Pauli exclusion operator and binding energy of nuclear matter

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Brueckner-Hartree-Fock calculations are performed for nuclear matter with an exact treatment of the Pauli exclusion operator in the Bethe-Goldstone equation. The differences in the calculated binding energy, compared to the angle-average approximation, which is commonly used, are non-negligible. These differences exhibit a specific density dependence, which shifts the calculated saturation point towards smaller densities. This effect is observed for various versions of modern models for the nucleon-nucleon interaction. [S0556-2813(99)02605-9]

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It is one of the very central and very old projects of nuclear structure theory to evaluate the saturation properties of nuclear matter from a realistic nucleon-nucleon (NN) interaction without any adjustment of a free parameter. The so-called hole-line expansion or Brueckner-Bethe-Goldstone theory has been one of the tools for solving this many-body problem, which has already been used for many years [1–4]. These early investigations were successful to some extent. The inclusion of NN correlations in the lowest order of the hole-line expansion, the Brueckner-Hartree-Fock (BHF) approach, turned out to be very important. Realistic models of the NN interaction like the Reid soft-core potential [5] yield an energy of nuclear matter around 150 MeV per nucleon if the effects of correlations are ignored in a mean-field or Hartree-Fock calculation. The BHF approach provides a drastic improvement leading to an energy per nucleon of -11 MeV, which was only by 5 MeV off from the empirical value of -16 MeV per nucleon. Attempts have been made to improve the description of the saturation point further by exploring different NN interactions. It turned out, however, that BHF calculations using these various NN interactions yield results for the saturation point, which fall on the so-called Coester band [6]. They either predict too small binding energy at the empirical value for the density, or about the correct energy at a density, which is too large by a factor of 2, or results in between. Comparison of BHF with variational calculations furthermore demonstrated that the inclusion of three-hole line contributions seems to be necessary to obtain a reliable estimate for the binding energy of nuclear matter [7,8].

During the last years some progress has been made in this field. It has been shown that a continuous choice for the particle spectrum [9,10] (see, also, the discussion below) accounts for the main part of the effects of three-body correlations. The discrepancy between the calculated saturation points of nuclear matter and the empirical one has significantly been reduced by considering relativistic effects within the Dirac-Brueckner-Hartree-Fock (DBHF) approach [11–13]. Finally, it should be mentioned that a new generation of realistic NN potentials has been developed [14–16], which yield very accurate fits of proton-neutron and proton-proton scattering. These new potentials, which are essentially phase-shift equivalent remove a large part of the discrepancies observed between older models of the NN interaction [17].

Because of these improvements, the time seems to be appropriate to test the reliability of approximations which are generally employed in the BHF calculations of nuclear matter. One of the central equations to be solved in the BHF approximation is the Bethe-Goldstone equation, which we may write in the momentum representation

$$G_{S,T}(\vec{k},\vec{k}',K,\omega)=V_{S,T}(\vec{k},\vec{k}')+\int d^3p\,V_{S,T}(\vec{k},\vec{p})\times\frac{Q(\vec{p},K)}{\omega-H_0}G_{S,T}(\vec{p},\vec{k}',K,\omega). \tag{1}$$

In this equation K represents the center-of-mass momentum of the interacting pair of nucleons while $\vec{k}$, $\vec{k}'$, and $\vec{p}$ stand for relative momenta, which are related to the single-particle momenta according to

$$\vec{K}=\frac{1}{2}(\vec{k}_1+\vec{k}_2) \quad \text{and} \quad \vec{k}=\frac{1}{2}(\vec{k}_2-\vec{k}_1), \tag{2}$$

ω denotes the starting energy, while $V_{S,T}$ and $G_{S,T}$ refer to the matrix elements of the bare interaction and G matrix, respectively, for two nucleons with total spin S and isospin T. The operator H_0 is used to define the energy spectrum of the intermediate two-particle state $(K,\vec{p})$. The conventional choice for these energies of particle states above the Fermi surface has been to replace H_0 by the kinetic energy of these states. In the so-called continuous choice, one assumes that the single-particle energies for these particle states as well as for the hole states are calculated from the kinetic energy plus a mean-field contribution, which is calculated in a self-consistent way from the G matrix by

$$\epsilon_q=\frac{q^2}{2m}+\int_{p\leq k_F} d^3p\langle\vec{q}\vec{p}|G(\omega=\epsilon_q+\epsilon_p)|\vec{q}\vec{p}\rangle\approx\frac{q^2}{2m^*}+U. \tag{3}$$

The term on the right-hand side exhibits a parametrization of these single-particle energies in terms of an effective mass and a constant potential, which is often used. The Pauli operator in the Bethe-Goldstone equation (1) prevents scattering into intermediate states with momenta $\vec{p}_1=\vec{K}-\vec{p}$ and $\vec{p}_2=\vec{K}+\vec{p}$, which are smaller than the Fermi momentum k_F. Therefore, the value of $Q(\vec{p},K)$ depends on the angle Ω between the center-of-mass momentum K and the relative momentum p. Employing a partial wave expansion of the two-particle states, the matrix elements for this Pauli operator can be written [18]

$$\langle (l'S)J'M|Q(p,K)|(lS)JM\rangle = \sum_{m_l,m_S} (l'm_lSM_s|J'M)(JM|lm_lSM_s) \times\langle l'm_l|Q(p,K)|lm_l\rangle$$

with

$$\langle l'm_l|Q(p,K)|lm_l\rangle = \int d\Omega\, Y^*_{l'm_l}(\Omega)Y_{lm_l}(\Omega)\Theta(|\vec{K}+\vec{p}|-k_F) \times\Theta(|\vec{K}-\vec{p}|-k_F), \quad (4)$$

with $\Theta(x)$ defining the step function. One finds that the Pauli operator is diagonal with respect to the modulus of the momenta K and p, the spin S and the projection quantum number m. It has nonvanishing matrix elements between states of different l and J with the restriction of parity conservation ($l+l'$ must be even) and its value depends on the projection quantum number M. This implies that also the solution of the Bethe-Goldstone equation is not diagonal with respect to the angular momentum quantum numbers l and J and depends on M,

$$\langle klJ|G_{STM}(\omega,K)|k'l'J'\rangle. \quad (5)$$

In order to simplify the calculation this Pauli operator is usually replaced by the so-called angle-average approximation

$$\langle l'm_l|Q^A(p,K)|lm_l\rangle=\delta_{l,l'}\begin{cases}0 & \text{for } p\leq\sqrt{k_f^2-K^2},\\ 1 & \text{for } p\geq k_F+K,\\ \dfrac{K^2+p^2-k_F^2}{2Kp}, & \text{otherwise.}\end{cases} \quad (6)$$

The angle-average approximation yields matrix elements for the Pauli operator which are diagonal in the l and J and independent on M. This means that the Bethe-Goldstone Eq. (1) can be solved separately for each partial wave and the resulting G matrix will be diagonal in J and independent of M.

The matrix elements of G can then be used to evaluate the total energy per nucleon. In the case of the exact Pauli operator this energy is given as

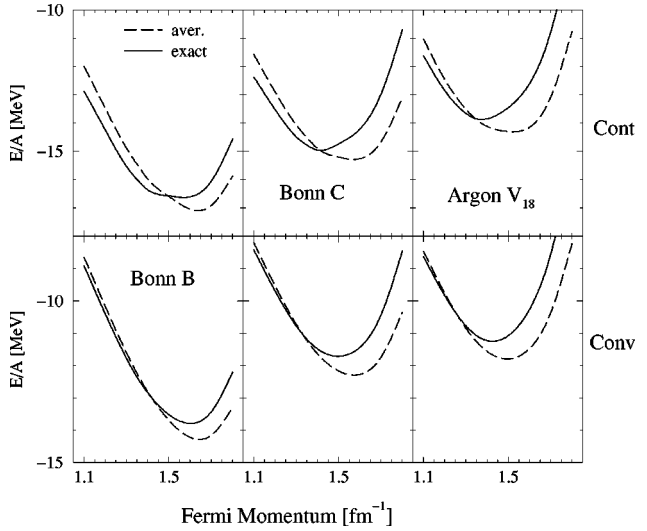

FIG. 1. Calculated binding energies per nucleon for nuclear matter as a function of the Fermi momentum k_F. Results are presented for the angle-average approximation of the Pauli operator (dashed lines) and the exact treatment (solid lines). The potentials Bonn B and C, defined in [19], as well as the neutron-proton part of the Argonne V_{18} potential [15] were used for the NN interaction. The continuous choice for the particle state spectrum in the Bethe-Goldstone Eq. (1) has been used to obtain the results displayed in the upper part, while the conventional choice has been used to calculate the results shown below.

$$\frac{E}{A}=\frac{3}{5}\frac{k_F^2}{2m}+\frac{6}{k_F^3}\sum_{\substack{T,S,M,l',l,\\ J',J,m_l,m_s}}(2T+1) \times\int k^2dk\int K^2dK\int d\Omega\langle klJ|G_{STM}(\omega,K)|kl'J'\rangle \times(l'm_lSm_S|J'M)(lm_lSm_S|JM)Y_{l'm_l}(\Omega) \times Y_{lm_l}(\Omega)\Theta(k_F-|\vec{K}+\vec{k}|)\Theta(k_F-|\vec{K}-\vec{k}|) \quad (7)$$

with Ω being the angle between the direction of the relative momentum $\vec{k}$ and the center-of-mass momentum $\vec{K}$. In the calculations discussed below we consider the coupling of partial waves up to $J,J'\leq 6$. For angular momenta larger than 6, the Born approximation is used. If the matrix elements of G are diagonal in the total angular momentum ($J=J'$) and independent of the projection quantum number M, as it is the case in the angle-average approximation for the Pauli operator, this expression can be rewritten as

$$\frac{E}{A}=\frac{3}{5}\frac{k_F^2}{2m}+\frac{6}{k_F^3}\sum_{T,S,l,J}(2T+1)(2J+1)\int_0^{k_F}dk\,k^2 \times\left[\int_0^{k_F-k}dK\,K^2+\int_{k_F-k}^{\sqrt{k_F^2-k^2}}dK\,K^2\frac{k_F^2-K^2-k^2}{2Kk}\right] \times\langle klJ|G_{ST}(\omega,K)|klJ\rangle, \quad (8)$$

which corresponds to the standard expression discussed, e.g., in [4].

Results for the calculated binding energy per nucleon as a function of the Fermi momentum are displayed in Fig. 1, considering various *NN* potentials. The continuous choice (figures in the upper half) as well as the conventional choice were used for the single-particle spectrum. For each density, *NN* interaction, and particle state spectrum, a self-consistent single-particle spectrum has been determined using the effective mass parametrization defined in Eq. (3). The total binding energy has then been calculated using the angle-average approximation for the Pauli operator (dashed lines) as well as the exact treatment (solid lines).

A general feature can be observed, which is independent of the *NN* interaction and the choice for the single-particle spectrum: The angle-average approximation tends to underestimate the binding energy per nucleon at low densities but overestimates it at higher densities. The effects of the exact treatment of the Pauli operator is not very large around and below the empirical value for the saturation density. This is in agreement with older studies of the angle-averaged approximation [18,20], in which matrix elements of G were compared at those small densities. The characteristic density dependence for the exact treatment of the Pauli operator, however, leads to a non-negligible shift in the calculated saturation, i.e., the minimum in the energy versus density curve. This correction moves the calculated saturation points to smaller densities and smaller energies. It is worth noting that the saturation points calculated for the Bonn C potential ($E=-14.97$ MeV at $k_F=1.42$ fm^{-1}) and the neutron-proton part of Argonne V_{18} potential ($E=-13.89$ MeV at $k_F=1.37$ fm^{-1}) are rather close to the empirical value.

The effects of an exact treatment of the Pauli operator are larger for the continuous choice of the single-particle spectrum than for the conventional one. This is quite plausible as the continuous choice yields a larger sensitivity to the proper treatment of states around the Fermi momentum. A similar argument can be used to explain the fact that the Pauli effects are larger for *NN* potentials which have a slightly stronger tensor force (Bonn C and Argonne V_{18}) than is observed for the Bonn B potential, which contains a weaker tensor component.

In summary we would like to point out that the effects of an exact treatment of the Pauli operator in the Bethe-Goldstone equation are not very dramatic in particular for nuclear matter at small densities. A characteristic density dependence of these Pauli corrections, however, lead to a non-negligible improvement in the calculated saturation points. Therefore, many-body calculations going beyond the BHF approximation should take these effects into account.

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[1] K. Brueckner, R. J. Eden, and N. C. Francis, Phys. Rev. **100**, 891 (1955).
[2] H. A. Bethe, Annu. Rev. Nucl. Sci. **21**, 933 (1971).
[3] B. D. Day, Rev. Mod. Phys. **39**, 719 (1967).
[4] M. I. Haftel and F. Tabakin, Nucl. Phys. **A158**, 1 (1970).
[5] R. V. Reid, Ann. Phys. (N.Y.) **50**, 411 (1968).
[6] F. Coester, S. Cohen, B. D. Day, and C. M. Vincent, Phys. Rev. C **1**, 769 (1970).
[7] V. R. Pandharipande and R. B. Wiringa, Rev. Mod. Phys. **51**, 821 (1979).
[8] B. D. Day, Phys. Rev. C **24**, 1203 (1981).
[9] H. Q. Song, M. Baldo, G. Giansiracusa, and U. Lombardo, Phys. Lett. B **411**, 237 (1997).
[10] J. P. Jeukenne, A. Lejeunne, and C. Mahaux, Phys. Rep. **25**, 83 (1976).
[11] M. R. Anastasio, L. S. Celenza, W. S. Pong, and C. M. Shakin, Phys. Rep. **100**, 327 (1983).
[12] R. Brockmann and R. Machleidt, Phys. Rev. C **42**, 1965 (1990).
[13] B. ter Haar and R. Malfliet, Phys. Rep. **149**, 207 (1987).
[14] V. G. J. Stoks, R. A. M. Klomp, C. P. F. Terheggen, and J. J. de Swart, Phys. Rev. C **49**, 2950 (1994).
[15] R. B. Wiringa, V. G. J. Stoks, and R. Schiavilla, Phys. Rev. C **51**, 38 (1995).
[16] R. Machleidt, F. Sammarruca, and Y. Song, Phys. Rev. C **53**, R1483 (1996).
[17] L. Engvik, M. Hjorth-Jensen, R. Machleidt, H. Müther, and A. Polls, Nucl. Phys. **A627**, 85 (1997).
[18] T. Cheon and E. F. Redish, Phys. Rev. C **39**, 331 (1989).
[19] R. Machleidt, Adv. Nucl. Phys. **19**, 189 (1989).
[20] W. Legindgaard, Nucl. Phys. **A297**, 429 (1978).