

AN APPLICATION OF SEMI-FREE GAS AND COLLECTIVE
COORDINATES MODELS ON FERMION SYSTEMS

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Abstract. Semi-free gas and collective coordinates models are used for description of the ground state of fermion systems.

1. I n t r o d u c t i o n. Semi-free gas model has been introduced in the theory of boson and fermion systems by Ljölje^{1,2)}.

This model treats correlative motion of every pair of particles by means of two-particle asymptotic wave function for short distances, leaving the particles to move freely in the rest of space.

The contribution of the greater inter-particle distances, for boson systems, has been taken into account by making use of collective motion with RPA (Random Phase Approximation)^{3,4,5)}.

The aim of this article is an application of these two methods for description of the ground state of fermion systems.

The energy of the ground state has been calculated by Iwamoto-Yamada method⁷⁾, taking for the symmetrical part of wave-function one of the eigen-functions of the Hamiltonian.

2. E x p e c t i n g v a l u e o f t h e H a m i l t o n i a n f o r f e r m i o n s y s t e m. The Hamiltonian of a fermion system has the form³⁾:

$$H = -\sum_i \frac{\hbar^2}{2m} \Delta_i + \frac{1}{2} \sum_{ij} V^1(r_{ij}) + \sum_{ij} V^2(r_{ij}) \quad (1)$$

where the potentials $V^1(r_{ij})$ and $V^2(r_{ij})$ describe the short-range and long-range interaction, respectively.

The wave functions of the observed system is written as a product of a symmetrical wave function, as in the case of boson systems^{3,4,5)}, and a determinant wave function, composed of one-particle functions; i.e. :

$$\Psi = \Psi_s \cdot \Phi \quad (2)$$

where is

$$\Phi = \frac{1}{\sqrt{N!}} \sum_P (-1)^P \prod_j \lambda_j(\vec{x}_j) \quad (3)$$

and

$$\lambda_j(\vec{x}_j) = \frac{1}{\sqrt{\Omega}} \exp(i \vec{k}_j \vec{r}_j) S_j(\vec{b}_j). \quad (4)$$

The functions $S_j(\vec{b}_j)$ are spin functions.

The symmetrical wave function is also written as a product

$$\Psi_s = \Psi_{sR} \cdot \Psi_{sL} \quad (5)$$

where the wave function Ψ_{sR} is given as a product of two-particle asymptotic wave functions for short inter-particle distances:

$$\Psi_{sR} = \exp(-\frac{1}{2} \sum'_{ij} f_{ij}). \quad (6)$$

The wave function, which describes the collective motion, can be also, written as a product of two-particle functions:

$$\Psi_{sL} = \exp(-\frac{1}{2} \sum'_{ij} \tilde{f}_{ij}). \quad (7)$$

By making use the following denotes:

$$\tilde{f}_{ij} = f_{ij} + \tilde{f}_{ij}, \quad F_{ij} = \exp(-f_{ij}) \quad (8)$$

the realation (2) becomes:

$$\Psi = \prod_{i < j} F_{ij} \frac{1}{\sqrt{N!}} \sum_{\substack{P_1 \dots P_N \\ \vec{r}_1 \dots \vec{r}_N}} \epsilon_P \prod_l \lambda_l(\vec{x}_l). \quad (9)$$

The expecting value of the Hamiltonian (1), regarding to the wave function (9), is given by

$$\langle H \rangle = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \quad (10)$$

3. Finding of the functions f_{ij} and \tilde{f}_{ij} . The function f_{ij} which describes the short-range interaction, is determined, in the semi-free gas model ¹⁾, in such way so as to cancel the strong repulsive short-range potential $V'(r_{ij})$. This condition leads to the equation:

$$2 \frac{\hbar^2}{m} (\nabla_i f_{ij})^2 = \frac{1}{2} V'(r_{ij}), \quad (11)$$

which has general solution ^{1,3)}:

$$f(r) = \pm \int_0^r \sqrt{\frac{m}{4\hbar^2} V'(r')} dr' + C. \quad (12)$$

The function ψ_{ij} , which describes collective oscillations of the system, is connected with long-range potential $V^2(r_{ij})$. This connection can be found by expanding ψ_{ij} and $V^2(r_{ij})$ with respect to the plane waves; i.e.:

$$V^2(r_{ij}) = \sum_k V_k \exp[i\vec{k}(\vec{r}_i - \vec{r}_j)]; \quad \psi_{ij} = \sum_k \psi_k \exp[i\vec{k}(\vec{r}_i - \vec{r}_j)] \quad (13)$$

Inserting (13) in (10) and introducing the collective coordinates

$$p_k = \sum_i \exp(i\vec{k}\vec{r}_i), \quad \vec{k} \neq 0, \quad (14)$$

the expecting value of the Hamiltonian is obtained, regarding to the collective coordinates. The request, that the coefficient, beside the square of collective coordinate vanishes, leads to the relation for the Fourier component ψ_k of long-range part of two-particle wave function ψ_{ij} .

This component reads

$$\psi_k = \frac{1}{2N} \left(\sqrt{1 + \frac{4m}{\hbar^2 k^2} \rho V_k^2} - 1 \right), \quad (15)$$

where is $V_k^2 = \Omega V_k^2$.

By making use the relation 6):

$$\int F(x) \sin x r dx = \frac{F(0)}{r} - \frac{F''(0)}{r^3} + \frac{F^{(4)}(0)}{r^5} - + \dots, \quad (16)$$

for the function $\psi(r)$ is obtained:

$$\psi(r) = \frac{A(x, \rho)}{r^2} + \frac{B(x, \rho)}{r^4} + \dots, \quad (17)$$

where $\rho = \frac{N}{\Omega}$ is the density of system and X designates variational parameters of separation of the potential $V(r_{ij})$.

The coefficient $A(x, \rho)$ and $B(x, \rho)$ have the values

$$A(x, \rho) = \frac{1}{\rho} \frac{\lambda}{4\hbar} \sqrt{\frac{4m}{\hbar^2 \lambda^2} \rho R(x-S)}; \quad B(x, \rho) = \frac{1 - \frac{8m}{\hbar^2 \lambda^2} \rho R(x-S)}{\sqrt{\frac{4m}{\hbar^2} \rho R(x-S)}}, \quad (18)$$

where λ, R, S and C are constances 6).

4. Using of Iwamoto-Yamada method. The calculation of expecting value of the Hamiltonian will be made by using of Iwamoto_Yamada method ⁷⁾.

Applying this method and taking only coefficients of cluster expansion, which give the contribution of the first power of density, it could be written:

$$\langle H \rangle = \xi \langle i | H(i) | i \rangle + \frac{1}{2} \sum_{ij} \langle ij - ji | H(i,2) F_{12}^2 | ij \rangle + \dots \quad (19)$$

where is

$$H(i) = H_i(\vec{x}_i) = -\frac{\hbar^2}{2m} \frac{\Delta \lambda_i(\vec{x}_i)}{\lambda_i(\vec{x}_i)} \quad ,$$

$$H(i,2) = H_{ij}(\vec{x}_i, \vec{x}_2) = -\frac{\hbar^2}{m} \left\{ \frac{\Delta F_{12}}{F_{12}} + \frac{\nabla \lambda_i(\vec{x}_i) \nabla F_{12}}{\lambda_i(\vec{x}_i) F_{12}} + \frac{\nabla \lambda_j(\vec{x}_2) \nabla F_{12}}{\lambda_j(\vec{x}_2) F_{12}} + V_{12}^1 + V_{12}^2 \right\} \quad (20)$$

In our case, we get

$$H(i) = \frac{\hbar^2 k_f^2}{2m}$$

$$H(i,2) = -\frac{\hbar^2}{m} \left\{ -\frac{d^2}{dr_{12}^2} f_{12} - \frac{2}{r_{12}} \frac{d}{dr_{12}} f_{12} - \frac{d^2}{dr_{12}^2} \gamma_{12} - \frac{2}{r_{12}} \frac{d}{dr_{12}} \gamma_{12} + 2 \frac{df_{12}}{dr_{12}} \cdot \frac{d\gamma_{12}}{dr_{12}} + \left(\frac{d}{dr_{12}} \gamma_{12} \right)^2 - i(\vec{k}_i - \vec{k}_j) \frac{\vec{r}_{12}}{r_{12}} \left(\frac{d}{dr_{12}} f_{12} + \frac{d}{dr_{12}} \gamma_{12} \right) \right\} + V_{12}^2 \quad (21)$$

After inserting (21) in (19) and ordering, the terms of (19) read as following .

The first:

$$\sum_i \langle i | H | i \rangle = N \frac{3\hbar^2}{10m} (3f)^{2/3} \cdot \rho^{2/3} \quad , \quad (22)$$

the second:

$$\frac{1}{2} \sum_{ij} \langle ij - ji | H(i,2) F_{12} | ij \rangle = \rho \frac{N\hbar^2}{m} \left\{ \int e^{-2\beta(r)} \cdot K(r) dr + \int e^{-2\beta(r)} \cdot R(r) dr \right\} + \frac{\rho}{(2\beta)^2} \left\{ \int e^{-2\beta(r)} \frac{1}{r^2} (\sin k_f r - k_f r \cos k_f r)^2 \cdot K(r) dr + \int R(r) \frac{1}{r^2} (\sin k_f r - k_f r \cos k_f r)^2 dr \right\} \quad (23)$$

where is

$$K(r) = \left[\frac{d^2}{dr^2} f(r) + \frac{2}{r} \frac{d}{dr} f(r) \right] ,$$

$$R(r) = \left[\frac{d^2}{dr^2} \gamma(r) + \frac{2}{r} \frac{d}{dr} \gamma(r) + \left(\frac{d}{dr} \gamma(r) \right)^2 + 2 \frac{d}{dr} f(r) \frac{d}{dr} \gamma(r) \right] + V^2(r) .$$

The expecting value of energy per particle, regarding to the density, is:

$$\begin{aligned} \frac{\langle H \rangle}{N} = & \frac{3\hbar^2}{10m} (3\pi^2)^{2/3} \cdot \rho^{2/3} + \rho \left\{ \frac{\hbar^2}{m} \left[\int e^{-2fr} \cdot K(r) dr^3 + \int e^{-2fr} \cdot R(r) dr^3 \right] + \right. \\ & \left. + \frac{1}{(2\pi)^3} \left[\int e^{-2fr} \cdot \frac{1}{r^6} (\sin k_r r - k_r \cos k_r r)^2 K(r) dr^3 + \int R(r) \cdot \frac{1}{r^6} (\sin k_r r - k_r \cos k_r r)^2 dr^3 \right] \right\} . \end{aligned}$$

This result could be applied on liquid He³ which is a representative example of fermion systems. Because of troubles in the numerical computation, this application is left for an other article.

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