PHYSICAL REVIEW E VOLUME 54, NUMBER 4 OCTOBER 1996

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Particle correlations in the generalized Thomas-Fermi approach

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(Received 18 April 1996)

This paper presents the Thomas-Fermi approach generalized to consider the particle correlations in many-body systems with non-Coulomb interaction potentials. The key points of the generalization consist in using integral formulation and extracting the radial distribution function. The latter has been found to obey the integral equation which, in the classical limit, is reduced to the well-known equation of Bogoliubov. So, the approach presented can be used to explore particle correlations in the quantum many-body systems with the interparticle potentials not having the Fourier transform, for example, with a Lennard-Jones potential. [S1063-651X(96)12309-6]

PACS number(s): 05.30.−d, 67.55.−s, 67.20.+k

It is known that the Thomas-Fermi approach [1] together with its particular variant for the classical many-body systems, the Debye-Hueckel method [2], is able to provide satisfactory results while investigating the correlation phenomena in the media with Coulomb interparticle potential. The advantage of this approach consists in the extreme transparency of understanding the physics of the particle correlations. But up to now the applications of the Thomas-Fermi method have been limited to the situation of the Coulomb type interactions. This paper presents the generalization of the approach to consider the many-body systems with constituents interacting by means of an arbitrary relevant potential.

To derive the generalization, let us take the system of some particles uniformly distributed with density n over a region of volume V. Let the potential of the particle interaction be $\Phi(r)$. Assume that a point object is placed into this region and interacts with the surroundings via the same potential. Further we shall treat the point of the object location as the origin of the coordinates. We are interested in the equilibrium structure produced around the origin point. This structure is specified by the quantity $n_{str}(r;\theta,n)$ being the density of the particles located in the vicinity of point $\vec{r}, r\equiv|\vec{r}|$. Here θ denotes the system temperature. Below we shall use $n_{str}(r)$ instead of $n_{str}(r;\theta,n)$ to simplify the formulas. According to the first ‘‘item’’ of the Thomas-Fermi approach, $n_{str}(r)$ can be calculated with the following condition:

$$\mu_{id}(n_{str}(r))+\Phi(r)+U(r)=\text{const} \quad (\forall\vec{r}), \tag{1}$$

where $\mu_{id}(\rho)$ is the chemical potential of the ideal gas of the considered particles at density ρ, and $U(r)$ is the energy of the interaction of the particle being at point $\vec{r}$ with the other particles of the system. The quantity on the left side of (1) can be named the total particle potential. To calculate $n_{str}(r)$ with (1), the connection of $U(r)$ with $n_{str}(r)$ should be fixed. In the case of the systems with Coulomb interparticle potential, this is realized by employing the neutralizing background and the Poisson equation [1,2]. But it is impossible for the case of non-Coulomb interactions. However, we can follow the other way based on the obvious integral relation

$$U(r)=\int_V \Phi(|\vec{r}-\vec{y}|)n_{str}(y)d\vec{y}. \tag{2}$$

At point $\vec{r}_{far}$ which is far enough from the origin of the coordinates, the total particle potential then takes the value

$$\mu_{id}(n)+n\int_V \Phi(|\vec{r}_{far}-\vec{y}|)d\vec{y}, \tag{3}$$

if, of course, we hold to the reasonable assumption that

$$\lim_{r\to\infty}\Phi(r)=0\ .$$

Note, that we consider $r_{far}\equiv|\vec{r}_{far}|\ll R$, where R is the minimal distance between the location point of the object and the system boundary. Thus any boundary effects can be ignored in our investigation. Equating (1) and (3) we can find

$$\mu_{id}(n)-\mu_{id}(n_{str}(r))=\Phi(r)+\int_V (n_{str}(y)-n)\Phi(|\vec{r}-\vec{y}|)d\vec{y}, \tag{4}$$

where the used relation

$$\lim_{V\to\infty}\frac{\int_V[\Phi(|\vec{r}_{far}-\vec{y}|)-\Phi(|\vec{r}-\vec{y}|)]d\vec{y}}{\int_V\Phi(|\vec{r}-\vec{y}|)d\vec{y}}=0 \tag{5}$$

is fulfilled for a lot of the known potentials, in particular, for the Coulomb potential as well as for the integrable ones. We should remark here that the differential version of Eq. (4) used for the electron many-body systems, has been derived within the WKB approximation [3]. Hence, one can expect that Thomas-Fermi approach is a semiclassical method which takes into account quantal phenomena by quantizing phase space into cells of volume h^f where f is the number of degrees of freedom of the system, and then integrating over momentum space to obtain the density in coordinate space.

Now we should realize the second ‘‘item‘‘ of the Thomas-Fermi method. It implies that using $n_{str}(r)$, we are able to study the space correlations in the many-body system made of the particles uniformly distributed with density n. The most important quantity calculated in the Thomas-Fermi approach and related with the particle correlations, is usually thought to be the screening radius. Of course, now we can not exploit this quantity, for it is tightly connected with the Coulomb interparticle potential and the neutralizing background. But there is one more correlation characteristic, no less important than the screening radius, that may be evaluated in the approach discussed. It is the radial distribution function $g(r;\theta,n)$ for which we have

$$g(r;\theta,n)=\frac{n_{str}(r;\theta,n)}{n}. \tag{6}$$

Using (4) and (6) we readily obtain the following integral equation for the radial distribution function:

$$\mu_{id}(n)-\mu_{id}(ng(r))=\Phi(r)+n\int_V(g(y)-1)\Phi(|\vec{r}-\vec{y}|)d\vec{y}, \tag{7}$$

where $g(r)\equiv g(r;\theta,n)$. To see to what extent this equation is adequate, let us explore its classical limit. In this case we have

$$\mu_{id}(n)-\mu_{id}(ng(r))=-\theta\ \ln g(r). \tag{8}$$

Therefore, relation (7) can be rewritten as

$$-\theta\ \ln g(r)=\Phi(r)+n\int_V(g(y)-1)\Phi(|\vec{r}-\vec{y}|)d\vec{y}. \tag{9}$$

Equation (9) makes it possible to generate the expansion in powers of n for $g(r;\theta,n)$

$$g(r;\theta,n)=g_0(r;\theta)+ng_1(r;\theta)+\cdots,$$

where

$$g_0(r;\theta)=\exp\left(-\frac{\Phi(r)}{\theta}\right),$$

$$g_1(r;\theta)=-\frac{1}{\theta}\exp\left(-\frac{\Phi(r)}{\theta}\right)\int_V\Phi(|\vec{r}-\vec{y}|)\times\left[\exp\left(-\frac{\Phi(y)}{\theta}\right)-1\right]d\vec{y}.$$

As is seen, $g_0(r;\theta)$ is in full agreement with the known result of the calculations in the Gibbs canonical ensemble [4]. But the expression for $g_1(r;\theta)$ coincides with the true value

$$\exp\left(-\frac{\Phi(r)}{\theta}\right)\int_V\left[\exp\left(-\frac{\Phi(|\vec{r}-\vec{y}|)}{\theta}\right)-1\right]\times\left[\exp\left(-\frac{\Phi(y)}{\theta}\right)-1\right]d\vec{y}$$

only at high temperatures. So, Eq. (9) gives the valid second virial coefficient at low temperatures, and the correct second and third ones at high temperatures. Note, that quite reasonable integral equations for $g(r)$ derived in the superposition approximation [5], are in error beyond the third virial coefficient [4,6]. Thus, the use of integral formulation for Thomas-Fermi approach instead of the differential one and the orientation to the radial distribution function, enable us to generalize this method to study the case of the non-Coulomb interactions. But the investigation goal has not been reached yet.

Indeed, Eq. (7) gives the possibility to consider particle correlations in, for example, nuclear matter, where the nucleon-nucleon potential is of Yukawa type $\exp(-y)/y$, or in the electron gas. But it is not the case for the potentials which are not integrable due to their behavior at small separations between interacting particles. For instance, if we take potential $1/r^m$ $(m>2)$ then the integrals in expressions (7) and (9) will not exist. This obstacle appears because particle correlations have been neglected while calculating $U(r)$. In particular, in above mentioned reasonings, quantity $U(r_{far})$ is given with the expression

$$U(r_{far})=n\int_V\Phi(|\vec{r}_{far}-\vec{y}|)d\vec{y}$$

that corresponds to the particle interactions taken in the Hartree approximation. The latter is well known not to take into account any correlations. To derive a more correct relation for quantity $U(r_{far})$, note, that it is nothing else but the interaction energy of a particle with the other particles uniformly distributed around with density n. Keeping this in mind, we estimate $U(r_{far})$ [7,8] as

$$U(r_{far})=n\int_V g(|\vec{r}_{far}-\vec{y}|)\Phi(|\vec{r}_{far}-\vec{y}|)d\vec{y}. \tag{10}$$

But now the problem arises how $U(r)$ can be specified, for we have fixed only its limit value at $\vec{r}_{far}$. A reasonable way to do this is to treat quantity $g(r)\Phi(r)$ as the effective interaction potential which should be substituted for $\Phi(r)$ in all the integrals in expressions (2)–(5). In this case we have

$$U(r)=\int_V g(|\vec{r}-\vec{y}|)\Phi(|\vec{r}-\vec{y}|)n_{str}(y)d\vec{y}. \tag{11}$$

Further, (1) and (11) together with (6) yield the equation

$$\mu_{id}(n)-\mu_{id}(ng(r))=\Phi(r)+n\int_V(g(y)-1)g(|\vec{r}-\vec{y}|)\times\Phi(|\vec{r}-\vec{y}|)d\vec{y}. \tag{12}$$

It is interesting to compare (12) with the well-known integral equations for the radial distribution function of the classical simple liquids. In such a situation expression (12) can be rewritten as

$$-\theta\ \ln g(r)=\Phi(r)+n\int_V(g(y)-1)g(|\vec{r}-\vec{y}|)\times\Phi(|\vec{r}-\vec{y}|)d\vec{y}. \tag{13}$$

This is very similar to the equation

$$-\theta\ \ln g(r)=\Phi(r)+n\int_V(g(y)-1)\tilde{\Phi}(|\vec{r}-\vec{y}|)d\vec{y} \tag{14}$$

derived in the superposition approximation by Bogoliubov [4]. Here

$$\tilde{\Phi}(|\vec{r}-\vec{y}|)\equiv g(|\vec{r}-\vec{y}|)\Phi(|\vec{r}-\vec{y}|)+\int_{|\vec{r}-\vec{y}|}^{\infty}\Phi(t)\frac{dg}{dt}dt.$$

Function $\Phi(t)\,dg/dt$ is oscillating around zero, so its integral, apparently, does not make an essential contribution into the expression for $\tilde{\Phi}(|\vec{r}-\vec{y}|)$. So, Eqs. (13) and (14) have to yield similar qualitative results. According to (14), we can expect that $\tilde{\Phi}$ (r) is more accurate an estimation of the effective interaction potential than $g(r)\Phi(r)$. The replacement of $g(r)\Phi(r)$ by $\tilde{\Phi}(r)$ in expression (12), results in the following integral equation:

$$\mu_{id}(n)-\mu_{id}(ng(r))=\Phi(r)+n\int_V(g(y)-1)\tilde{\Phi}(|\vec{r}-\vec{y}|)d\vec{y}, \tag{15}$$

which gives the Bogoliubov equation (14) in the classical limit. Thus, we have now derived integral Eqs. (13) and (15) that allow us to explore particle correlations even in the many-body systems with the interaction potentials behaving at small distances as $1/r^m$ $(m>2)$.

In conclusion, let us take notice of the most important points of the paper once more. The article presents the generalization of the Thomas-Fermi method to investigate particle correlations in the many-body systems with non-Coulomb interactions of their constituents. The essentials of the generalization consist in using integral formulation and operating with the radial distribution function. The paper results in the integral equations for $g(r)$ which correspond to the different ways of considering particle interactions. The most interesting of them, (15), is reduced to Bogoliubov equation (14) in the classical limit and can be used to investigate particle correlations for the quantum liquids with the interaction potential not having the Fourier transform, for example, with Lennard-Jones potential. Of course, it is also necessary to explore other possible evaluations of $U(r)$ and corresponding integral equations for the radial distribution function. This investigation will be presented in a forthcoming paper.

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