Comment on Baker, Brueckner, and Jastrow energies in nuclear matter

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The R matrix calculation of Baker, Hind, and Kahane for the energy of nuclear matter is reanalyzed. We find that because of the Padé summation used, the R matrix theory is qualitatively similar to the usual Brueckner theory with self-energies. Both theories differ qualitatively from variational theories using Jastrow correlation functions.

[NUCLEAR STRUCTURE Nuclear matter; compared Baker, Brueckner, and Jastrow (FHNC) energies.]

Several years ago, Baker, Hind, and Kahane (BHK)[1] calculated nuclear-matter (NM) energies for a hard-core plus attractive square well potential through fourth order in a regularized Brueckner reaction matrix, the R matrix. The calculation further differs from usual Brueckner calculations in that no self-energy corrections are made on single-particle (s.p.) states. It was found that the calculated energy does not converge by fourth order in R, as shown order by order in Table I for $k_F = 1.56$ fm^{-1}. However, a [2,2] Padé approximant gives -25.6 MeV/A as the estimated sum of the series.[1] This is to be compared with an energy[1] of only -16.8 MeV in the lowest-order Brueckner theory (LOBT), which is a two-hole approximation with self-energy corrections. The conclusion was that there is substantial attraction missed by the LOBT.

Recently, the NM energy for this potential at the same density was also calculated by Clark *et al.*,[2] who use a variational state-independent Jastrow correlation function and the Fermi hypernetted-chain (FHNC) method[3] for Fermi liquids. A FHNC energy of -23.8 MeV/A is obtained. Another $-(1-3)$ MeV should be added to this result to correct the inadequacies of Jastrow wave functions.[2] Thus a remarkable agreement appears to exist between the variational and the R matrix results. The conclusion appears to be that this agreement gives additional support for the FHNC results.

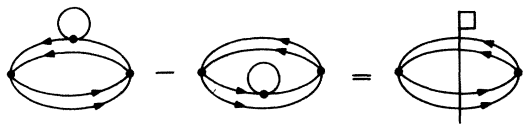
The purpose of this note is to point out that the R matrix theory with Padé summations is qualitatively similar to Brueckner theory with self-energies, and that they both differ qualitatively from the FHNC result in the neglect of higher-order terms. Unlike the Brueckner theory, the use of Padé summations was not motivated by physical considerations. Although it is not inconceivable that the [2,2] Padé approximant used is actually more efficacious in estimating the contributions of the neglected terms than Brueckner and Bethe-Faddeev sums in spite of the complications of the energy expression,[4,5] this possibility has not been demonstrated. Consequently, R matrix results should be viewed with a great deal of reservation.

We begin by commenting briefly on the R matrix results of BHK at $k_F = 1.56$ fm^{-1}, which are shown in Table I. The small second-order energy E_2^R is the leading contribution to the small differences between the G and the R matrices. It may be neglected for the purpose of the present discussion. The large third- and fourth-order energies show that a straightforward perturbation expansion does not work. Their major contributions are items (a), (b), and (c) of Table I, which correspond respectively to diagrams (a), (b), and (c) of Fig. 1. They turn out to be precisely those effects which the Brueckner theory attempts to handle in a convergent fashion by self-energy corrections [diagrams (a) and (b)], and by the Bethe-Faddeev summation of the three-body contribution[6,7] [diagram (c)]. According to Rajaraman[6] and Bethe,[7] the fourth-order diagram (c) is the first nontrivial term of a divergent series and should not be isolated from the rest of the series.

In BHK, the "divergence" problem is handled by Padé summations. Now in the approximation $E_2^R = 0$, the [2,2] Padé approximant simplifies to

TABLE I. R matrix perturbation energies of orders $n = 0$ to $n = 4$ for nuclear matter at $k_F = 1.56$ fm^{-1}, as reported in Ref. 1. Contributions (a), (b), and (c) correspond to Figs. 1(a), 1(b), and 1(c).

n	E_n^R (MeV)	Major contributions
0	30.38	Kinetic energy per particle
1	−64.59	
2	0.13	
3	32.4	(a) 33.4 MeV
4	−74.6	(b) −29.0 MeV (c) −39.3 MeV



(a) Diagram F3 of BHK

(b) Diagram IV·1 (c) Diagram IIA·1

FIG. 1. Hugenholtz diagrams in the R matrix, as classified by Baker, Hind, and Kahane (Ref. 1).

$$E([2,2]) = E_0^R + E_1^R/(1+2\kappa^R),$$
$$\kappa^R = -\frac{1}{2}\frac{E_3^R/E_1^R}{(1-E_4^R/E_3^R)}. \quad (1)$$

The result is similar in form to that for LOBT in the sense that certain higher-order effects have been included in the "self-energy" correction [4] $(1+2\kappa^R)^{-1}$. Here κ^R plays the role of an effective pair excitation parameter. Equation (1) differs from a "standard" LOBT calculation as follows: (i) Self-consistency has not yet been achieved. (ii) Bubble insertions on particle lines are already included as parts of the "flag" insertions of diagrams (a) and (b), while they are absent in the standard LOBT. (iii) A leading fourth-order contribution, diagram (c), to the Bethe-Faddeev three-body energy has been included through κ^R.

How different is this [2,2] Padé approximant of the leading R matrix perturbation terms from Brueckner results? To answer this question, we note that when both E_3^R and E_4^R are neglected, we have $E_0^R + E_1^R = -34$ MeV. If only E_4^R is neglected, Eq. (1) gives just a [1,1] Padé approximant with E_3^R as the third term of the series. The result is -12.6 MeV (or $\kappa^R = 0.25$). If in addition we keep the "flag" contribution (b) in E_4^R, but leave out the questionable contribution (c) and all other $n=4$ contributions, we get -20.7 MeV ($\kappa^R = 0.13$), as compared with -25.6 MeV for the original approximant when everything is included. These numbers oscillate around the LOBT energy of -16.8 MeV and are reminiscent of the oscillatory approach to self-consistency in LOBT calculations. We should also note that self-consistency with respect to flag insertions in the R matrix expansion will be achieved when "flag" diagrams of all orders are included. The self-consistent result will probably differ somewhat from the "standard" LOBT result because of the R matrix inclusion of s.p. potentials on particle lines. (Our guess for the former is -18 or -19 MeV.)

We now come to contribution (c) of E_4^R, which accounts for a little more than half of the additional attraction beyond LOBT in the Padé-summed R matrix result. The Padé approximant (1) treats it effectively as part of a self-energy correction. In the Bethe-Brueckner theory, on the other hand, contribution (c) is summed with all other three-hole contributions by the Bethe-Faddeev equation before it is used to modify s.p. energies.[6,7] Its effect on the total energy is then greatly reduced, according to available calculations.[8] We should add that in these "standard" Brueckner-Bethe calculations the third-order particle-insertion part of diagram (a) is included in the Bethe-Faddeev three-body energy rather than in the flag insertion.

We therefore conclude that the R matrix result should be treated with extreme caution until its accuracy is verified. Consequently, the additional attraction obtained in Ref. 1 does not appear to have been firmly established. It is related to convergence problems in the R matrix expansion and can be understood on purely technical grounds, without introducing any new physical mechanisms not yet discussed or calculated in the Brueckner theory.

This situation is in contrast to the FHNC calculations, which include explicitly certain correlational effects involving many, many bodies. The finding of Ref. 2, that the R matrix and FHNC results are in close agreement, suggests the possibility of finding interesting features in the Baker procedure. The most obvious possibility is that implied by Eq. (1), namely that an independent-pair picture is valid when the self-energy of the pair is defined by assuming that third- and higher-order R matrix terms form a simple geometrical series in their effect on κ^R. It is not clear, however, why this simple procedure is actually equivalent to the much more complicated FHNC summation. Additional studies of higher-order R matrix energies will be needed to establish the validity and to determine the physical meaning of this and other possible features of the Baker procedure.

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