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Choice of finite-temperature single-particle potential and preservation of thermodynamic relations

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A method for choosing and deriving a suitable single-particle potential for many-body calculations at finite temperature is suggested. With this potential one can readily determine the self-consistent correlated chemical potential and consequently the resulting equations of state rigorously satisfy a number of basic thermodynamic relations. Application of our method to a Brueckner-Hartree-Fock nuclear matter calculation yields results in remarkably good agreement with the Hugenholtz–Van Hove theorem.

Introduction. Nuclear matter equations of state (EOS) are a subject of much current interest.[1] There have been numerous attempts to derive them microscopically, starting from a given nuclear Hamiltonian. In doing so, there is nevertheless a basic and rather subtle difficulty. Clearly we cannot calculate the various thermodynamic quantities of nuclear matter exactly; we must make some approximations such as the Hartree-Fock (HF) and the Brueckner-Hartree-Fock (BHF) approximation. Many of these approximations are, however, nonconserving[2] in the sense that the thermodynamic quantities obtained with these approximations are not compatible with certain fundamental thermodynamic relations.

A well-known case is the zero-temperature BHF theory of nuclear matter; it very seriously violates[2–4] the Hogenholtz–Van Hove (HVH) theorem.[5] Several authors[6,2–4] have suggested that this violation may be largely reduced if certain two-body cluster contributions to the mass operator are included. To carry out finite-temperature EOS calculations one has to first find a suitable method to overcome the above nonconserving difficulty; to our knowledge rather little seems to have been done in this area.

In this Brief Report we wish to propose a general and fairly convenient method for choosing an auxiliary single particle (s.p.) potential U such that the resulting EOS and several related thermodynamic quantities can rigorously satisfy certain basic thermodynamic relations. We shall describe the definition and derivation of such a potential in the next section. A main point is that this U must be chosen in consistence with the approximations adopted in the calculation of the thermodynamic potential Ω. For example, if one chooses to calculate Ω with certain classes of ring diagrams[7] summed up to all orders, then one should employ a corresponding ring-diagram s.p. potential U^{Ring}. And if one decides to calculate Ω using a HF approximation, then a corresponding HF s.p. potential U^{HF} must be employed. A central advantage of doing so is that we can determine the self-consistent correlated potential rigorously and with convenience. It is primarily because of this that we are able to preserve a number of basic thermodynamic relations. We have carried out some preliminary numerical calculations to verify the validity of our method. As presented in the application and discussion section, the results of our nuclear matter calculations using the Bonn (k-space) (Ref. 8) potential fulfill the HVH theorem remarkably well. Some additional results and general discussions related to our approach are also presented in this section.

Formalism. A standard starting point for carrying out microscopic calculations of many-body systems at finite temperature is the thermodynamic potential Ω which can be expressed as a linked-diagram expansion.[7] Let us introduce an auxiliary s.p. potential U and rewrite the nuclear Hamiltonian H as $(T_{\text{KE}}+U)+(V_{NN}-U)\equiv H_0+H_1$. T_{KE} and V_{NN} represent respectively the kinetic energy and the nucleon-nucleon (NN) interaction. The s.p. energies and wave functions defined by H_0 are denoted respectively by ϵ_i and $|i\rangle$. One hopes to choose a U such that certain important properties of H are well approximated by those of H_0. But how to choose such a U? For the zero-temperature case this problem has been rather extensively studied.[9,10] Here we wish to study a method for deriving a suitable U for finite-temperature many-body calculations.

The unperturbed thermodynamic potential Ω_0 corresponding to H_0 is

$$\Omega_0=\sum_k \tilde{\epsilon}_k f_k+\frac{1}{\beta}\sum_k (f_k \ln f_k+\bar{f}_k \ln \bar{f}_k) \;, \tag{1}$$

where f_k is the Fermi-Dirac distribution function $[1+\exp(\beta\tilde{\epsilon}_k)]^{-1}$, $\bar{f}_k=1-f_k$, and β is the inverse temperature $1/(k_B T)$, k_B being the Boltzmann constant. Note that $\tilde{\epsilon}_k=\epsilon_k-\mu$ where μ is the chemical potential. For simplicity, it has been a common practice to determine μ from the familiar relation

$$\rho=\frac{1}{V}\sum_k f_k \;, \tag{2}$$

where ρ is the density of the system and V its volume. This gives only the zeroth order chemical potential μ_0. [Eq. (2) is equivalent to $\rho V=-(\partial\Omega_0/\partial\mu)_{\text{TV}}$ if $(\partial\epsilon_k/\partial\mu)_{\text{TV}}=0$.] Rigorously, one should derive μ from the relation $\rho V=-(\partial\Omega/\partial\mu)_{TV}$ where Ω is the full thermodynamic potential corresponding to H. As given in Fetter and Walecka,[11] corrections to μ_0 may be studied via a perturbation expansion $\mu=\mu_0+\mu_1+\mu_2+\cdots$ where μ_n denotes the correction nth order in the interaction. We shall discuss in the following a different and simpler approach for determining μ in a self-consistent way. We have found, as to be discussed later, that μ and μ_0 can in general be very different from each other and it is essential to employ μ calculated in consistence with Ω in EOS calculations.

The thermodynamic potential Ω corresponding to H can be written as a linked-diagram expansion[7]

$$\Omega=\Omega_0+\Omega_{\rm int}=\Omega_0-\sum_k U_k f_k+\Omega'_{\rm int} \ . \tag{3}$$

Some representative diagrams of $\Omega_{\rm int}$, the interacting part of Ω, are given in Fig. 1. Because $H_1=V_{NN}-U$, $\Omega_{\rm int}$ contains diagrams with $-U$ vertices. The lowest-order diagram of this type is diagram (i) given by $\sum_k U_k f_k$. We define $\Omega'_{\rm int}$ as $\Omega_{\rm int}$ with diagram (i) subtracted. Diagram (ii) is the familiar HF interaction diagram. Diagram (iii) is a fourth-order particle-particle hole-hole ring diagram[7] of $\Omega_{\rm int}$.

For a given $\Omega_{\rm int}$, let us require that the chosen s.p. potential satisfy the subsidiary condition

$$\sum_k U_k \left[\frac{\partial f_k}{\partial \mu}\right]_{TV}=\left[\frac{\partial \Omega'_{\rm int}}{\partial \mu}\right]_{TV} . \tag{4}$$

This condition and Eq. (1) imply that

$$\rho=-\frac{1}{V}\left[\frac{\partial}{\partial\mu}(\Omega_0+\Omega_{\rm int})\right]_{TV}=\frac{1}{V}\sum_k f_k \ , \tag{5}$$

which is a rather important result. It means that with the s.p. potential chosen according to Eq. (4) the true or correlated chemical potential μ given by $\rho V=-(\partial\Omega/\partial\mu)_{TV}$ is exactly reproduced by the "unperturbed" μ_0 obtained by Eq. (2). In other words, the above choice of U ensures $\mu=\mu_0$. Equation (5) has also the important implication that the physical density corresponding to Ω is given by $(1/V)\sum_k f_k$. Note that in deriving Eq. (5) we have made use of the relation $(\partial\epsilon_k/\partial\mu)_{TV}=(\partial U_k/\partial\mu)_{TV}$.

The above choice of U also ensures that the free energy density given by $f=(\Omega_0+\Omega_{\rm int})/V+\mu\rho$ rigorously satisfies the fundamental relation

$$\left[\frac{\partial f}{\partial \rho}\right]_T=\mu \ . \tag{6}$$

The independent variables used in most finite-temperature calculations are ρ and T. Thus one customarily calculates p by way of the free energy F, namely $p=-(\partial F/\partial V)_{TN}=\rho(\partial f/\partial\rho)_T-f$. In so doing, however, we must employ the appropriately calculated F. We may calculate it by way of $F=\Omega+\mu N$ where μ must be determined in consistence with Ω. Our present choice of the s.p. potential enables us to obtain readily such a μ and consequently F can be readily calculated. Thus, the validity of Eq. (6) is assured and the above expression for pressure becomes

$$p=\rho\mu-f=-\frac{\Omega}{V} \ . \tag{7}$$

Hence, our present method entitles us to calculate p using either $-(\partial F/\partial V)_{TN}$ or simply $-\Omega/V$. The latter is clearly more direct and convenient as the calculation of Ω is usually the first step in any finite-temperature many-body calculation.

As temperature tends to zero, Eq. (7) becomes

$$\frac{p}{\rho}=\epsilon_F-\frac{E_0}{N} \ , \tag{8}$$

where ϵ_F is the Fermi energy obtained with our present s.p. potential, which ensures $\mu=\mu_0$, and E_0/N is the ground-state energy per particle. Note that Eq. (8) is just the familiar HVH theorem.[5] Thus our choice of the s.p. potential ensures that this theorem is automatically satisfied.

The above choice of the s.p. potential also leads to a simpler formula for evaluating the compression modulus K. From Eqs. (6) and (7), we have

$$K=9\left[\frac{\partial p}{\partial \rho}\right]_T=9\rho\left[\frac{\partial \mu}{\partial \rho}\right]_T . \tag{9}$$

The correlated μ can be calculated rather simply in the present approach. Thus Eq. (9) provides a more convenient way for calculating K than the usual method where one needs to evaluate the second-order derivative of f with respect to the density.

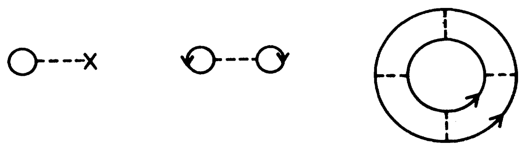
We have now seen that there are a number of advantages in choosing a s.p. potential U_k which satisfies Eq. (4). Let us now turn to the solution of U_k from Eq. (4). This may be easily carried out. We can rewrite $(\partial\Omega'_{\rm int}/\partial\mu)_{TV}$ in a functional derivative form as

$$\sum_k(\partial f_k/\partial\mu)_{TV}(\delta\Omega'_{\rm int}/\delta f_k)_{TV} \ .$$

Then

$$U_k=\left[\frac{\delta\Omega'_{\rm int}}{\delta f_k}\right]_{TV} \tag{10}$$

is clearly a solution of Eq. (4). It is of interest that this U_k may be considered as a finite-temperature extension of the quasiparticle potential employed in Landau's Fermi liquid at zero temperature. As to be discussed later, Eq.



(i) (ii) (iii)

FIG. 1. Some linked diagrams of $\Omega_{\rm int}$.

(4) does *not* give a unique solution for U_k. It should be of interest to look for its other solutions as well. The solution given by Eq. (10) appears, however, to be a convenient and physically appealing one. We note that Eq. (10) is a self-consistent equation for determining U.

Application and discussion. Let us first apply our method to a HF nuclear matter EOS calculation using effective Skyrme interactions.[12] In this case we have $\Omega'_{\rm int}=\frac{1}{2}\sum_{mn}f_m f_n\langle mn|V_{NN}|mn\rangle$. Here V_{NN} stands for the Skyrme interaction. Since the physical density is now given by Eq. (5), Eq. (10) gives $U_k=U_k^{\rm HF}+R$ where $U_k^{\rm HF}-\sum_m f_m\langle km|V_{NN}|km\rangle$ and R is the rearrangement potential

$$\frac{1}{2V}\sum_{mn}\left\langle mn\left|\frac{\partial V_{NN}}{\partial\rho}\right|mn\right\rangle f_m f_n \; .$$

The Skyrme interaction has a density-dependent term $\frac{1}{6}t_3\rho^\alpha\delta(\mathbf{r}_1-\mathbf{r}_2)$. Hence R is simply $\frac{1}{16}\alpha t_3\rho^{\alpha+1}$. Then the EOS is readily given by

$$p=-\frac{1}{V}\left[\Omega_0+\Omega'_{\rm int}-\sum_k f_k(U_k^{\rm HF}+R)\right]$$

which is just

$$p=\frac{3}{8}\left[t_0+\frac{\alpha+1}{6}t_3\rho^\alpha\right]\rho^2 -\frac{\Omega_0}{V}\left[\frac{5}{2}-\frac{3/2}{1+(m\rho/8)(3t_1+5t_2)}\right], \tag{11}$$

where the t's are the parameters of the Skyrme interaction[12] and m is the nucleon mass. The above EOS agrees with that given by other authors (see Ref. 12 and references quoted therein), but the present derivation is much simpler and clearer.

Next we apply our method to a BHF calculation of nuclear matter. As recently discussed by several authors,[2-4] the HVH theorem is not satisfied by the conventional BHF theory of nuclear matter. We may write the BHF $\Omega'_{\rm int}$ as[7]

$$\Omega_{\rm int}^{\rm BHF}=\frac{1}{2}\sum_{kl\in P}K_{klkl}(\tilde{\epsilon}_{kl})f_k f_l \; , \tag{12}$$

where K is the familiar reaction matrix and $\tilde{\epsilon}_{kl}-2\mu$ and $\epsilon_{kl}=\epsilon_k+\epsilon_l$. P is a chosen model space such as the momentum space with $k\le k_F$, the Fermi momentum. Substituting this into Eq. (10), we have

$$U_k=\sum_{l\in P}K_{klkl}(\tilde{\epsilon}_{kl})f_l +\frac{1}{2}\sum_{mn\in P}\left[\frac{\delta}{\delta f_k}K_{mnmn}(\tilde{\epsilon}_{mn})\right]_{\rm TV}f_m f_n \; , \tag{13}$$

where the first term is the well-known BHF s.p. potential $U_k^{\rm BHF}$ and the second term may be referred to as the arrangement potential. Because of Eq. (5), we can replace $(\delta/\delta f_k)_{\rm TV}$ by $(1/V)(\partial/\partial\rho)_T$. This leads to the rather interesting and simple result

$$\begin{aligned}U_k&=U_k^{\rm BHF}\\&\quad+\frac{1}{4V}\sum_{\substack{ij\in P\\ mn\in Q}}f_i f_j|K_{ijmn}(\tilde{\epsilon}_{ij})|^2\left[\frac{1}{e}\frac{\partial Q_{mn}}{\partial\rho}-\frac{Q_{mn}}{e^2}\frac{\partial e}{\partial\rho}\right]\\&\equiv U_k^{\rm BHF}+R_Q+R_E \; ,\end{aligned} \tag{14}$$

where e stands for $(\epsilon_{ij}-\epsilon_{mn})$. Q is the Pauli exclusion operator with $Q_{mn}=(1-f_m)(1-f_n)$.

As mentioned earlier Eq. (4) does not uniquely determine the s.p. potential U. There may be many solutions for U, and in the above we have actually selected one "most convenient" for calculation. By directly evaluating the second term of Eq. (13) we can obtain a different set of rearrangement terms $R_Q(k)$ and $R_E(k)$, the former corresponding to diagram (a) or (b) of Fig. 2 which is just the M_2 diagram of Refs. 2–4 and the latter corresponding to higher order diagrams such as (c) of Fig. 2. It is numerically more complicated to use $R_Q(k)$ and $R_E(k)$, because they both are momentum dependent and we have to carry out additional self-consistent calculations to determine an entirely new s.p. potential. In contrast our chosen solutions R_Q and R_E are momentum independent; they just provide a density-dependent constant shift to $U_k^{\rm BHF}$. It may be mentioned, however, that the use of $R_Q(k)$ and $R_E(k)$ may be more desirable in terms of the cancellation of the self-energy diagrams. The convergence property of the diagrammatic expansion of $\Omega_{\rm int}$ is a matter of much importance. Ideally one would like to choose a s.p. potential which may improve the convergence of the above expansion. Studies in this direction will be very useful.

The HVH theorem should be satisfied within the present framework. Let us now check if this is so. In the present work, we consider only the zero-temperature case. We first perform the conventional BHF nuclear matter calculation[13,14] using the Bonn (k-space) potential. Then the nuclear matter pressure is calculated using both $p=-(dE_0/dV)_N$, where E_0 is the ground-state energy of nuclear matter, and $p_0=\rho(\epsilon_F^{\rm BHF}-E_0/N)$. As shown in Table I, p and p_0 are vastly different. Clearly the HVH theorem is badly violated here.

Next we repeat the above calculation using the s.p. potential proposed in the present work. In this way the

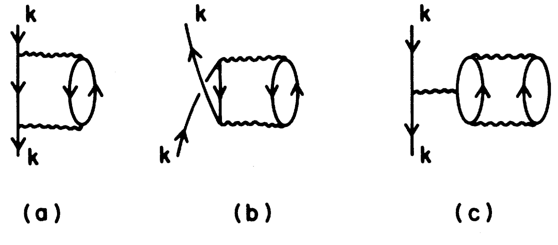


FIG. 2. Diagrams of the rearrangement single-particle potential.

TABLE I. Rearrangement potential and the fulfillment of the Hugenholtz–Van Hove theorem. Calculations are performed for symmetric nuclear matter at zero temperature with the Bonn (k-space) potential. The units for the various entries are k_F (fm^{-1}), ρ (fm^{-3}), columns 3–6 (MeV), and columns 7–9 ($\mathrm{MeV\,fm}^{-3}$).

k_F	ρ	$\epsilon_F^{\mathrm{BHF}}$	E_0/N	R_Q	R_E	$p=-dE_0/dV$	p_0	p_R
1.1	0.090	−18.65	−8.76	1.93	2.68	−0.487	−0.890	−0.475
1.2	0.117	−21.12	−10.10	2.23	3.01	−0.669	−1.289	−0.676
1.3	0.148	−23.19	−11.59	2.75	3.41	−0.836	−1.717	−0.805
1.4	0.185	−24.56	−12.69	3.23	3.84	−0.866	−2.196	−0.888
1.5	0.228	−25.05	−13.48	3.97	4.34	−0.686	−2.638	−0.743
1.6	0.277	−24.41	−13.91	5.05	4.87	−0.196	−2.909	−0.161
1.7	0.332	−22.28	−13.68	6.41	5.42	1.102	−2.855	1.073

pressure is given by $p_R=\rho(\epsilon_F^R-E_0/N)$ where $\epsilon_F^R=\epsilon_F^{\mathrm{BHF}}+R_Q+R_E$; here $\epsilon_F^{\mathrm{BHF}}$ and E_0 are the same as those of p_0. As usual we have employed a partial-wave representation and angle averaged Pauli exclusion operator[13] to calculate R_Q and R_E. As shown in Table I, p_R is very much closer to p than p_0. (The slight difference between p_R and p are probably mainly due to the average angle approximation used in our calculations.) Clearly our results agree with the HVH theorem remarkably well. Note that the rearrangement terms R_Q and R_E, arising respectively from the density dependence of the Pauli exclusion operator and of the s.p. spectrum, are of nearly equal importance in achieving this agreement.

In summary, we have proposed a probably useful and convenient method for choosing and deriving a "conserving" s.p. potential for finite-temperature many-body calculations. This potential must be determined in consistence with the approximation scheme adopted for the calculation of the thermodynamic potential. A main advantage of our method is that the correlated chemical potential can be rigorously determined from the occupation of the s.p. levels. It is primarily because of this that a number of basic thermodynamic relations are automatically fulfilled by the present framework. In addition our formalism also ensures the fulfillment of the relation

$$(\mu_b-\mu_a)_T=\left[\int_a^b \frac{1}{\rho}\,dp\right]_T ;$$

without which the frequently used Maxwell construction for phase coexistence would become disallowed. We have recently calculated certain ring diagrams of the nuclear matter thermodynamic potential.[15] The corresponding ring-diagram chemical potential and EOS may also be obtained using the present method.

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