Eur. Phys. J. A **11**, 271–275 (2001)

THE EUROPEAN PHYSICAL JOURNAL A

Thermodynamic consistency for nuclear matter calculations

P. Bożek[a] and P. Czerski

Institute of Nuclear Physics, PL-31-342 Kraków, Poland

Received: 8 February 2001 / Revised version: 4 June 2001
Communicated by A. Molinari

Abstract. We investigate the relation between the binding energy and the Fermi energy and between different expressions for the pressure in cold nuclear matter. For a self-consistent calculation based on a Φ derivable T-matrix approximation with off-shell propagators, the thermodynamic relations are well satisfied unlike for a G-matrix or a T-matrix approach using quasi-particle propagators in the ladder diagrams.

PACS. 21.65.+f Nuclear matter

1 Introduction

Nuclear matter calculations are usually performed using Brueckner-type resummation of ladder diagrams. Works using realistic interactions lead to reasonable results for the saturation density and the binding energy at the saturation point. However, in violation of the Hugenholz-Van Hove theorem the resulting Fermi energy $E_{\rm F}$ at the saturation point is usually very different from the binding energy per particle E/N. It is a manifestation of a general violation of thermodynamic consistency by the G-matrix approximation. The problem was discussed in the literature [1,2] and improvements due to rearrangement terms were invoked but without removing the discrepancy altogether. Improvement of the fulfillment of the Hugenholz-Van Hove property with respect to the G-matrix approximation is observed when using the quasi-particle T-matrix approach, or correction from hole-hole lines [1,2].

On the other hand, it is known that the exact theory [3–5] should fulfill certain thermodynamical relations. The simplest one being the exact equality of the Fermi momenta for the free and the interacting theory. Another statement that we shall consider in the present work is the equivalence of two ways of calculating the pressure in a system at zero temperature:

$$P = \rho^2 \frac{\partial (E/N)}{\partial \rho} = \tag{1}$$

$$\rho (E_{\rm F} - E/N) \,, \tag{2}$$

where ρ is the nuclear matter density. From the above relation follows that, at the saturation point where (E/N) has a minimum,

$$E_{\rm F} = E/N \,, \tag{3}$$

i.e., the Hugenholz-Van Hove property. These relations are satisfied by the exact theory and can also be satisfied in a perturbative calculation to a given order of the expansion parameter.

Non-perturbative approximations schemes which are thermodynamically consistent are known [5]. Baym has shown that the condition of the thermodynamical consistency of an approximation can be related to the so-called Φ derivability. The self-energy is constructed as a functional derivative of a functional Φ of dressed propagators $G(k)$ and bare vertices

$$\Sigma(k) = \frac{\delta \Phi}{\delta G(k)} \,. \tag{4}$$

The approximate functional Φ is defined by a set of two-particle irreducible diagrams. Φ derivable approximations to the self-energy are also termed as conserving approximations since they lead to conservation laws in corresponding transport equations [6]. In particular, different types of non-perturbative approximations can be identified for the generating functional. Below, we shall consider two of them: the Hartree-Fock approximation and the T-matrix approximation (fig. 1). Diagrams for the corresponding self-energies obtained by taking a functional derivative are also shown in fig. 1. It must be stressed again that the propagators in the diagrams for Φ are dressed self-consistently by the self-energy (4). For the Hartree-Fock approximation it means only a shift in the single-particle energies, but for the T-matrix approach one has to take into account the full spectral function for the propagators in the calculation of Φ or Σ. Calculations involving off-shell propagators in the T-matrix ladder have been recently performed [7–10] both in the normal and in the superfluid phase. Below, we shall restrict ourselves to zero-temperature normal nuclear matter.

[a] e-mail: bozek@solaris.ifj.edu.pl

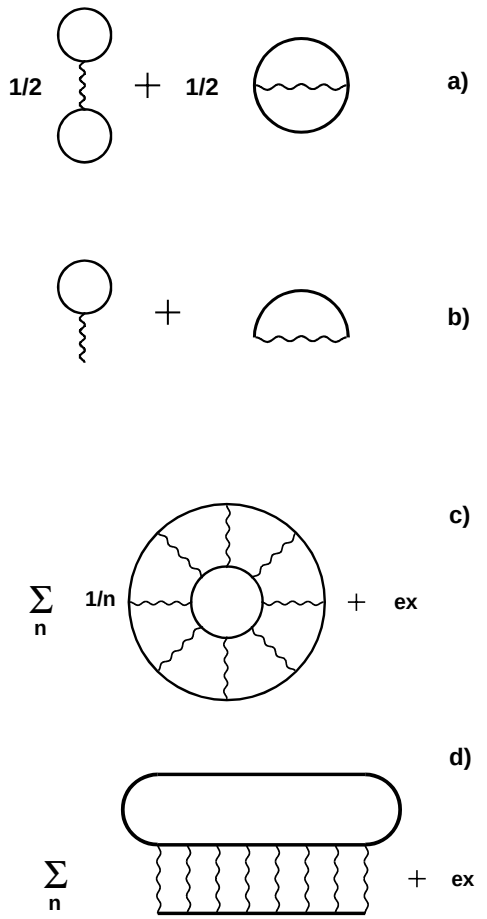

Fig. 1. Diagrams contributing to the generating functional Φ in the Hartree-Fock approximation (a)) and in the T-matrix approximation (c)). The corresponding diagrams for the self-energy are shown in parts b) and d), respectively.

2 Approximations for the nuclear matter problem

We shall compare different calculation of cold nuclear matter with a model interaction. We choose a separable rank two parameterization of Mongan type [11] in the S wave with softened repulsive core

$$V_\alpha(k,p) = \lambda^r_\alpha g^r_\alpha(k) g^r_\alpha(p) - \lambda^a_\alpha g^a_\alpha(k) g^a_\alpha(p), \qquad (5)$$

with $g^{r,a}(p) = \frac{1}{p^2+\beta^2_{r,a}}$ and

$$\begin{aligned} &\lambda^r = 29.6\,\mathrm{GeV}^2, && \beta^r = 639\,\mathrm{MeV}, \\ &\lambda^a = 2.91\,\mathrm{GeV}^2, && \beta^a = 352\,\mathrm{MeV}, \quad \text{for} \quad \alpha = S^1_0, \\ &\lambda^r = 5.27\,\mathrm{GeV}^2, && \beta^r = 471\,\mathrm{MeV}, \\ &\lambda^a = 4.78\,\mathrm{GeV}^2, && \beta^a = 376\,\mathrm{MeV}, \quad \text{for} \quad \alpha = S^3_1. \end{aligned} \qquad (6)$$

With this interaction, nuclear matter properties will be calculated within the following approximations:

– Brueckner resummation of particle-particle ladder diagrams with in medium G-matrix

$$\begin{aligned} \langle \mathbf{p}|G(\mathbf{P},\Omega)|\mathbf{p}'\rangle &= V(\mathbf{p},\mathbf{p}') \\ &+ \int \frac{\mathrm{d}^3q}{(2\pi)^3} V(\mathbf{p},\mathbf{q}) \frac{(1-f(\omega_{p_1}))(1-f(\omega_{p_2}))}{\Omega - \omega_{p_1} - \omega_{p_2}} \\ &\times \langle \mathbf{q}|G(\mathbf{P},\Omega)|\mathbf{p}'\rangle, \end{aligned} \qquad (7)$$

where $\mathbf{p}_{1,2} = \mathbf{P}/2 \pm \mathbf{q}$. G-matrix resummation allows to define single-particle energies and gives relatively good results for the saturation properties of nuclear matter. In the above equation and in the following we skip the spin, isospin indices which are implicitly summed over. Medium effects enter through the Pauli blocking factors $1 - f(\omega_p)$ in the numerator and single-particle energies ω_p in the denominator ($f(\omega_p) = \Theta(E_\mathrm{F} - \omega_p)$). The single-particle energies ω_p, are self-consistently defined by the G-matrix

$$\omega_p = \frac{p^2}{2m} + U(p,\omega_p), \qquad (8)$$

where

$$\begin{aligned} U(p,\omega) &= \int \frac{\mathrm{d}^3k}{(2\pi)^3} f(\omega_k) \\ &\times \langle (\mathbf{p}-\mathbf{k})/2|G(|\mathbf{p}+\mathbf{k}|, \omega_k + \omega)|(\mathbf{p}-\mathbf{k})/2\rangle. \end{aligned} \qquad (9)$$

For the G-matrix approach, much more realistic potentials are commonly used in nuclear matter calculations. However, the aim of the present paper is to compare different approximation schemes for a simple separable potential. The violation of the Hugenholz-Van Hove theorem is general for all G-matrix calculation independent of the potential assumed [1,12], also for realistic non-separable potentials. There is some dependence on the assumed single-particle energies [1].

– In the quasi-particle T-matrix approximation [13,14], the ladder diagrams include both particle-particle and hole-hole propagation. The Pauli blocking factor $(1 - f(\omega_{p_1}))(1 - f(\omega_{p_2}))$ in the G-matrix equation is replaced by $1 - f(\omega_{p_1}) - f(\omega_{p_2})$ in the equation for the retarded T-matrix

$$\begin{aligned} \langle \mathbf{p}|T(\mathbf{P},\Omega)|\mathbf{p}'\rangle &= V(\mathbf{p},\mathbf{p}') \\ &+ \int \frac{\mathrm{d}^3q}{(2\pi)^3} V(\mathbf{p},\mathbf{q}) \frac{(1-f(\omega_{p_1})-f(\omega_{p_2}))}{\Omega - \omega_{p_1} - \omega_{p_2} + i\epsilon} \\ &\times \langle \mathbf{q}|T(\mathbf{P},\Omega)|\mathbf{p}'\rangle. \end{aligned} \qquad (10)$$

The imaginary part of the retarded self-energy in the T-matrix approximation is

$$\begin{aligned} \mathrm{Im}\Sigma(p,\omega) &= \int \frac{\mathrm{d}^3k}{(2\pi)^3} \Big(f(\omega_k) + b(\omega + \omega_k) \Big) \\ &\times \langle (\mathbf{p}-\mathbf{k})/2|\mathrm{Im}T(|\mathbf{p}+\mathbf{k}|, \omega_k + \omega)|(\mathbf{p}-\mathbf{k})/2\rangle, \end{aligned} \qquad (11)$$

where $b(\omega)$ is the Bose distribution. The above formula can be obtained using the spectral representation for the nucleon Green's function and for the T-matrix (here the Bose function appears) [15]. The real part of the self-energy consists of the Hartree-Fock self-energy and a dispersive contribution obtained from $\mathrm{Im}\Sigma$:

$$\mathrm{Re}\Sigma(p,\omega) = \Sigma_\mathrm{HF}(p) + \mathcal{P} \int \frac{\mathrm{d}\omega'}{\pi} \frac{\mathrm{Im}\Sigma(p,\omega')}{\omega' - \omega}\,. \qquad (12)$$

The imaginary part of the self-energy is neglected leading to the quasi-particle approximation for the two-nucleon propagator in the T-matrix (eq. (10)).

– Allowing for off-shell propagation of nucleons and taking the self-energy self-consistently (also its imaginary part) requires the use of full spectral functions in the calculation resulting in more complicated expressions for the T-matrix and the self-energy [7,8]:

$$\langle \mathbf{p}|T(\mathbf{P},\Omega)|\mathbf{p}^{'}\rangle = V(\mathbf{p},\mathbf{p}^{'}) + \int \frac{\mathrm{d}\omega_1}{2\pi}\int \frac{\mathrm{d}\omega_2}{2\pi}\int \frac{\mathrm{d}^3q}{(2\pi)^3} V(\mathbf{p},\mathbf{q}) \frac{\big(1-f(\omega_1)-f(\omega_2)\big)}{\Omega-\omega_1-\omega_2+i\epsilon} \times A(p_1,\omega_1)A(p_2,\omega_2)\langle \mathbf{q}|T(\mathbf{P},\Omega)|\mathbf{p}^{'}\rangle, \quad (13)$$

and

$$\mathrm{Im}\Sigma(p,\omega) = \int \frac{\mathrm{d}\omega_1}{2\pi}\int \frac{\mathrm{d}^3k}{(2\pi)^3} A(k,\omega_1) \times \langle (\mathbf{p}-\mathbf{k})/2|\mathrm{Im}T(\mathbf{p}+\mathbf{k},\omega+\omega_1)|(\mathbf{p}-\mathbf{k})/2\rangle \times \Big(f(\omega_1)+b(\omega+\omega_1)\Big), \quad (14)$$

where

$$A(p,\omega) = \frac{-2\mathrm{Im}\Sigma(p,\omega)}{\Big(\omega - p^2/2m - \mathrm{Re}\Sigma(p,\omega)\Big)^2 + \mathrm{Im}\Sigma(p,\omega)^2} \quad (15)$$

is the self-consistent spectral function of the nucleon.

– Finally, we present results for a simple Hartree-Fock approximation. It is certainly not well suited for realistic applications in nuclear matter. However, this approach is Φ derivable and it is illustrative to check its thermodynamic consistency explicitly. The Hartree-Fock approximation with parameters given by eq. (6) shows no saturation. We reduced the repulsive part of the interaction λ_α^r by 1.15 for the Hartree-Fock calculation. This rescaling mimics the effect of ladder resummation which leads to a reduction of the repulsive core.

Equations for all the approximations schemes have to be solved iteratively, with a constraint on the total density. The numerical method for the solution of the T-matrix equation with off-shell propagators [9] has been generalized to the case of low and zero temperature. The details of the numerical procedure will be given elsewhere.

3 Results for thermodynamic properties around the saturation point

Only within the self-consistent T-matrix calculation is the momentum distribution of nucleons

$$n(p) = \int_{-\infty}^{\mu} \frac{\mathrm{d}\omega}{2\pi} A(p,\omega) \quad (16)$$

different from the Fermi-Dirac distribution (fig. 2). Clearly, a Fermi-liquid behavior is observed in the T-matrix approximation, with a jump in the fermion density

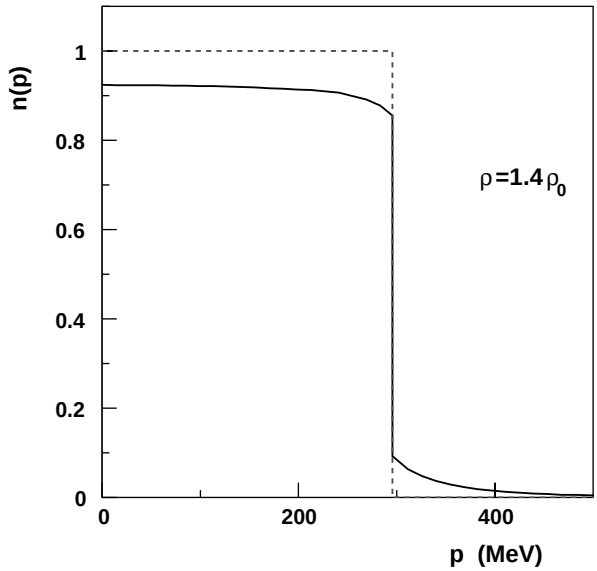

Fig. 2. Momentum distribution of nucleons for the full T-matrix calculation compared to the free fermion distribution.

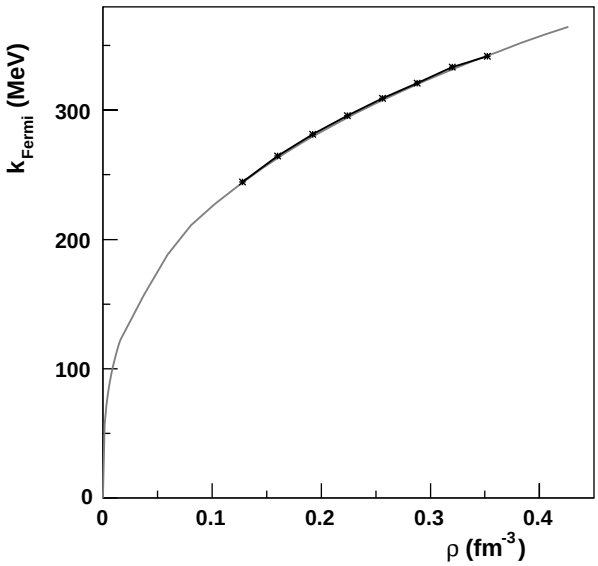

Fig. 3. Fermi momentum as obtained in the full T-matrix calculation (points) compared to the Fermi momentum of the free fermion gas (solid line).

of $\left(1-\frac{\partial \mathrm{Re}\Sigma(p_\mathrm{F},\omega)}{\partial\omega}|_{\omega=E_\mathrm{F}}\right)^{-1} \simeq 0.7$ at the Fermi momentum. In the calculation, the chemical potential $\mu = E_\mathrm{F}$ is fixed by the constraint on the total density

$$\int_{-\infty}^{\mu} \frac{\mathrm{d}\omega}{2\pi}\int \frac{\mathrm{d}^3p}{(2\pi)^3} A(p,\omega) = \rho\,. \quad (17)$$

The corresponding Fermi momentum p_F is defined by $E_\mathrm{F} = \omega_{p_\mathrm{F}}$. For a conserving approximation, the Fermi momentum should be the same as the Fermi momentum of a free fermion gas [16,5]. Indeed, it is well satisfied for a range of densities for the self-consistent T-matrix calculation (fig. 3). All the other approximation discussed in

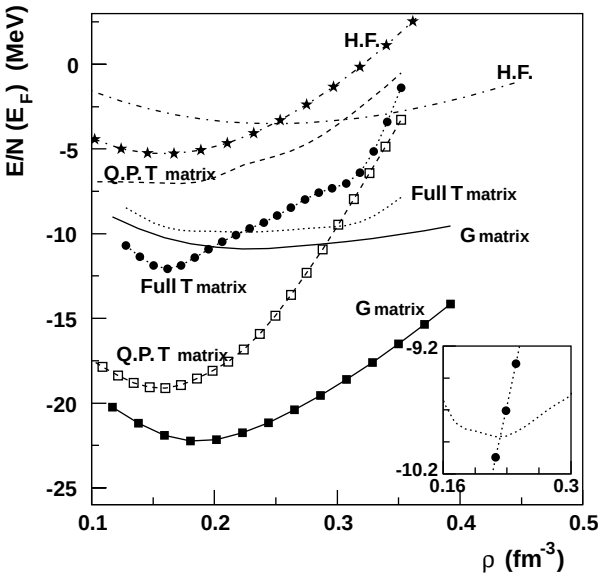

Fig. 4. Binding energy per particle for the G-matrix calculation (solid line), the on-shell T-matrix calculation (dashed line), the full T-matrix calculation (dotted line) and the Hartree-Fock calculation (dash-dotted line) as a function of the density. The corresponding Fermi energies are denoted by the same lines with solid boxes, open boxes, full circles and stars for the G-matrix, on-shell T-matrix, full T-matrix and Hartree-Fock results, respectively. In the insert is shown a blow-up of the region around the saturation point for the full T-matrix calculation.

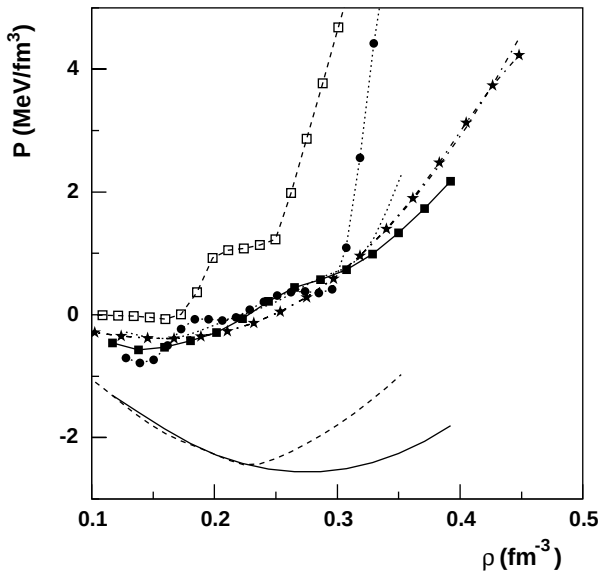

Fig. 5. Pressure obtained using eq. (2) for the G-matrix calculation (solid line), the on-shell T-matrix calculation (dashed line), the full T-matrix calculation (dotted line) and the Hartree-Fock calculation (dash-dotted line) as a function of the density. The corresponding pressures obtained as a derivative of the binding energy (eq. (1)) are denoted by the same lines with solid boxes, open boxes, full circles and stars for the G-matrix, on shell T-matrix, full T-matrix and Hartree-Fock results, respectively.

Table 1. Saturation density, Fermi energy, binding energy and compression modulus for different approximations discussed in the text.

approximation	ρ_s/ρ_0	$E_{\rm F}$ (MeV)	E/N (MeV)	$\mathcal{K}$ (MeV)
Hartree-Fock	1.55	−3.5	−3.5	87
G-matrix	1.42	−21.6	−10.9	107
T-matrix on shell	1.08	−18.9	−7.0	103
T-matrix	1.39	−9.9	−9.9	103

this work fulfill this relation trivially since they use quasi-particles.

The energy per particle in the different approximations can be obtained from the standard form of the energy density

$$E/N = \frac{1}{\rho}\int \frac{\mathrm{d}^3p}{(2\pi)^3}\int_{-\infty}^{\mu}\frac{\mathrm{d}\omega}{2\pi}\frac{1}{2}\left(\frac{p^2}{2m}+\omega\right)A(p,\omega)\,. \quad (18)$$

Only for the self-consistent T-matrix the spectral function and the ω integration are non-trivial. For the other approximation schemes the spectral function is a delta function. In that case, the energy per particle can be expressed in the usual way using the single-particle potential and kinetic energies.

In fig. 4 is plotted the energy per particle for different approximations for a range of densities around the saturation density. The G-matrix and the full T-matrix calculations give very similar results for the binding energy. The T-matrix with quasi-particle propagators gives somewhat different results, with lower saturation density and smaller binding energy. This behavior is due to very strong modifications of the effective mass around the Fermi momentum in the quasi-particle T-matrix approach. This effect is caused by the appearance of the pairing singularity in the T-matrix [14,17,9]. In fact, the quasi-particle T-matrix approximation is oversensitive to the presence of the pairing singularity, since the use of full spectral functions reduces the influence of the Cooper pair bound state on the nucleon spectral function and the single-particle energies [9,18].

In table 1 are shown the corresponding binding energies and saturation densities. The Hartree-Fock approximation gives significantly different results. It has a saturation point only after a change of the parameters. The Fermi energy obtained for different densities depends very much on the approximation chosen. Only for consistent approaches, *i.e.* Hartree-Fock and self-consistent T-matrix, is the Hugenholz-Van Hove condition at the saturation point satisfied. The difference between $E_{\rm F}$ and E/N at the saturation point is zero within numerical accuracy for the Hartree-Fock and the self-consistent T-matrix calculations, and becomes as large as 10.7 MeV for the G-matrix and 10.9 MeV for the quasi-particle T-matrix approximations. In the case where the pairing effect is strong (as in this work), the use of the quasi-particle T-matrix does not cure the violation of the Hugenholz-Van Hove property and moreover deforms the results for the binding

energy and the effective mass [17,18]. It is different from ref. [2] where the use of on-shell (*i.e.* non-self-consistent) T-matrix approximation instead of the G-matrix reduces the violation of the Hugenholz-Van Hove theorem at the saturation point. It should be noted that, besides the strong pairing force in our calculation, the overall violation of the Hugenholz-Van Hove is stronger in the G-matrix approach than for relativistic interactions used in ref. [2]. We observe a very good fulfillment of the Hugenholz-Van Hove condition in the numerical solutions for Φ derivable approaches with self-energies self-consistently taken into account, which means for the T-matrix calculation the use of self-consistent spectral functions in the propagators.

The pressure can be calculated for a range of densities by two methods (eqs. (1),(2)) which should be equivalent. However, only for the consistent approximations, we find an approximate equivalence between the two formulas, with very good agreement for the Hartree-Fock calculation (fig. 5). On the other hand, non-consistent approaches give very different results. In particular, the point where the pressure equals zero and the slope of the pressure *vs.* density comes out differently for the two ways of calculating the pressure. The slope of the pressure as a function of the density defines the compression modulus of nuclear matter

$$\mathcal{K} = 9\frac{\partial P}{\partial \rho}\,, \tag{19}$$

which should be positive at the saturation point, as a condition of stability.

As expected [19], non-consistent approximations give reasonable results for the binding energy and not for the Fermi energy. Thus, one should use eq. (1) for the calculation of thermodynamic properties (in particular $\mathcal{K} = 9\frac{\partial}{\partial\rho}\left(\rho^2\frac{\partial}{\partial\rho}\left(\frac{E}{N}\right)\right)$). The compression modulus for different approximations is given in table 1. Its value is similar for different approximations using ladder resummation. The values of $\mathcal{K}$ obtained are smaller than in usual nuclear matter calculations because we reduced the strength of the repulsive core.

4 Conclusion

We have investigate the thermodynamical consistency of different approximations for nuclear matter. The Φ derivable T-matrix approximation with off-shell propagators is thermodynamically consistent (conserving) and fulfills these relations. The same is true for the simple Hartree-Fock approximation. On the other hand, the usual G-matrix approximation violates badly the Hugenholz-Van Hove relation for pressure at zero temperature. The disagreement is not reduced when using a simplified version of the T-matrix approach, *i.e.* when using the T-matrix with on-shell quasi-particle propagators. The full T-matrix and the G-matrix calculations give similar results for E/N. The binding energy is a physical result that can be used for the calculation of the pressure or compression modulus also in the non-consistent G-matrix approach. The same is not true for the Fermi energy which, for non-consistent approaches, is unreliable and leads often to unphysical results, if used in the thermodynamical relations. We note that the use of the quasi-particle approximation in the T-matrix resummation can lead to wrong results for the the binding and Fermi energies if the effect of pairing is important. This is true in the normal phase, slightly above T_c [17,18] and in the expansion around the normal state at zero temperature, as in this work. This leads to results significantly different both from the usual G-matrix and from the full self-consistent T-matrix calculation. The self-consistent T-matrix and the G-matrix calculations are less sensitive to the fact that we have neglected the superfluid transition for cold nuclear matter [2,8,18].

This work was supported in part by the Polish Committee for Scientific Research (KBN) under Grant 2P03B02019.

References

1. M. Baldo, F. Bombaci, G. Giansiracusa, U. Lombardo, C. Mahaux, R. Sartor, Phys. Rev. C **41**, 1748 (1990).
2. F. de Jong, R. Malfliet, Phys. Rev. C **44**, 998 (1991).
3. N.M. Hugenholz, L. Van Hove, Physica **24**, 363 (1958).
4. J.M. Luttinger, J.C. Ward, Phys. Rev. **118**, 1417 (1960).
5. G. Baym, Phys. Rev. **127**, 1392 (1962).
6. L.P. Kadanoff, G. Baym, Phys. Rev. **124**, (1961) 287; L.P. Kadanoff, G. Baym, *Quantum Statistical Mechanics* (Benjamin, New York, 1962).
7. W.H. Dickhoff, Phys. Rev. C **58**, 2807 (1998); W.H. Dickhoff, C.C. Gearhart, E.P. Roth, A. Polls, A. Ramos, Phys. Rev. C **60** (1999), 4319.
8. P. Bożek, Phys. Rev. C **59**, 2619 (1999).
9. P. Bożek, Nucl. Phys. A **657**, 187 (1999).
10. Y. Dewulf, D. Van Neck, M. Waroquier, nucl-th/0012022.
11. T.R. Mongan, Phys. Rev. **178**, 1597 (1969).
12. P. Czerski, A. Molinari, A. de Pace, work in preparation.
13. B.E. Vonderfecht, W.H. Dickhoff, A. Polls, A. Ramos, Nucl. Phys. A **555**, 1 (1993).
14. T. Alm, G. Röpke, A. Schnell, N.H. Kwong, H.S. Kohler, Phys. Rev. C **53**, 2181 (1996).
15. T. Alm, G. Röpke, A. Schnell, H. Stein, Phys. Lett. B **346**, 233 (1995).
16. J.M. Luttinger, Phys. Rev. **119**, 1153 (1960).
17. A. Schnell, G. Röpke, P. Schuck, Phys. Rev. Lett. **83**, 1926 (1999).
18. P. Bożek, Phys. Rev. C **62**, 054316 (2000).
19. A.L. Fetter, J.D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971).