in such a way that $V(a')=\nu\beta$ with $\nu>0$. Since it has been assumed that $V(r)$, and thus $\omega^2(\varepsilon,r)$, are decreasing functions of r in the core region, the contribution of the domain $a'<r<a$ to $\langle\omega^2\rangle$ is obviously smaller than $\nu^2\beta^2$. The only contribution which then remains to be studied is that of the region $0<r<a'$.

In order to take advantage of inequality (32), one may notice from Eqs. (26), (28), and (30) that the behavior of $n(\varepsilon,c,b)$ is dominated by the exponential

$$x=\exp[2k(b)(b-c)]\ . \tag{33}$$

It therefore looks reasonable to maximize x with respect to b and, for that purpose, to choose b only slightly larger than c. As an ansatz, let this variational parameter b be given a value $\hat{b}(c)$ defined by

$$\omega^2[\varepsilon,\hat{b}(c)]=\tfrac{1}{2}[\omega^2(\varepsilon,c)+\omega^2(\varepsilon,a')]\ . \tag{34}$$

This locates $\hat{b}$ between c and a', because ω^2 decreases monotonically. It is also clear from Eq. (34) that $2k(\hat{b})$ is larger than $\sqrt{2}k(c)$. The next step then consists in finding a lower bound for $(\hat{b}-c)$, to be inserted into Eq. (33).

From Eqs. (34) and (17′) one obtains

$$V(\hat{b})=\frac{V(c)+\omega^2(\varepsilon,a')[1+\eta V(c)]}{2+\eta V(c)-\eta\omega^2(\varepsilon,a')[1+\eta V(c)]}\ , \tag{35}$$

hence

$$V(c)-V(\hat{b}) =[1+\eta V(c)]\frac{V(c)-\omega^2(\varepsilon,a')[1+\eta V(c)]}{2+\eta V(c)-\eta\omega^2(\varepsilon,a')[1+\eta V(c)]}\ . \tag{36}$$

Let a'' be defined by the condition $V(a'')=\eta^{-1}$. When $a''<c<a'$, then $\eta V(c)<1$ and one obtains readily from Eq. (36) the inequality

$$V(c)-V(\hat{b})>\frac{V(c)-2\omega^2(\varepsilon,a')}{3} \tag{37}$$

or

$$V(c)-V(\hat{b})>\frac{V(c)-2V(a')}{3}\ . \tag{38}$$

If one assumes that there is a second-order derivative $V''(r)$ which furthermore is positive in the core region (this is true in most practical cases), then the modulus $|V'(r)|$ of the first-order derivative is smaller, when $c<r<\hat{b}$, than $|V'(c)|$. This can be also seen trivially in Fig. 3 and yields

$$\hat{b}-c>|V'(c)|^{-1}[V(c)-V(\hat{b})]\ , \tag{39}$$

hence, together with inequality (38),

$$\hat{b}-c>\tfrac{1}{3}|V'(c)|^{-1}[V(c)-2V(a')]\ . \tag{40}$$

In the region $a''<c<a'$, the condition $\eta V(c)<1$ also implies, as shown by Eq. (17′), that $\omega^2(\varepsilon,c)$ is larger than $\frac{1}{2}V(c)$. Since, as seen after Eq. (34), the quantity $2k(\hat{b})$ is larger than $\sqrt{2}k(c)$, it is then larger than $[V(c)]^{1/2}$. The exponential x defined by Eq. (33) therefore obeys the inequality

$$x>\exp\{\tfrac{1}{3}|V'(c)|^{-1}[V(c)]^{1/2}[V(c)-2V(a')]\}\ . \tag{41}$$

For most practical cases, this result, inequality (41), shows that x^{-1} vanishes faster than the divergence of any power of V (or ω, *a fortiori*). To give only one example, if V behaves like an inverse power r^{-m}, with $m>2$, then x^{-1} behaves like $\exp(-r^{1-m/2})$. It is now clear that the inequality

$$\xi_\varepsilon^2(c)<\{n[\varepsilon,c,\hat{b}(c)]\}^{-1},\quad a''<c<a' \tag{42}$$

provides a stringent upper bound to the corresponding contribution to $\langle\omega^2\rangle$. It would provide an upper bound for any power of ω as well. The only contribution left for investigation corresponds to $0<r<a''$. Since in that region $\omega(\varepsilon,r)$ is smaller than η^{-1}, and also $\xi_\varepsilon^2(r)$ is smaller than $\xi_\varepsilon^2(a'')$, the corresponding contribution is obviously smaller than $\eta^{-2}\{n[\varepsilon,a'',\hat{b}(a'')]\}^{-1}a''$.

To summarize this long argument, there are four contributions to $\langle\omega^2\rangle$. The contribution from the outer region ($r>a$) and that from a transition region ($a'<r<a$) can be easily bounded because $|\omega|$ can be uniformly bounded there by a fixed number $\mu\beta$ or $\nu\beta$. The contribution from the steep region of ω, defined by $a''<r<a'$ with $\omega(a'')=\frac{1}{2}\eta^{-1}$, is smaller than

$$\int_{a''}^{a'} dc\,\omega^2(\varepsilon,c)\{n[\varepsilon,c,\hat{b}(c)]\}^{-1}\,.$$

The remainder, corresponding to the smoothed part of ω, is smaller than $\eta^{-2}\{n[\varepsilon,a'',\hat{b}(a'')]\}^{-1}a''$. We have thus obtained a handy numerical, and to a great extent analytical, calculation of the counterterm.

From the many physical aspects hidden in the details of the mathematical argument set out in this section, we emphasize that the exponential convergence imposed by $n(\varepsilon,c,\hat{b})$ only reflects the physical fact that the stronger the repulsion, the smaller the wave function. The main tool in the proof is the nature of the curvature of the wave function. That curvature demands so fast an increase of the wave function that the norm function is pushed "exponentially" out of the repulsive barrier. It is likely that a larger class of potentials V than that admitted in the present section could be handled along similar lines. The class in which V is monotonic and has a curvature of fixed sign is, however, quite sufficient for practical purposes. It is likely that many results derived in this paper are also valid for a class of regular potentials.

For partial waves of the two-body problem with a larger orbital momentum than the s wave, it is trivial to find that the same upper bounds to $\langle\omega^2\rangle$ as those found for the s wave are valid, because the centrifugal barrier increases the repulsion and thus crushes even more the wave function.

The reader will notice that the exact value of binding energy plays no role at all (besides being negative) in the derivation of an upper bound of $\langle\omega^2\rangle$. In other words, the upper bound of $\langle\omega^2\rangle$ which has been derived in this section is *uniformly* valid for any bound state of this local potential.

We now consider the N-body problem. The derivation of an upper bound to the N-body counterterm is slightly more involved and it is the subject of the paper[5] which precedes this one. But the argument essentially goes along the same lines. For each pair (ij) one defines the probability density $\rho(r)$ for that pair to be at distance r. One finds an inequality $\rho''(r)\geq\mathcal{U}(r)\rho(r)$ where $\mathcal{U}$ is positive. Hence an upper bound to ρ is found, in a way identical to the argument leading to Eq. (32). Thus finally an upper bound to $\langle\omega_{ij}^2\rangle$ is found.

V. NUMERICAL APPLICATION AND DISCUSSION

To illustrate the method introduced in this paper let us consider a two-nucleon s wave with a potential given by

$$V(r)=A\left[\frac{1}{r^6}-B\frac{e^{-\mu r}}{\mu r}\right], \tag{43}$$

where $A=2.8$ MeV fm^6, $B=31.8$ fm^{-6}, and $\mu=0.7$ fm^{-1}. This potential is simply a Yukawa potential to which we added a r^{-6} repulsive part in order to test the method of regularization.

We fixed the value of B such that $V(r)$ vanishes at $r=0.5$ fm, and that of A such that $V(r)$ has a unique bound state at the deuteron binding energy $E=-2.2$ MeV. The inverse length μ takes here the usual one pion exchange potential (OPEP) value $\mu=0.7$ fm^{-1}. The potential $V(r)$ reaches a minimum of -88 MeV at $r=0.72$ fm.

As mentioned above we define a' such that $V(a')=40$ MeV. This choice fixes $a'=0.48$ fm and the region $a'<r<a$ thus contains already a certain amount of repulsion due to the beginning of the core. Finally, one may consider $\Omega=100$ MeV and $\gamma=50$ MeV as typical parameters for the alternative potential and set $\varepsilon_M=0.8$ which defines $\eta_M^{-1}=75$ MeV.

We adopt another manner of regularizing the original two-body potential. There is no need to regularize $V(r)$ for $r>a'$, since this is a perfectly well bounded and moderate size (by definition of a') part of the potential. It is therefore reasonable to restrict the regularization of $V(r)$ to $r<a'$ only. This serves to modify the definition, Eq. (17'), of ω into

$$\omega(\varepsilon,r)=\frac{V(r)}{1+\eta V(r)}\Theta(a'-r)+V(r)\Theta(r-a')\,. \tag{17''}$$

(We notice that the introduction of a local approximation of G enables us to regularize V locally, i.e., for specific regions only.) The advantage of this new definition of ω is that $\langle\omega^2\rangle$ is smaller, because its defining integral is taken from 0 to a' only. The change in the definition of ω does not affect the content of the previous sections. No complication arises from the discontinuity at $r=a'$ of the potential defined by Eq. (17'').

The upper bound to $\langle\omega^2\rangle$ based upon Eq. (42) has been calculated for various values of η. Although very simple to obtain, numerical results turned out to give too large a bound. Therefore Eqs. (41) and (42) provide us with a mathematical proof of existence of a bound for $\langle\omega^2\rangle$, but not with a practical tool. This does not affect, however, the main argument of this paper, namely the estimate of a counterterm, for (i) it is clear that Eq. (42) is not the best upper bound that mathematicians can derive [indeed, the difficulty of estimating $\int_0^a dr\,\xi_\varepsilon^2(r)$ forced us to use $1=\int_0^\infty dr\,\xi_\varepsilon^2(r)$ in the left-hand side of inequality (29), whereas it can be seen on numerical examples that the former integral hardly exceeds 10^{-2}], and in some partic-

ular choices of V a stricter bound for this integral might be easy to find, then (ii) special cases might be more adapted to Eq. (42), and finally, (iii) "exact numerical" integration of the two-body Schrödinger equation governed by ω is even easier to obtain than that for V.

Table I gives several values of the two-body counterterm $E-\mathscr{E}(\varepsilon)$. The results are gratifying, for the counterterm hardly exceeds a few MeV or even tenths of MeV. Other numerical experiments based on reasonable potentials differing from that chosen above give similar counterterms.

It will be noticed that our alternative potential ω, and the resulting estimate of the counterterm, are defined only for values of $(-\omega)$ which are on the left side of the "poles." It has been pointed out[9] to us, however, that is very useful to allow $(-\omega)$ to take on values which belong to a region corresponding to the single-particle energies of occupied orbitals. In other words, one would like $(-\omega)$ to be in the "hole pole region." In so far as numerical calculations for the two-body problem are feasible, nothing prevents us from calculating a G matrix for such values of $(-\omega)$, then using that G matrix as an interaction for two particles and generating the corresponding binding energy for an N-body system.

All the results of this paper, which have been derived for distinct particles, can be readily extended for identical bosons, because the same value of the regularization parameters $\Omega_{ij}\varepsilon^{-1}$ can be associated to all particle pairs.

The question remains as to whether all these results apply to identical fermions. In that case, the bare interactions V_{ij} from which the G matrices are calculated are the same for all particle pairs. The G matrices can therefore differ only from each other through the starting energies $\varepsilon^{-1}\Omega_{ij}$ and the single-particle potentials U_i and U_j (with the corresponding parameters γ_i and γ_j). This defines for each pair a parameter η_{ij} and the corresponding ω_{ij}.

Since the G matrices are different, the resulting lack of symmetry of $H(\varepsilon)$ and $\mathscr{H}(\varepsilon)$ with respect to exchange between particle labels might concern us. The difficulty is only apparent, because $H(\varepsilon)$ and $\mathscr{H}(\varepsilon)$ must be restricted to the subspace of totally antisymmetric wave functions in the same way as their limit when $\varepsilon\to 0$, namely H. In other words, under the condition of projection into the "antisymmetric" subspace, a nonsymmetric Hamiltonian can describe a system of identical fermions. The N-body counterterm is then just given by Eq. (12′).

By reformulating the above theory in a framework in which indices such as i and j would refer to single-particle orbitals rather than particle themselves, however, one might find a more satisfactory point of view. A second quantization framework would indeed be better. This problem is under study and will give rise to a future paper in the case of success. It must be stressed, however, that the validity of the counterterm which has been derived above is not affected by the lack of antisymmetrization which remains in the theory at the present stage.

TABLE I. Values of the two-body counterterm deduced from the alternative potential ω. First row contains the energy η^{-1} which characterizes the cutoff. Then one finds the regularization parameter ε, the expectation value $\langle\omega^2\rangle_{a'}$, the coefficient by which it must be multiplied to generate [see Eq. (12′)] the derivative of the counterterm, and, finally, the counterterm.

	η^{-1} (MeV)			
	800	400	200	100
ε	0.12	0.22	0.40	0.67
$\langle\omega^2\rangle_{a'}$	6.98	4.33	2.42	1.31
$\dfrac{\Omega}{(\Omega-\varepsilon\gamma)^2}$	0.011	0.013	0.016	0.026
$\mathscr{E}(0)-\mathscr{E}(\varepsilon)$	1.27	1.86	2.46	2.96

VI. CONCLUSION

Several properties have been established in this work. The G-matrix regularization has been proved to be "monotonic" in a certain domain of starting energies, at least on the left-hand side from the pole region. A suitable counterterm can be added to the regularized Hamiltonian in order to generate a *rigorous* variational principle with respect to *both* trial functions *and* starting energies in that domain. A very simple, projector-free, local potential can be exhibited, which takes care of many relevant properties of the G matrix. It shows in particular how the G matrix practically consists in a cutoff of the repulsion of V beyond the energy η^{-1}.

A practical numerical procedure has been proposed for the calculation of the counterterm. Actually we have shown that the whole method reduces to the search for a reasonable counterterm. As matter of fact, we would like to propose, as a consequence of our study, that any strong repulsive core be regularized in the following way:

$$V_\varepsilon(r)=V(\varepsilon)\Theta(\varepsilon-r)+V(r)\Theta(r-\varepsilon)\ . \tag{44}$$

This is because we have found that the other regularizations finally amount to the latter, Eq. (44); and clearly the latter is the simplest possible and retains all the desired physical and mathematical properties.[5]

Progress can be made in two directions, namely, (i) antisymmetrization at the beginning of the theory, and (ii) closer bounds than those generated from ω. Better counterterms and large domains for ε are certainly to be found. Our rigorous solution is now under study for further refinements.

ACKNOWLEDGMENTS

Stimulating exchanges with B. R. Barrett, D. Bessis, M. Chemtob, H. Cornille, G. Giraud, H. M. Hofmann, M. W. Kirson, P. Moussa, H. Müther, M. Pelicoro, E. Osnes, and M. Villani and gratefully acknowledged. We are very grateful to the late Guy Giraud for his stimulating interaction with us at the beginning of this project. It is a pleasure for one of us (B.G.G.) to thank especially M. Villani for an invitation to the University of Bari which helped to unlock a path to the solution shown in Sec. IV. We wish to thank particularly C. Verneyre for her handling of the numerical tests of the theory.

APPENDIX A

The various conditions which define the domain available for ε can be listed as follows:

(i) all operators $Q(\Omega_{ij}\varepsilon^{-1}+t_i+t_j+U_i+U_j+V_{ij})Q$ and, if necessary, all operators $Q(\Omega_{ij}\varepsilon^{-1}+t_i+t_j+U_i+U_j)$ must be positive definite in the subspace conserved by Q;

(ii) all operators $\{\Omega_{ij}\varepsilon^{-1}+t_i+t_j+U_i+U_j+[Q(\lambda)]^{1/2}V_{ij}[Q(\lambda)]^{1/2}\}$ and, if necessary, all operators $(\Omega_{ij}\varepsilon^{-1}+t_i+t_j+U_i+U_j)$ must be positive definite;

(iii) all operators $(\Omega_{ij}\varepsilon^{-1}-\gamma_i-\gamma_j V_{ij})$ must be positive definite; and

(iv) all numbers $\beta_{ij}(\Omega_{ij}\varepsilon^{-1}-\gamma_i-\gamma_j)(\Omega_{ij}\varepsilon^{-1}-\gamma_i-\gamma_j-\beta_{ij})^{-1}$ must be smaller than $\mu\beta_{ij}$, with $\mu>1$.

Since t_i and t_j are positive and since U_i, U_j, and V_{ij} (and *a fortiori* $[Q(\lambda)]^{1/2}V_{ij}[Q(\lambda)]^{1/2}$) are larger than $(-\gamma_i)$, $(-\gamma_j)$, and $(-\beta_{ij})$, respectively, it is trivial to check that all conditions (i), (ii), and (iii) are satisfied if

$$\varepsilon^{-1}>\max_{i,j}[\Omega_{ij}^{-1}(\gamma_i+\gamma_j+\beta_{ij})]\ . \tag{A1}$$

As regards conditions (iv), they are fulfilled if

$$\varepsilon^{-1}>\max_{i,j}\left[\Omega_{ij}^{-1}\left[\gamma_i+\gamma_j+\frac{\mu}{\mu-1}\beta_{ij}\right]\right]\ , \tag{A2}$$

which is even more restrictive than (A1) since $\mu>1$ and $\beta_{ij}>0$.

It is clear that conditions (i)—(iv) are not independent from each other, some of them including the others. Depending on the specific problem under study, some of these conditions (i)—(iv) might become unnecessary, and the value ε_M deduced from (A2) would than appear as a conservative boundary for the domain of ε.

APPENDIX B

Since the functions $\xi_\varepsilon(r)$ and $\xi_\varepsilon(c)\chi(r)$ are regular solutions of Eqs. (19) and (22), respectively, and since $\chi(c)=1$, their Wronskian at point c reads

$$\xi_\varepsilon(c)[\xi_\varepsilon'(c)-\xi_\varepsilon(c)\chi'(c)]=\xi_\varepsilon(c)\int_0^c dr[\omega(\varepsilon,r)-\omega(\varepsilon,c)-\mathscr{E}]\xi_\varepsilon(r)\chi(r)\ . \tag{B1}$$

The right-hand side of Eq. (B1) is a positive number, because $\mathscr{E}$ is negative, ξ_ε and χ are positive and curved upwards, and $\omega(\varepsilon,r)$ is a decreasing function of r in the core region. Therefore the derivative of $\xi(r)$ is larger than the derivative of $\xi_\varepsilon(c)\chi(r)$ at that point c where the graphs of those functions cross each other. Before that point, $\xi_\varepsilon(r)$ must be smaller than $\xi_\varepsilon(c)\chi(r)$.

APPENDIX C

Because of their boundary conditions at point c, $\xi_\varepsilon(r)$ and $\xi_\varepsilon(c)\ \varphi(r)$ are the unique solutions of the inhomogeneous Volterra equations

$$\xi_\varepsilon(r)=\xi_\varepsilon(c)+(r-c)\xi_\varepsilon(c)+\int_c^r dr'(r-r')[\omega(\varepsilon,r')-\mathscr{E}]\xi_\varepsilon(r')\ , \tag{C1}$$

and

$$[\xi_\varepsilon(c)\varphi(r)]=\xi_\varepsilon(c)+(r-c)\xi_\varepsilon(c)\chi'(c)+\int_c^r dr'(r-r')\omega(\varepsilon,b)[\xi_\varepsilon(c)\varphi(r')]\ , \tag{C2}$$

respectively.

As seen just above, both the inhomogeneous term and the kernel of Eq. (C1) are larger (when $c<r<b$) than those of Eq. (C2), respectively. It is well known that these equations can be solved by iterations, which involves here positive quantities only. Each iteration of Eq. (C1) thus generates a larger term than the same step for Eq. (C2), and thus $\xi_\varepsilon(r)$ must be larger than $\xi_\varepsilon(c)\varphi(r)$.

[1]W. M. Frank, D. J. Land, and R. M. Spector, Rev. Mod. Phys. **43**, 36 (1971), and references therein.

[2]H. Cornille, Nuovo Cimento **38**, 1243 (1965); **39**, 557 (1965); **43**, 786 (1966).

[3]W. M. Frank (unpublished).

[4]B. G. Giraud and E. Osnes, Phys. Rev. C **16**, 453 (1977).

[5]B. G. Giraud and E. Osnes, preceding paper, Phys. Rev. A **32**, 64 (1985).

[6]K. A. Brueckner, C. A. Levinson, and H. M. Mahmoud, Phys. Rev. **95**, 217 (1954); K. A. Brueckner and C. A. Levinson, *ibid.* **97**, 1344 (1955); K. A. Brueckner, *ibid.* **97**, 1353 (1955); J. Goldstone, Proc. R. Soc. London, Ser. A **239**, 267 (1957). An introduction to Brueckner theory, containing more references, can be found in the review article by B. D. Day, Rev. Mod. Phys. **39**, 719 (1967).

[7]V. R. Pandharipande, R. B. Wiringa, and B. D. Day, Phys. Lett. **57B**, 205 (1965); J. C. Owen, R. F. Bishop, and J. M. Irvine, *ibid.* **61B**, 147 (1976).

[8]C. Bloch and J. Horowitz, Nucl. Phys. **8**, 91 (1958). The review article by B. R. Barrett and M. W. Kirson, Adv. Nucl. Phys. **6**, 219 (1973), contains a general introduction to the theory of effective operators.

[9]We thank G. E. Brown for this remark.