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APPLICATION OF URSELL-MAYER METHOD IN THE MODEL OF SEMI-FREE GAS OF LIQUID ⁴He

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1. K. Ljolje¹) has shown that short range correlations of each pair of particles secure a bound state of liquid ⁴He in low density limit. Evaluation of relevant integrals were performed by making use of hard-sphere method. Here we want to apply Ursell-Mayer method in the evaluation of these integrals, that means of the expectation value of the energy, in order to obtain exact expansion with respect to density, and to compare the result with that of K. Ljolje in the low density limit.

2. The expression of expectation value of the energy of liquid ⁴He in the stated paper reads

$$E_{o} = n (n-1) (n-2) \frac{\int \psi^{2} \Phi(123) \overrightarrow{dr_{1} \dots dr_{n}}}{\int \psi^{2} \overrightarrow{dr_{1} \dots dr_{n}}} + n (n-1) \frac{\int \psi^{2} f(12) \overrightarrow{dr_{1} \dots dr_{n}}}{\int \psi^{2} \overrightarrow{dr_{1} \dots dr_{n}}}.$$
(1)

The notations are the same as in the paper¹). We define the functions:

$$G_2 - V^2 e^{-2Be^{-\frac{\alpha}{2}r_{12}}} \cdot \frac{1}{I_n} \cdot \int \psi^2 d\vec{r_3} \cdots d\vec{r_n}, \qquad (2)$$

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$$G_{s} = V^{s} e^{-\frac{\alpha}{2}r_{12}} - 2Be^{-\frac{\alpha}{2}r_{13}} - 2Be^{-\frac{\alpha}{2}r_{23}} \cdot \frac{1}{I_{n}} \cdot \int \psi^{2} d\vec{r_{4}} \cdots d\vec{r_{n}}, \quad (3)$$

where

$$I_n = \int \psi^2 \, dr_1 \dots dr_n \; ; \tag{4}$$

and similarly we introduce

$$I_{n-2} = \int \psi^2 (3...n) \, dr_3...dr_n , \qquad (5)$$

$$I_{n-3} = \int \psi^2 (4 \dots n) \, dr_4 \dots dr_n \, . \tag{6}$$

After the Mayer's supstitution²⁾

$$f'(r_{ij}) \equiv f'_{ij} = e^{-2Be^{-\frac{\alpha}{2}}r_{ij}} - 1, \qquad (7)$$

we have

$$\Psi^{\mathbf{a}} = \sum_{\mathbf{v}_{kl}} \prod_{k=0,1}^{n \ge 1 \ge 3} \prod_{\substack{k=1,2\\kl}}^{r_{v} \ge 1} f_{kl}^{r_{kl}} e^{-2Be^{-\frac{\alpha}{2}r_{12}}} \Psi^{\mathbf{a}}(3...n) \cdot$$
(8)

Let us first consider the function G_2 . After supstitution of (8) in (2), let us concentrate our attention to one term in the sum. Let be the term in which the function f' with m particles have $v_{kl} \neq 0$ (the particles 1 and 2 are excluded here).

Integral over other particles multiplied with V^m/I_{n-2} is

$$F_m = \frac{V^m}{I_{n-2}} \int \psi^2 (3 \dots n) \, dr_{m+3} \dots dr_n \, . \tag{9}$$

Since the integrals of each set of m particles are equal, and

$$\frac{(n-2-m)! \ m!}{(n-2)!} \sim \frac{n^m}{m!} \ (\text{for } m < n),$$

we obtain:

$$G_{2} = \frac{V^{2}I_{n} - 2}{I_{n}} \left\{ 1 + \sum_{n \gg m \ge 1} \frac{\rho^{m}}{m!} \int \prod_{l=3}^{m+2} \left| e^{-\sum_{k=1}^{2} 2Be^{-\frac{a}{2}r_{kl}}} - 1 \right] \cdot F_{m} d\vec{r_{s}} \cdots d\vec{r_{m+2}} + \cdots \right\}$$
(10)

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Performing similar procedures one obtains

$$G_{8} = \frac{V^{8}}{l_{n}} \frac{l_{n}}{l_{n}} = 3 \left\{ 1 + \sum_{n \gg m \geqslant 1} \frac{e^{m}}{m!} \int \prod_{l=4}^{m+3} \left[e^{-\sum_{k=1}^{3} 2Be^{-\frac{\alpha}{2}r_{kl}}} -1 \right] \cdot F'_{m} d\vec{r_{4}} \cdots d\vec{r_{m+3}} + \cdots \right\} \cdot (11)$$

$$= \frac{l_{n}}{l_{n-2}} = \int e^{-2Be^{-\frac{\alpha}{2}r_{12}}} \left\{ 1 + \sum_{n \gg m \geqslant 1} \frac{\rho_{m}}{m!} \int \prod_{l=4}^{m+3} \cdot \left(1 + \sum_{n \gg m \geqslant 1} \frac{\rho_{m}}{m!} \int \prod_{l=4}^{m+3} \cdot \left(1 + \sum_{l=4}^{2} 2Be^{-\frac{\alpha}{2}r_{kl}} -1 \right] \cdot F_{m} d\vec{r_{3}} \cdots d\vec{r_{m+2}} + \cdots \right\} d\vec{r_{1}} d\vec{r_{2}} , (12)$$

$$= \frac{l_{n}}{l_{n-3}} = \int e^{-2Be^{-\frac{\alpha}{2}r_{12}}} -2Be^{-\frac{\alpha}{2}r_{13}} -2Be^{-\frac{\alpha}{2}r_{23}}$$

$$= \left\{ 1 + \sum_{n \gg m \geqslant 1} \frac{\rho^{m}}{m!} \int \prod_{l=4}^{m+3} \left[e^{-\sum_{k=1}^{3} 2Be^{-\frac{\alpha}{2}r_{kl}}} -1 \right] + \sum_{n \gg m \geqslant 1} \frac{\rho^{m}}{m!} \int \prod_{l=4}^{m+3} \left[e^{-\sum_{k=1}^{3} 2Be^{-\frac{\alpha}{2}r_{kl}}} -1 \right] + \sum_{n \gg m \geqslant 1} \frac{\rho^{m}}{m!} \int \prod_{l=4}^{m+3} \left[e^{-\sum_{k=1}^{3} 2Be^{-\frac{\alpha}{2}r_{kl}}} -1 \right] + \sum_{n \gg m \geqslant 1} \frac{\rho^{m}}{m!} \int \prod_{l=4}^{m+3} \left[e^{-\sum_{k=1}^{3} 2Be^{-\frac{\alpha}{2}r_{kl}}} -1 \right] + \sum_{n \gg m \gg 1} \frac{\rho^{m}}{m!} \int \prod_{l=4}^{m+3} \left[e^{-\sum_{k=1}^{3} 2Be^{-\frac{\alpha}{2}r_{kl}}} -1 \right] + \sum_{l=4}^{m+3} \left[e^{-\sum_{k=1}^{3} 2Be^{-\frac{\alpha}{2}r_{kl}}} -1 \right] + \sum_{l=4}^{m} \left[e^{-\sum_{k=1}^{3} 2Be^{-\frac{\alpha}{2}r_{kl}} -1 \right] + \sum_{l=4}^{m} \left[e^{-\sum_{k=1}^{3} 2Be^{-\frac{\alpha}{2}r_{kl}}} -1 \right] + \sum_{l=4}^{m} \left[e^{-\sum_{k=1}^{3} 2Be^{-\frac{\alpha}{2}r_{kl}} -1 \right] + \sum_{l=4}^{m} \left[e^{-\sum_{k=1}^{3} 2Be^{-\frac{\alpha}{2}r_{kl}}} -1 \right] + \sum_{l=4}^{m} \left[e^{-\sum_{k=1}^{3} 2Be^{-\frac{\alpha}{2}r_{kl}}} -1 \right] + \sum_{l=4}^{m} \left[e^{-\sum_{k=1}^{3} 2Be^{-\frac{\alpha}{2}r$$

with

$$F'_{m} = \frac{V^{m}}{I_{n-3}} \int \psi^{2} (4 \dots n) \, \overrightarrow{dr_{m+4} \dots dr_{n}} \,. \tag{14}$$

The supstitution of (10) and (11) in Eq. (1) gives the expansion of the expectation value of the energy with respect to the density.

3. In the limit of low density $(\varrho \rightarrow 0)$ it follows

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$$\frac{E_{o}}{n} = \varrho I_{1} + \varrho^{2} (I_{2} + I'_{2} + \gamma I_{1}) , \qquad (15)$$

where

$$I'_{2} = V^{-1} \int e^{-2Be^{-\frac{\alpha}{2}r_{12}}} f(12) \left[e^{-2Be^{-\frac{\alpha}{2}r_{13}}} - 2Be^{-\frac{\alpha}{2}r_{23}} - \frac{1}{2} \right] dr_{1} dr_{2} dr_{3} dr_{3},$$

$$\gamma = -2 \int f'(r) dr.$$

Other notations are the same as in the paper¹).

We see that the first term of Eqs. (15) and (16) in the paper¹) are equal. For real densities of liquid ⁴He the first two powers of ϱ are not enough.

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References

K. Ljolje, Fizika, 1 (1968) 11;
 J. E. Mayer and M. G. Montroll, J. Chem. Phys. 9 (1941) 1.