Saturation properties and liquid-gas phase transition of nucleus

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Abstract

Saturation properties and liquid-gas phase transition of nucleus are analysed in the framework of Hatree-Fock theory. We modify Hill-Wheller formula with a finite-size-effect parameter by fitting the zero-temperature properties of nucleus. Employing Gogny effective interaction and phenomenological expression of Coulomb energy, we give the critical temperature of liquid-gas phase transition of nucleus being about 12 MeV, which agrees with the result extracted from heavy-ion collision experiments. It is pointed out that a phenomenological formula of surface energy of hot nucleus is not available in the region where nucleon density is far away from the normal density.

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I. Introduction

The developments of heavy-ion physics have evoked great interest on the studies about statistic properties of infinite nuclear matter and nucleus, especially about equation of state (EOS) and liquid-gas phase transition. There have been a lot of calculations of infinite nuclear matter in the framework of Hatree-Fock theory (HFT), in which finite-size-effect and Coulomb interaction were ignored [1-10]. The finite-size-effect of nucleus and Coulomb interaction in nucleons should play important roles in realistic heavy-ion collisions. Refs. [11, 12] took into account the finite-size-effect with the help of Hill-Wheller formula and Coulomb effect in the use of a phenomenological expression in the calculation of finite nuclear matter. It was found that the finite-size-effect leads to a reduction of critical temperature of liquid-gas transition in finite nuclear matter by about $5 \sim 10$ MeV, and Coulomb effect leads to a reduction about $1 \sim 3$ MeV. In our opinion, any approach which is applied to study hot nucleus though infinite nuclear matter approximation should be able to give reasonable zero-temperature saturation properties of nucleus also. Basing on the calculations of six typical nuclei (from $^{40}\text{Ca}$ to $^{238}\text{U}$) with several Skyrme effective interactions, Wang and Yang [14] found that it is impossible to give correct bound energies and other saturation properties of nucleus by adopting Hill-Wheller formula directly as that in Refs. [11, 12]. There is a general agreement that Gogny effective interaction [15] is able to describe the long-range and medium-range behaviours of nucleon-nucleon interaction more reasonable than Skyrme interaction. In this paper, we will modified Hill-Wheller formula with a finite-size-effect parameter through the studies on the zero-temperature saturation properties of nucleus with Gogny interaction. Employing the modified Hill-Wheller formula, we study the liquid-gas transition of hot nucleus. We also analyse the applicability of a widely used phenomenological expression of surface energy of hot nucleus.

The paper is organized as follows. In section II, we modified Hill-Wheller formula by fitting the zero-temperature properties of nucleus. We study the stability character and liquid-gas phase transition of hot nucleus in section III. The surface energy of nucleus is discussed in section IV. As usual, the last section is reserved for summary.

II. Formalism

Let us begin with a brief review of Hatree-Fock theory of infinite nuclear matter system with Gogny interaction. Gogny D1 effective interaction is expressed as [15]

$$V(r) = \sum_{i=1,2} (W_i + B_i P_\sigma - H_i P_\tau - M_i P_\sigma P_\tau) \exp\left(-r^2/\mu_i^2\right) + t_0 (1 + X_0 P_\sigma) \rho^\alpha \delta(r) + iW_{LS}(\sigma_1 + \sigma_2) \cdot \nabla \times \delta(r) \nabla,$$

where $\rho$ is nucleon density and $P_\sigma, P_\tau$ are exchange operators of spin and isospin respectively. In Eq. (1), the part with $\delta$ function is zero-range interaction which is density-dependent and the part with Gauss function is finite-range interaction which is density-independent. The parameters of Gogny D1 interaction are listed in table 1.
The Hatree-Fock single particle spectrum with Gogny D1 interaction is

\[ \epsilon_q = \frac{\hbar^2 q^2}{2m} + u_q + u_D, \]

\[ u_q = \sum_{q'} (qq' | V | qq' - q'q) f_{q'}, \]

\[ u_D = \frac{1}{2V} \sum_{i \neq j} \left( q_i q_j \left| \frac{\partial V}{\partial \rho} \right| q_i q_j - q_j q_i \right) f_{q_i} f_{q_j}, \]

\[ f_q = \frac{1}{1 + \exp \left[ \beta (t_q + u_q + u_D - \mu) \right]}, \]  

(2)

where \( V \) is the volume of nuclear matter system, \( \mu \) the chemical potential, \( T \) the temperature, \( \beta = 1/(k_B T) \), \( u_q \) the usual HF single particle potential, and \( u_D \) the rearrangement potential. It has been pointed out that the introduction of rearrangement potential is necessary to guarantee the density relation \( \rho = \frac{1}{V} \sum_q f_q \) and give correct chemical potential \[16\]. Then EOS can be readily obtained from Eq. (2) \[6, 12, 13\].

Now we turn to the approach to respect finite-size-effect and Coulomb interaction in finite nuclear matter system. In Hatree-Fock theory, the calculation of infinite nuclear matter is simplified by taking plane wave function as single particle wave function, in which the state number between \( k \) and \( k + dk \) in the momentum space reads

\[ dN_k = V \frac{k^2 dk}{2\pi^2}. \]  

(3)

To study the liquid-gas phase transition in finite nuclear matter system, Jaqaman, Mekjian and Zamick \[11\] proposed that the finite-size-effect can be taken into account in the theory framework of infinite nuclear matter system by Hill-Wheller formula

\[ dN_k = V \left[ \frac{k^2 dk}{2\pi^2} - \frac{S}{V} \frac{k dk}{8\pi} + \frac{L}{V} \frac{dk}{8\pi} \right], \]  

(4)

where \( S \) and \( L \) are the measures of the average surface and linear of finite nuclear matter system respectively. For a spherical system with radius \( R \), \( S = 4\pi R^2 \), \( L = 2\pi R \). The effects of zero-point motion and quantization of wave number in a finite-size system were taken into account in Eq. (4). In fact, Eq. (4) is derived from a simple model, a finite-size system with free particles. Strictly speaking, it cannot be applied to the study of nucleus directly. The reason is as following: Because there are interactions in nucleons, the single particle wave function in nucleus is not plane wave function as that in the finite-size system without interaction, and different for the nucleus with different shell. Eq. (4) is a approximate approach to study finite-size-effect in the theory framework of nuclear matter system. In our opinion, any approach which is applied to study the liquid-gas phase transition of nucleus through the infinite nuclear matter approximation should be able to give reasonable zero-temperature saturation properties of nucleus also. The calculations of the six typical nuclei show that Eq. (4) can not satisfy this constrain (see table 2). It can be found that the bound energies per nucleon
of the nuclei calculated with Eq. (4) are much smaller than the experimental data and this divergence becomes more and more serious as the nucleon number decrease, so that $^{40}$Ca can not combine any more. This shows that the finite-size-effect isn’t considered suitably with Eq. (4). As a result, it is hardly to believe the calculations of EOS and liquid-gas transition of finite nuclear matter system given in Refs. [11, 12]. We may add a finite-size-effect parameter $a_F$ to the second and third terms in Eq. (4) to respect the fact that the single particle wave function in nucleus is different from that in the finite system with free particle,

$$
dN_k = V \left\{ \frac{k^2 dk}{2\pi^2} + a_F \left[ -\left( \frac{4\pi \rho}{3A} \right)^{\frac{3}{2}} \frac{3kd\rho}{8\pi} + \left( \frac{4\pi \rho}{3A} \right)^{\frac{1}{2}} \frac{3d\rho}{16\pi} \right] \right\},$$

where $a_F$ is decided by fitting the experimental data of bound state energies of nuclei. Eq. (5) becomes Eq. (4) when we take $a_F = 1$ and becomes Eq. (3) as $A \rightarrow \infty$. By fitting the experimental data, we find that to take the finite-size-effect parameter $a_F = 0.35$ in Eq. (5), the bound energies of the nuclei from light to heavy agree with the experimental data very well and the saturation densities $\rho_0$ of the six typical nuclei are about 0.13, which has mild dependence on the nucleon number $A$ (see table 2). This agrees with the saturation character. With this $\rho_0$, through the phenomenological formula $R = r_0A^{\frac{1}{3}}$ of the effective radius $R = (3/4\pi \rho_0)^{\frac{1}{2}}$, we obtain $r_0 = 1.21 \sim 1.22$, which agrees with the experimental result also. All of these show that it is reasonable with Eq. (5) to study the finite-size-effect of nucleus.

Coulomb interaction is a long-range interaction, adopting it directly in the calculation of matrix between plane wave functions will bring divergent result. So, for simplicity, we use a phenomenological expression of Coulomb energy per proton to respect Coulomb effect [11, 12],

$$E_C = a Z^2 \left[ 1 - 5 \left( \frac{3}{16\pi Z} \right)^{\frac{3}{2}} - \frac{1}{Z} \right] \rho^{\frac{3}{2}}A^{-\frac{1}{3}}. \quad (6)$$

We take $a = 1.50$ in order to fit the experimental data more well, which is slight different with the usual value $a = 1.39$.

### III. Stability character and liquid-gas phase transition of hot nucleus

For discussing the stability character of hot nucleus, limit temperature $T_l$ is defined, which is the highest temperature below that free energy has a minimum. Nucleon density corresponding with the minimum of free energy at $T_l$ is called limit density $\rho_l$. When the temperature is larger than $T_l$, the pressure of the system is always larger than zero. The condensation phase and the nucleon-gas phase can not arrive phase equilibrium without extra pressure. The values of $T_l$ and $\rho_l$ of the six typical nuclei are listed in table 3. It can be found that $T_l$ and $\rho_l$ are not sensitive to nucleon number $A$. $T_l$ is about 9.0 $\sim$ 9.5 MeV, and $\rho_l$ is about 0.075 fm$^{-3}$.

Liquid-gas phase transition of hot nucleus is another interesting question. Strictly speaking, a phase transition can only occur in a system with infinite number of particles,
which is reflected in the singularity behavior of some thermodynamic quantities. For example, the specific heat displays a sharp $\lambda$-type singularity at the critical temperature $T_c(\infty)$ for a liquid-gas phase transition in an infinite particles system. The specific heat of finite particles system does not exhibit such a sharp singularity, but it has a large peak at a temperature $T_c(A)$ which approaches to $T_c(\infty)$ as the particle number $A \rightarrow \infty$. The temperature $T_c(A)$ can be regarded as the critical temperature of a finite particle system. For a finite particles system, it is convenient to determine the critical point by the inflection point condition of $\mu \sim \rho$ isothem rather than $P \sim \rho$ isothem:

$$\left. \frac{\partial \mu}{\partial \rho} \right|_{\gamma,T_c,\rho_c} = \left. \frac{\partial^2 \mu}{\partial \rho^2} \right|_{\gamma,T_c,\rho_c} = 0,$$

where $\mu$ is the average chemical potential

$$\mu = \frac{1}{\rho}(\rho_p \mu_p + \rho_n \mu_n) = \frac{1 - \gamma}{2} \mu_p + \frac{1 + \gamma}{2} \mu_n$$

with $p$ denotes parton and $n$ neutron. To study the finite-size-effect, we calculate the EOS and liquid-gas transition critical point of symmetrical infinite nuclear matter system with different nucleon number and without Coulomb interaction. Figs. 1 and 2 display $\mu \sim \rho$ isotherms at temperature $T = 6$ MeV and 14 MeV. As it is known, liquid phase and gas phase can coexist at low temperature, while only gas phase can exist at high temperature. It can be found that there is a critical nucleon number $A_c(T)$ for a certain temperature. As $A \leq A_c(T)$, only gas phase can exist. Table 4 lists the critical temperatures $T_c$ and densities $\rho_c$ of the symmetrical nuclear matter with different nucleon number $A$. $T_c$ and $\rho_c$ decrease with $A$ decreasing. Here again we find that for the realistic nucleus system ($A \leq 250$) the liquid-gas critical points calculated with Eq. (5) and $a_F = 0.35$ are very different from that with Eq. (4) obviously. Coulomb interaction and neutron-proton asymmetry are another two factors which decrease the critical temperature. Table 3 gives the critical temperatures $T_c$ and densities $\rho_c$ of the six typical nuclei. It can be found that with Eq. (5) and $a_F = 0.35$, finite-size-effect, Coulomb interaction and asymmetry effect reduce the critical temperature $T_c$ by about $3 \sim 4$ MeV comparing with that of the symmetrical infinite nuclear matter. $T_c$ and $\rho_c$ are insensitive to nucleon number $A$, which is very different from the results with Eq. (4). As exhibited in section II, we can obtain reasonable zero-temperature saturation properties of nuclei with Eq. (5) and $a_F = 0.35$ while we cannot with Eq. (4). Thus the critical temperatures $T_c$ obtained in the present work are reasonable and reliable. $T_c$ has mild dependence on nucleon number $A$. In fact, all of the finite-size-effect, Coulomb interaction and neutron-proton asymmetry play the roles to weaken the nucleus combination and reduce $T_c$. The finite-size effect becomes weak with $A$ increasing, while Coulomb interaction and neutron-proton asymmetry effect play more and more important roles. As a result, $T_c$ is not sensitive to the nucleon number $A$, $T_c \approx 12$ MeV. Our results are close to that with Skyrme effective interaction [14].
Panagiotou et al. \cite{17} extracted the critical temperatures of nuclei by analyzing the mass distribution of multi-fragments in intermediate-energy heavy-ion collisions basing on the condensation theory, which gave $T_c \approx 12$ MeV. Bondorf et al. \cite{18} obtained $T_c \approx 11$ MeV for $A=100$ system basing on the Monte Carlo calculation. Our calculations are consistent with these results.

IV. Surface energy of nucleus

A phenomenological surface energy expression was applied to study the stable properties and dynamical properties of nucleus in some works \cite{19,20},

$$E_S = \frac{4\pi R^2 \sigma}{A} = 4\pi \left( \frac{3A^{\frac{2}{3}}}{4\pi \rho} \right)^{\frac{2}{3}} \frac{\sigma}{A},$$

(9)

where $\sigma$ is the tension coefficient $\sigma \approx 1.2$ MeV·fm$^{-2}$ which is derived from the surface energy term in the bound energy phenomenological formula of nucleus. This approach takes the tension coefficient being independent of density, which gives the relation $E_S \sim \rho^{-\frac{2}{3}}$. In the present calculations, the surface energy coming from the finite-size-effect can be derived naturally from the bound energy of nucleus and that of infinite symmetric nuclear matter,

$$\Delta E = E(A, \rho) - E(A \to \infty, \rho).$$

(10)

The surface energy of $^{90}_{40}$Zr obtained with Eqs. (9) and (10) are plotted in Fig. 3. Although Eqs. (9) and (10) present similar results in the neighborhood of normal nucleon density $\rho_0$, their behaviors are very different in the other density regions. The saturation curves $(E/A) \sim \rho$, pressure-density curves $P \sim \rho$ calculated with Eq. (9) are plotted in Figs. 4 and 5, which are very different form that obtained form HFT. The saturation properties of nucleus calculated with Eq. (9) are given table 2. We find that according to Eq. (9), the bound energies agree with the experiment data, but the saturation densities of the nuclei are general larger than that of infinite nuclear matter and reduce as mass number $A$ increasing, which is not reasonable obviously. All of these show that Eq. (9) is not available for the region where the nucleon density is far away from the normal nucleon density. We find that Eq. (10) can be expressed by the following formula

$$E'_S = C_1 \rho^\frac{2}{3} A^{-\frac{1}{3}} + C_2 \rho^\frac{5}{3} A^{-\frac{1}{3}},$$

(11)

where $C_1 = 53.0$ MeV·fm$^2$ and $C_2 = 108$ MeV·fm$^5$. In Eq. (11) the first term is derived from the fermion gas model and the finite-size-effect is taken into account by the second term. The density dependence of Eq. (11) which reads $E'_S \sim \rho^\frac{2}{3}$ is very different form that of Eq. (9). Tables 2 and 4 give the saturation properties and critical temperature in the use of Eq. (11), which agree with the results with Eq. (9) very well. The calculations also show that the surface energy Eq. (11) is not sensitive to temperature. Thus, Eq. (11) can be employed in the study about EOS of nucleus.
V. Summary and discussion

We analyse the saturation properties and liquid-gas phase transition of nucleus and infinite nuclear matter in the framework of Hatree-Fock theory. At first, in order to give reasonable zero-temperature properties of nucleus, we modify Hill-Wheller formula which is used to respect the finite size effect of nucleus. Employing Gogny effective interaction and phenomenological Coulomb energy, we obtain the critical temperatures of liquid-gas phase transition of nucleus being about 12 MeV, which is consistent with the result extracted from heavy-ion collisions. The critical temperature of liquid-gas phase transition of nucleus has mild dependence on nucleon number $A$ due to the cooperation of finite-size-effect, Coulomb interaction and neutron-proton asymmetry. In addition, the surface energy of nucleus is analysed. It is pointed out that a widely used phenomenological expression of surface energy is not available in studying hot nucleus.

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\[
\begin{array}{cccccc}
\begin{array}{|c|c|c|c|c|}
\hline
i & \mu_i (\text{fm}) & W_i (\text{MeV}) & B_i (\text{MeV}) & H_i (\text{MeV}) & M_i (\text{MeV}) \\
\hline
1 & 0.7 & -402.4 & -100 & -496.2 & -23.56 \\
2 & 1.2 & -21.3 & -11.77 & 37.24 & -68.81 \\
\hline
\end{array}
\end{array}
\]

\[
t_0 = 1350 \text{ MeV-fm}^4, \: \alpha = 1/3, \: W_{LS} = 115 \text{ MeV-fm}^5, \: X_0 = 1.
\]

Table 1. Parameters of Gogny D1 effective interaction.

| & \( ^{40}\text{Ca} \) & \( ^{56}\text{Ni} \) & \( ^{90}\text{Zr} \) & \( ^{156}\text{Sm} \) & \( ^{208}\text{Pb} \) & \( ^{238}\text{U} \) |
|---|---|---|---|---|---|---|
| Exp. Bound energy (MeV) | 8.55 | 8.64 | 8.71 | 8.25 | 7.87 | 7.57 |
| Eq. (5) | 8.97 | 8.82 | 8.72 | 8.02 | 7.45 | 7.15 |
| Eq. (4) | -1.01 | -0.36 | 0.66 | 1.20 | 1.30 | 1.29 |
| Eq. (5) | 8.77 | 8.70 | 8.70 | 8.00 | 7.41 | 7.28 |
| Eq. (4) | 8.76 | 8.72 | 8.73 | 8.11 | 7.56 | 7.27 |
| \( \rho_0 (\text{fm}^{-3}) \) Equ. (5) | 0.131 | 0.132 | 0.134 | 0.134 | 0.134 | 0.133 |
| Eq. (4) | 0.185 | 0.180 | 0.177 | 0.173 | 0.170 | 0.176 |
| Eq. (5) | 0.129 | 0.130 | 0.133 | 0.133 | 0.133 | 0.133 |

Table 2. Zero-temperature saturation properties of the six typical finite nuclei.
Table 3. The limit temperature $T_l$, density $\rho_l$ and liquid-gas phase transition critical temperature $T_c$, density $\rho_c$ of six typical nuclei. (1) without Coulomb interaction; (2) with Coulomb interaction. SINM=symmetric infinite nuclear matter.

Table 4. Size dependence of critical point of liquid-gas transition in symmetric infinite nuclear matter.
Figure Captions

**Fig. 1** The $\mu \sim \rho$ isotherms of infinite symmetric nuclear matter at $T = 6.0$ MeV evaluated with nucleon number $A = 100$ (solid line), $A = 200$ (dashed line), $A = 1000$ (dotted line) and $A = \infty$ (dash-dotted line) respectively.

**Fig. 2** Similar as Fig. 1 and $T = 14.0$ MeV.

**Fig. 3** Surface energy of $^{90}_{40}$Zr at temperature $T = 0.0$ MeV evaluated with Eqs. (10) and (5) with $a_F = 0.35$ (solid line); Eqs. (10) and (4) (dashed line); Eq. (3) (dotted line); and Eq. (11) (dash-dotted line) respectively.

**Fig. 4** The saturation curves $(E/A) \sim \rho$ calculated with Eq. (3) (solid line), Eq. (4) (dashed line), Eq. (9) (dotted line) and Eq. (11) (dash-dotted line) respectively.

**Fig. 5** The $P \sim \rho$ isotherms. The explanation of the curves is similar to Fig. 4.
Fig. 1
Fig. 2
Fig. 5