Thermodynamic consistency for nuclear matter calculations

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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 $\Phi$ 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.

Key words. nuclear matter – saturation point – thermodynamic properties – Hugenholz-Van Hove theorem

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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 $E_F$ 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 \cite{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 \cite{1,2}. On the other hand it is known that the exact theory \cite{3,4,5} 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:

\[ P = \rho^2 \frac{\partial (E/N)}{\partial \rho} \]

\[ = \rho (E_F - E/N) , \]

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

\[ E_F = E/N , \]

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 \cite{3}. Baym has shown that the condition of the thermodynamical consistency of an approximation can be related to the so called $\Phi$ derivability. The self-energy is constructed as a functional derivative of a functional $\Phi$ of dressed propagators $G(k)$ and bare vertices

\[ \Sigma(k) = \frac{\delta \Phi}{\delta G(k)} . \] (4)

The approximate functional $\Phi$ is defined by a set of two-particle irreducible diagrams. $\Phi$ derivable approximations to the self-energy are also termed as conserving approximations since they lead to conservation laws in corresponding transport equations \cite{3}. 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. \ref{fig:1}). Diagrams for the corresponding self-energies obtained by taking a functional derivative of $\Phi$ are also shown in Fig. \ref{fig:1}. It must be stressed again that the propagators in the diagrams for $\Phi$ are dressed self-consistently by the self-energy \cite{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 $\Phi$ or $\Sigma$. Calculations involving off-shell propagators in the $T^{-}$ matrix ladder have been recently performed \cite{8,9,10,11} both in the normal and in the superfluid phase. Below we shall restrict ourselves to zero temperature normal nuclear matter.
Fig. 1. Diagrams contributing to the generating functional $\Phi$ 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 in the $S$ wave with softened repulsive core

$$V_{\alpha}(k, p) = \chi_{\alpha} g_{\alpha}^r(k) g_{\alpha}^r(p) - \chi_{\alpha} g_{\alpha}^a(k) g_{\alpha}^a(p)$$

with $g^{\alpha\alpha}(p) = 1/p^2 + \beta_{\alpha\alpha}$ and

$$\chi^r = 29.6 GeV^2, \quad \beta^r = 639 MeV$$
$$\chi^a = 2.91 GeV^2, \quad \beta^a = 352 MeV \quad \text{for} \quad \alpha = S_0$$
$$\chi^r = 5.27 GeV^2, \quad \beta^r = 471 MeV$$
$$\chi^a = 4.78 GeV^2, \quad \beta^a = 376 MeV \quad \text{for} \quad \alpha = S_1$$

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

$$< p | G(\mathbf{P}, \Omega) | p' > = V(p, p') +$$
$$+ \int \frac{d^3q}{(2\pi)^3} V(p, q) \frac{(1 - f(\omega_{p_1}))(1 - f(\omega_{p_2}))}{\Omega - \omega_{p_1} - \omega_{p_2}}$$

$$< q | G(\mathbf{P}, \Omega) | p' > ,$$

where $p_{1,2} = P/2 \pm q$. $G$-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 $\omega_{p}$ in the denominator. The single particle energies $\omega_{p}$, are self-consistently defined by the G-matrix

$$\omega_{p} = \frac{p^2}{2m} + U(p, \omega_{p})$$

where

$$U(p, \omega) = \int \frac{d^3k}{(2\pi)^3} f(\omega_k)$$

$$< (p - k)/2 | G([p + k], \omega_k + \omega)(p - k)/2 > .$$

- In the quasi-particle $T$-matrix approximation 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

$$< p | T(\mathbf{P}, \Omega) | p' > = V(p, p') +$$
$$+ \int \frac{d^3q}{(2\pi)^3} V(p, q) \frac{(1 - f(\omega_{p_1}) - f(\omega_{p_2})}{\Omega - \omega_{p_1} - \omega_{p_2} + i\epsilon}$$

$$< q | T(\mathbf{P}, \Omega) | p' > .$$

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

$$\text{Im} \Sigma(p, \omega) = \int \frac{d^3k}{(2\pi)^3} \left( f(\omega_k) + b(\omega + \omega_k) \right)$$

$$< (p - k)/2 | \text{Im} T([p + k], \omega_k + \omega)(p - k)/2 >$$

where $b(\omega)$ is the Bose distribution. The real part of the self energy consists of the Hartree Fock self-energy and a dispersive contribution obtained from $\text{Im} \Sigma$

$$\text{Re} \Sigma(p, \omega) = \text{Re} \Sigma_{HF}(p) + \mathcal{P} \int \frac{dw}{\pi} \frac{\text{Im} \Sigma(p, w)}{w - \omega}.$$
– 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 \[ [9] \]

\[
\langle p|T(P, \Omega)|p'\rangle = V(p, p') + \int \frac{d\omega_1}{2\pi} \int \frac{d\omega_2}{2\pi} \int \frac{d^3q}{(2\pi)^3} V(p, q) \frac{(1 - f(\omega_1) - f(\omega_2))}{\Omega - \omega_1 - \omega_2 + i\epsilon} \]

\[
A(p_1, \omega_1)A(p_2, \omega_2) < q|T(P, \Omega)|p' >
\]

and

\[
\text{Im}\Sigma(p, \omega) = \int \frac{d\omega_1}{2\pi} \int \frac{d^3k}{(2\pi)^3} A(k, \omega_1)
\]

\[
< (p-k)/2|\text{Im}T(p+k, \omega+\omega_1)|(p-k)/2 >
\]

\[
\left( f(\omega_1) + b(\omega + \omega_1) \right)
\]

where

\[
A(p, \omega) = \frac{-2\text{Im}\Sigma(p, \omega)}{\left( \omega - p^2/2m - \text{Re}\Sigma(p, \omega) \right)^2} + \text{Im}\Sigma(p, \omega)^2
\]

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 $\Phi$ 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 $\lambda_\pi^r$ 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 \[ [10] \], 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

\[
n(p) = \int_{-\infty}^{\mu} \frac{d\omega}{2\pi} A(p, \omega)
\]

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 of

\[
1 - \left( 1 - \frac{\partial \text{Re}\Sigma(p, \omega)}{\partial \omega} \right) \bigg|_{\omega=E_F}^{-1} \simeq .7
\]
at the Fermi momentum.

In the calculation the chemical potential $\mu = E_F$ is fixed by the constraint on the total density

\[
\int_{-\infty}^{\mu} \frac{d\omega}{2\pi} \int \frac{d^3p}{(2\pi)^3} A(p, \omega) = \rho
\]

The corresponding Fermi momentum $p_F$ is defined by $E_F = \omega_{pF}$. For a conserving approximation the Fermi
momentum should be the same as the Fermi momentum of a free fermion gas. Indeed it is well satisfied for a range of densities for the self-consistent $T$-matrix calculation. 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. In the insert is shown a blow up of the region around the saturation point for the full $T$-matrix calculation.

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

$$E/N = \frac{1}{\rho} \int \frac{d^{3}p}{(2\pi)^{3}} \frac{d\omega}{2\pi} \left( \frac{p^{2}}{2m} + \omega \right) A(p, \omega) f(\omega).$$

Only for the self-consistent $T$-matrix the spectral function and the $\omega$ integration is nontrivial. For the other approximations 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. 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.

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. 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 versus density comes out differently for the two ways of calculating the pressure. The slope of the pressure as function of density defines the compression modulus of

| Approximation     | $\rho_{s}/\rho_{0}$ | $E_{F}$ (MeV) | $E/N$ (MeV) | $K$ (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       |

Table 1. Saturation density, Fermi energy, binding energy and compression modulus for different approximations discussed in the text.
The disagreement is reduced but not cured completely when using the superfluid transition for cold nuclear matter.

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