Comments

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Many fermion energy calculations

George A. Baker, Jr.*
Centre d'Études Nucleaires-Saclay, Boite Postale No. 2, 91190 Gif-sur-Yvette, France
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It is pointed out that because of the omission of residue terms from the basic Green's function, the two hole-line approximation to the ground state energy of infinite nuclear matter with self-consistent intermediate state energies for hole lines only differs from the corresponding physical energy in a completely uncontrolled manner. This interpretation is in contrast to that of Wong.

[NUCLEAR STRUCTURE Ground-state energy nuclear matter correctness 2 methods calculation assessed.]

Wong,[1] in considering the 1970 R-matrix method calculation[2] of the many-fermion binding energy (in spite of its excellent agreement with recent calculations of Clark *et al.*[3] using a variational state-independent Jastrow correlation function and the Fermi hypernetted chain method) concludes "that the R-matrix result should be treated with extreme caution until its accuracy is verified. Consequently the additional attraction obtained in Ref. 2 does not appear to have been firmly established." While no one, to my knowledge, has contended that the work of Refs. 2 and 3 is definitive, it is well to understand that the R-matrix method is at the very least, not known to be wrong in principle, while the standard of comparison, "lowest-order Brueckner theory" (called LOBT by some authors), used by Wong is, even if carried out to *all orders*, known to be wrong in principle.[4] The difficulty arises with the choice[5] of self-consistent energies for hole lines only for the intermediate state energy denominators. Attention in the LOBT approach cannot be confined solely to the size of higher-order corrections, as has been done in the past, but must also be directed to its errors of principle. From the calculations of Refs. 2 and 3 we can gain a notion of the *general order of magnitude* to anticipate for these latter corrections.

The fundamental question addressed here is "what is the limiting ground-state energy per particle of an infinitely large system of particles which obey the Schrödinger equation and interact by means of a specified two-body potential?" The answer to this question is beset by numerous difficulties. Most of these difficulties are related to real physical effects. The phenomenon of nuclear collapse when the sign of a usual-shaped potential is reversed causes the perturbation series to be at best asymptotic[6] rather than convergent. The problem of the nuclear hard-core necessitates rearrangement of the perturbation series in potential strength.[7] The possibility of superfluidity in some physical system led to the occurrence of Emery singularities[8] in the initial rearrangement. This occurrence has been treated in several ways, for example, the numerical expedient of Brueckner and Gammel[9] and the more systematic R-matrix rearrangement of Baker and Kahane.[10] Generally speaking as most of the currently known results have been reviewed at great length[11-15] we will confine our attention here to the R-matrix expansion[2,10] and the hole-line approach.

One other method[5] which has been used widely to speed convergence, simplify computation, and eliminate the Emery singularities in the hole-line approach is to include a self-consistent energy correction for the hole-line intermediate states, but not for the particle states. This further rearrangement cannot be justified by the methods of the general theory[11] because it makes a separation in fourth and higher orders of diagrams with two or more self-energy corrections on the same hole line (see Fig. 1) from the corresponding diagrams with self-energy corrections on the same particle line. That is, a finite contribution is

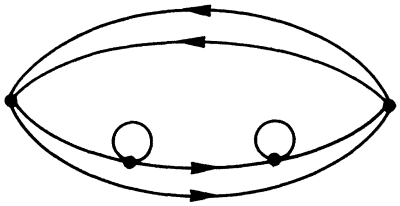

FIG. 1. A Hugenholtz diagram of a divergent contribution to the many-fermion energy.

split into two infinite ones. The reason is, since all the propagators in Fig. 1 are the same, there is a third-order singularity in the denominator which cannot be canceled, as could a second order one, by a three-space momentum integration. Consequently, this rearrangement has infinite coefficients in fourth and higher order. This unpleasantness is avoided in the V series by cancellation with the bubbles on the particle lines. Thus for this rearrangement, not all the conditions in the general theory[11] of rearrangements of the V series are met. So we cannot be assured from the start that this further rearrangement will lead to the physically correct sum. Nevertheless, it is possible to assign a valid meaning to the sum of all the diagrams for the two-hole-line approximation with self-consistent intermediate state hole energies, provided a path from a very weak potential to the potential of interest can be found that crosses no singularities of the function. This sum is embodied in the usual Green's function equations. Baker and Gammel[4] have carried out this investigation for the Baker-Hind-Kahane[2] potential. They found that it was necessarily so, that zeros of the energy denominator in the Green's function cross the usual contour of integration. Thus the Green's function equations normally written down[5] are incomplete, and one must add by Cauchy's theorem the residue of the poles which have crossed the integration contour. Baker and Gammel[4] were not able to find self-consistent solutions to the completed equations in the physical region, but when the complete and incomplete equations were both solved at the same potential (complex) for comparison's sake, they found that the results were definitely different; a ratio of 3 to 2 between the solutions represents a typical assessment of the type of difference found.

Thus the conclusion is that LOBT with self-energy corrections on hole lines only differs from the corresponding physical energy in a *completely uncontrolled manner*. The comparisons of Wong[1] between the results of my previous paper[2] which gives

$$E_{\mathrm{BHK}} = -25.6 \text{ MeV},$$

those of Clark *et al.*[3] who used a variational state-independent, Jastrow correlation function and the Fermi hypernetted chain method to compute

$$E_C = -23.8 \text{ MeV}$$

for the same potential and density, and the LOBT result of

$$E_{\mathrm{LOBT}} = -16.8 \text{ MeV}$$

are perhaps better interpreted as an estimate of the neglected residue terms just discussed.

The numerical comparison "oscillating around the LOBT energy" made by Wong retaining different subsets of terms does not seem to me to be appropriate, since one can rearrange such a series to approach any desired result. Certainly the rearrangement of a divergent series is not something which can be done carelessly! The elementary textbook example of a conditionally convergent series

$$1 - \tfrac{1}{2} + \tfrac{1}{3} - \tfrac{1}{4} + \tfrac{1}{5} - \tfrac{1}{6} + \cdots,$$

which can be rearranged to give any answer one pleases, can be used to rearrange at $x = 1$ the divergent series

$$\begin{aligned}\int_0^\infty \frac{e^{-t}\,dt}{1+xt} &= 1 - 1!x + 2!x^2 - 3!x^3 + \cdots \\ &= 2 - (1! + \tfrac{1}{2})x + (2! + \tfrac{1}{3})x^2 - (3! + \tfrac{1}{4})x^3 + \cdots \quad -1 + \tfrac{1}{2}x - \tfrac{1}{3}x^2 + \tfrac{1}{4}x^3 - \cdots \\ &= \int_0^\infty \frac{[e^{-t} + \theta(t-1)]\,dt}{1+t} - 1 + \tfrac{1}{2} - \tfrac{1}{3} + \tfrac{1}{4} - \tfrac{1}{5} + \cdots,\end{aligned}$$

where $\theta(y) = 1$, $y < 0$ and 0 for $y > 0$. The last equality is meant for $x = 1$ only.

In any event, it has been shown[11] that the R-matrix rearrangement used by Baker *et al.*[2] with unperturbed intermediate-state energy denominators uniquely determines the correct physical ground-state energy at least for the class of purely repulsive bounded finite-range potentials.

Having understood that LOBT as widely computed is an inadequate approach, we return to the orig-

inal question. Since the physics of the hole-line approach appears sensible, it is reasonable to attempt to use it with a different choice of intermediate energy denominator. Calculations of this sort are reported by Lejuene and Mahaux[16] using the original Brueckner-Gammel[9] approximation of a self-consistent energy depending only on the momentum of the state. The results of these calculations are such as to move very strongly from E_{LOBT} towards the Baker *et al.*[2] and Clark *et al.*[3] results. It seems to me, that a reasonable avenue of approach is now to implement the calculation of the sum of all the nonintrinsically three-body terms. That is to say, to choose for the intermediate state energy, a self-consistent energy which, for the particles, depends on the excitation of the Fermi sea as well as the momentum state. The details of this procedure appear in Appendix A of Brueckner and Gammel,[9] and while it was not practical in 1958, it should now be.

Since the appearance of Baker *et al.*,[2] both the Padé approximant method and the Borel-Padé method which they used for series summation have received considerable attention and have generally been found to be quite satisfactory[17] in accelerating the convergence of such series. As far as has been found to date, the reasons behind the convergence of the Padé approximants are related to powerful analyticity properties that occur in physical problems. While interpretations of low-order Padé approximants in pseudodiagrammatic terms such as Wong's[1] can and have been made, I feel that it is the deeper analyticity properties which are responsible for the large cancellations which otherwise seem so surprising. See, also the recent results of Wilson *et al.*[18] on the special invariance properties of the $[N+1/N]$ Padé approximant.

The author is happy to have had helpful discussions of this subject with J. L. Gammel, B. Giraud, C. Mahaux, and H. J. Pirner.

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*On leave from Theoretical Division, Los Alamos Scientific Laboratory, Los Alamos, New Mexico 87545.

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