ОБЪЕДИНЕННЫЙ
ИНСТИТУТ
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ

Дубна

E17-96-139

V.N.Minasyan, G.V.Turyan[1]

ON THE MODEL HAMILTONIAN OF LIQUID HELIUM He-4

Submitted to «ЖЭТФ»

[1]National Renewable Energy Laboratory, Golden, USA

1996

In this paper, we develop a consistent quantum theory of liquid $He-4$ at temperatures $T \leq T_0$ (T_0 is the temperature of Bose–condensation). The theory is based on the effective model of the Bose–Einstein interacting gas that differs from the Bogoliubov model for a weakly nonideal gas [1]. Like in the Bogoliubov model, the liquid $He-4$ is considered as a rarefied nonideal gas of identical spinless Bose-particles. The gas is so rarefied that only binary collisions of atoms are allowed. Let us denote the atomic momenta before collision by $\vec{p_1}$ and $\vec{p_2}$ and those upon collision by $\vec{p_1}'$ and $\vec{p_2}'$. The method of second quantization supplemented with the conservation law for a pair of atoms gives the following Hamiltonian:

$$\hat{H} = \sum_{\vec{p}} \frac{p^2}{2m} \hat{a}^+_{\vec{p}} \hat{a}_{\vec{p}} + \frac{1}{2V} \sum_{\vec{p_1},\vec{p_2},\vec{p_1}',\vec{p_2}'} U_{\vec{p}} \hat{a}^+_{\vec{p_1}} \hat{a}^+_{\vec{p_2}} \hat{a}_{\vec{p_2}'} \hat{a}_{\vec{p_2}'} \qquad (1)$$

with

$$\vec{p} = \vec{p_1} - \vec{p_1}' = \vec{p_2}' - \vec{p_2}$$

where $\vec{p}$ is the momentum change in collision, m is the mass of an atom, $U_{\vec{p}}$ is the pair potential of interaction of the Bose-gas atoms in the momentum space; $\hat{a}^+_{\vec{p}}$ and $\hat{a}_{\vec{p}}$ are the "creation" and "annihilation" operators of a free particle with momentum $\vec{p}$; V is the volume of the gas.

Let us transform the Hamiltonian to the form

$$\begin{aligned} \hat{H} &= \sum_{\vec{p}\neq 0} \frac{p^2}{2m} \hat{a}^+_{\vec{p}} \hat{a}_{\vec{p}} + \frac{1}{2V} \sum_{\vec{p}\neq 0} \sum_{\vec{p_1}} \sum_{\vec{p_2}} U_{\vec{p}} \hat{a}^+_{\vec{p_1}} \hat{a}^+_{\vec{p_2}} \hat{a}_{\vec{p_1}-\vec{p}} \hat{a}_{\vec{p_2}+\vec{p}} + \\ &+ \frac{U_0}{2V} \sum_{\vec{p_1}} \sum_{\vec{p_2}} \hat{a}^+_{\vec{p_1}} \hat{a}^+_{\vec{p_2}} \hat{a}_{\vec{p_1}} \hat{a}_{\vec{p_2}} \end{aligned} \qquad (2)$$

We will approximate the Hamiltonian under the following assumptions:

1. In a liquid $He-4$ at temperatures $T \leq T_0$, the number of atoms in the condensate $N_{0,T}$ is far larger than 1; in this case, the operators $\hat{a}^+_0 \simeq N_{0,T}{}^{1/2}$ and $\hat{a}_0 \simeq N_{0,T}{}^{1/2}$ can be considered c–numbers.

2. The presence of the condensate in the liquid helium at temperatures $T \leq T_0$ results in strong dominance of interactions between quantum state with momentum $\vec{p} \neq 0$ into the condensate state $\hat{\tau}_{\vec{p}} \ll \hat{\rho}_{\vec{p}}$,

where

$$\hat{\rho}_{\vec{p}} = \hat{a}_0^+ \hat{a}_{-\vec{p}}$$

is the component of the density fluctuation operator for the condensate particles with the momentum $\vec{p}$, and the other term

$$\hat{\tau}_{\vec{p}} = \sum_{\substack{\vec{p}_1 \neq 0, \\ \vec{p}_1 \neq \vec{p}}} \hat{a}_{\vec{p}_1}^+ \hat{a}_{\vec{p}_1 - \vec{p}}$$

is the operator of density fluctuations of above-condensate particles with the momentum $\vec{p}$.

3. Experimental data obtained by the method of neutron inelastic scattering on liquid $He-4$ demonstrate that the density of Bose condensate is temperature- dependent [2]. In the ground state of liquid $He-4$, the condensate contains less than 0.1 of all atoms. Therefore, at temperatures $T \leq T_0$, the number of atoms in the condensate $N_{0,T}$ is far smaller than the total number of particles in the gas N. Consequently, it can be assumed that the total number of particles in the gas N is much larger than the number of particles filling a certain quantum state with the momentum $N_{0,T}$ $(N \gg N_{\vec{p}})$.

Owing to these assumptions, the model Hamiltonian in zeroth approximation as a function of the Bose–condensate density $\frac{N_{0,T}}{V}$ takes the following form

$$\hat{H} = \sum_{\vec{p} \neq 0} \frac{p^2}{2m} \hat{a}_{\vec{p}}^+ \hat{a}_{\vec{p}} + \frac{1}{2V} \sum_{\vec{p} \neq 0} U_{\vec{p}} N_{0,T} \left(\hat{a}_{\vec{p}}^+ \hat{a}_{-\vec{p}}^+ + \hat{a}_{\vec{p}} \hat{a}_{-\vec{p}} + 2\hat{a}_{\vec{p}}^+ \hat{a}_{\vec{p}} \right) + \frac{U_0 N^2}{2V} \quad (3)$$

Now we will show that the chemical potential of the gas model under consideration can be considered zero. To this end, we take the Hamiltonian of a large canonical Gibbs ensemble $\hat{G}$

$$\hat{G} = \hat{H} - \mu \hat{N} \quad (4)$$

and transform it to the form

$$\hat{G} = \sum_{\vec{p} \neq 0} \left(\frac{p^2}{2m} - \mu \right) \hat{a}_{\vec{p}}^+ \hat{a}_{\vec{p}} + \frac{1}{2V} \sum_{\vec{p} \neq 0} U_{\vec{p}} N_{0,T} \left(\hat{a}_{\vec{p}}^+ \hat{a}_{-\vec{p}}^+ + \hat{a}_{\vec{p}} \hat{a}_{-\vec{p}} + 2\hat{a}_{\vec{p}}^+ \hat{a}_{\vec{p}} \right) - \mu N_{0,T} + \frac{U_0 N^2}{2V} \quad (5)$$

To carry the Hamiltonian $\hat{G}$ into the diagonal form, we take advantage of the Bogoliubov transformation

$$\hat{a}_{\vec{p}} = \frac{\hat{b}_{\vec{p}} + L_{\vec{p},T} \hat{b}_{-\vec{p}}^+}{\sqrt{1 - L_{\vec{p},T}^2}} \quad (6)$$

where $L_{\vec{p},T}$ is a real symmetric function of the momentum $\vec{p}$; $\hat{b}_{\vec{p}}^+$, $\hat{b}_{\vec{p}}$ are "creation" and "annihilation" operators of a quasiparticle with the momentum $\vec{p}$.

Then, the Hamiltonian $\hat{G}$ assumes the form

$$\hat{G} = \sum_{\vec{p} \neq 0} \varepsilon_{\vec{p},T} \hat{b}_{\vec{p}}^+ \hat{b}_{\vec{p}} + \frac{1}{2} \sum_{\vec{p} \neq 0} \left(\varepsilon_{\vec{p},T} - \frac{p^2}{2m} - \frac{N_{0,T} U_{\vec{p}}}{V} + \mu \right) - \mu N_{0,T} + \frac{U_0 N^2}{2V} \quad (7)$$

where $\varepsilon_{\vec{p},T}$ is the energy of the quasiparticle with momentum $\vec{p}$ at temperature T

$$\varepsilon_{\vec{p},T} = \left[\left(\frac{p^2}{2m} - \mu \right)^2 + \frac{p^2 N_{0,T} U_{\vec{p}}}{mV} - \frac{2\mu N_{0,T} U_{\vec{p}}}{V} \right]^{1/2} \quad (8)$$

and the function $L_{\vec{p},T}^2$ is given by

$$L_{\vec{p},T}^2 = \left(-\varepsilon_{\vec{p},T} + \frac{p^2}{2m} + \frac{N_{0,T} U_{\vec{p}}}{V} - \mu \right) \Big/ \left(\varepsilon_{\vec{p},T} + \frac{p^2}{2m} + \frac{N_{0,T} U_{\vec{p}}}{V} - \mu \right) \quad (9)$$

In this model of liquid $He-4$, the chemical potential tends to zero. Actually, it is known from experiment that when $\vec{p} \to 0$, $\varepsilon_{\vec{p},T} \to 0$, therefore from (8) it follows that μ can be considered zero.

So, the Hamiltonian of the system and energy of quasiparticles take the following form

$$\hat{H} = \sum_{\vec{p} \neq 0} \varepsilon_{\vec{p},T} \hat{b}_{\vec{p}}^+ \hat{b}_{\vec{p}} + \frac{1}{2} \sum_{\vec{p} \neq 0} \left(\varepsilon_{\vec{p},T} - \frac{p^2}{2m} - \frac{N_{0,T} U_{\vec{p}}}{V} \right) + \frac{U_0 N^2}{2V} \quad (10)$$

where

$$L_{\vec{p},T}^2 = \left(-\varepsilon_{\vec{p},T} + \frac{p^2}{2m} + \frac{N_{0,T} U_{\vec{p}}}{V} \right) \Big/ \left(\varepsilon_{\vec{p},T} + \frac{p^2}{2m} + \frac{N_{0,T} U_{\vec{p}}}{V} \right) \quad (11)$$

$$\varepsilon_{\vec{p},T} = \left[\left(\frac{p^2}{2m} \right)^2 + \frac{p^2 N_{0,T} U_{\vec{p}}}{mV} \right]^{1/2} \quad (12)$$

Experimentally, it is known [3] that the specific heat of liquid helium around the absolute zero is proportional to T^3. In view of this fact, Landau postulated that in the vicinity of absolute zero, quasiparticles in liquid helium are longitudinal phonons, which means that at the absolute zero of temperature, the energy of a quasiparticle with momentum $\vec{p}$ is of the form

$$\varepsilon_{\vec{p},0} = pv \quad (13)$$

where v is the velocity of phonons. With (13) substituted into (12), for $U_{\vec{p}}$ we derive the following expression

$$U_{\vec{p}} = \left(mv^2 - \frac{p^2}{4m}\right)\frac{V}{N_{0,0}} \tag{14}$$

where $N_{0,0}$ is the number of particles at rest at $T = 0$.

The energy of interaction between a pair of atoms in the coordinate space separated by the distance r from each other, $U_{12}(r)$, is of the form

$$U_{12}(r) = \frac{1}{V}\sum_{\vec{p}} U_{\vec{p}} \exp\left(-\frac{i2\pi\vec{p}\vec{r}}{h}\right) \tag{15}$$

Since our problem is to study the thermodynamic properties of a gas, we should always take account of the thermodynamic limit when $V \to \infty$, $N \to \infty$, and the specific volume $v_0 = \frac{V}{N}$ remains constant. Substituting $U_{\vec{p}}$ from (14) into (15) and performing the thermodynamic transition, it is easy to show that the sum in (15) diverges. To provide the divergence of that sum and obtain the expression for the interaction energy $U_{12}(r)$, one should introduce the concept of a boundary momentum for the liquid $He-4$ atoms. The boundary momentum for particles of a nonideal gas is connected with the characteristic length of interaction between a pair of atoms that is a minimal distance between two interaction atoms. Atoms with a momentum exceeding the boundary momentum $\vec{p_0}$ do not participate in the process of scattering. Therefore when $p \geq p_0$: $U_{\vec{p}} = 0$, and, thus, $U_{\vec{p}=\vec{p_0}} = 0$. Equating $U_{\vec{p}}$ obtained by formula (14), for we obtain for the boundary momentum the value $p_0 = 2mv$. In this case, for the interaction energy $U_{12}(r)$ (15) we arrive at the following expression

$$U_{12}(r) = \frac{V\hbar^2}{4\pi^2 r^5 N_{0,0} m}\left|3 - \left(\frac{2mvr}{\hbar}\right)^2\right|\left(1 + \frac{2mvr}{\hbar}\right)\sin\left\{\frac{2mvr}{\hbar} + \mathrm{arctg}\left(\frac{2mvr}{\hbar}\right)\right\} \tag{16}$$

So from the Landau postulate it follows that there exists a quantum state occupied with atoms with the boundary momentum $\vec{p_0}$. It is the boundary between quantum states occupied with atoms participating in the scattering process and free atoms. As a result, the Hamiltonian of the system can be written in the form

$$\hat{H} = \sum_{0<p\leq p_0} \varepsilon_{\vec{p},T}\hat{b}^+_{\vec{p}}\hat{b}_{\vec{p}} + \frac{1}{2}\sum_{0<p\leq p_0}\left(\varepsilon_{\vec{p},T} - \frac{p^2}{2m} + \frac{N_{0,T}U_p}{2V}\right) + \sum_{p>p_0}\frac{p^2}{2m}\hat{a}^+_{\vec{p}}\hat{a}_{\vec{p}} \tag{17}$$

Note that the model Hamiltonian and the energy of a quasiparticle will be determined only when the temperature dependence is known for the Bose- condensate. Now, we will theoretically look for the temperature dependence of $\frac{N_{0,T}}{N_{0,0}}$. To this end we will make use of the formula ($N \gg N_{0,T}$)

$$\sum_{0<p\leq p_0}\overline{N}_{p,T} + \sum_{p>p_0}\overline{N}_{p,T} = N \tag{18}$$

where $\overline{N}_{p,T}$ is the mean number of atoms in the quantum state with momentum $\vec{p}$ at temperature T. The chemical potential for the model under consideration of liquid helium is zero, therefore, the mean number of free atoms with the momentum $\vec{p}$ in the state of statistical equilibrium is represented in the form

$$\overline{N}_{p>p_0,T} = \overline{\hat{a}^+_{\vec{p}}\hat{a}_{\vec{p}}} = \frac{1}{\exp(\frac{p^2}{2mkT}) - 1} \tag{19}$$

with k is the Boltzmann constant.

To find the mean number in a quantum state with the momentum $\vec{p}$ from the interval $0 < p \leq p_0$ at temperature T we will apply to the Bogoliubov transformation, which gives

$$\overline{N}_{0<p\leq p_0,T} = \overline{\hat{a}^+_{\vec{p}}\hat{a}_{\vec{p}}} = \frac{1 + L^2_{p,T}}{1 - L^2_{p,T}}\overline{\hat{b}^+_{\vec{p}}\hat{b}_{\vec{p}}} + \frac{L^2_{p,T}}{1 - L^2_{p,T}}\left(\overline{\hat{b}^+_{\vec{p}}\hat{b}^+_{-\vec{p}}} + \overline{\hat{b}_{\vec{p}}\hat{b}_{-\vec{p}}}\right) + \frac{L^2_{p,T}}{1 - L^2_{p,T}} \tag{20}$$

where

$$\overline{\hat{b}^+_{\vec{p}}\hat{b}^+_{-\vec{p}}} = \overline{\hat{b}_{\vec{p}}\hat{b}_{-\vec{p}}} = 0 \tag{21}$$

Then

$$\overline{N}_{0<p\leq p_0,T} = \frac{1 + L^2_{p,T}}{1 - L^2_{p,T}}\overline{n}_{p,T} + \frac{L^2_{p,T}}{1 - L^2_{p,T}} \tag{22}$$

where $\overline{n}_{p,T}$ is the mean number of the quasiparticle in the quantum state with momentum $\vec{p}$ at temperature T

$$\overline{n}_{p,T} = \overline{\hat{b}^+_{\vec{p}}\hat{b}_{\vec{p}}} = \frac{1}{\exp(\frac{\varepsilon_{\vec{p},T}}{kT}) - 1} \tag{23}$$

Next, inserting (22) into (18) and $U_{\vec{p}}$ (14) into (11) and (12) we obtain the equation for $\frac{N_{0,T}}{N_{0,0}}$

$$\frac{N}{V} = \frac{1}{V}\sum_{0<p\leq p_0}\frac{1 + L^2_{p,T}}{1 - L^2_{p,T}}\overline{n}_{p,T} + \frac{1}{V}\sum_{0<p\leq p_0}\frac{L^2_{p,T}}{1 - L^2_{p,T}} + \frac{1}{V}\sum_{p>p_0}\overline{N}_{p,T} \tag{24}$$

where

$$\frac{1+L_{p,T}^2}{1-L_{p,T}^2}=\frac{\frac{p^2}{2m}+\left(mv^2-\frac{p^2}{4m}\right)\frac{N_{0,T}}{N_{0,0}}}{\varepsilon_{\vec{p},T}} \tag{25}$$

$$\frac{L_{p,T}^2}{1-L_{p,T}^2}=\frac{-\varepsilon_{\vec{p},T}+\frac{p^2}{2m}+\left(mv^2-\frac{p^2}{4m}\right)\frac{N_{0,T}}{N_{0,0}}}{2\varepsilon_{\vec{p},T}} \tag{26}$$

$$\varepsilon_{\vec{p},T}=\left[\left(\frac{p^2}{2m}\right)^2\left(1-\frac{N_{0,T}}{N_{0,0}}\right)+p^2v^2\frac{N_{0,T}}{N_{0,0}}\right]^{1/2} \tag{27}$$

If liquid helium is in the ground state, $\overline{n}_{p,0}=0$ and $\overline{N}_{p>p_0,0}=0$. Therefore, equation (24) assumes the form

$$\frac{N}{V}=\frac{1}{V}\sum_{0<p\leq p_0}\frac{L_{p,0}^2}{1-L_{p,0}^2} \tag{28}$$

where

$$L_{p,0}^2=\left(1-\frac{2mv}{p}\right)^2/\left(1+\frac{2mv}{p}\right)^2 \tag{29}$$

In the thermodynamic limit, for the phonon velocity at $T=0$ we have

$$\frac{2\pi v_0 m^3 v^3}{3h^3}=1 \tag{30}$$

Then the phonon velocity equals $v=209.4m/s$ that slightly differs from the experimental result $v=237m/s$. At the value $v=209.4m/s$, the characteristic length $\frac{h}{p_0}$ related to the boundary momentum equals $4,75A$.

At the temperature of Bose-condensation T_0: $\frac{N_{0,T_0}}{N_{0,0}}=0$, equation (24) becomes

$$\frac{4\sqrt{2}\pi v_0(mk)^{3/2}T_0^{3/2}}{h^3}\int_0^\infty\frac{x^{1/2}dx}{e^x-1}=1 \tag{31}$$

Solving this equation for T_0, we obtain the known value $T_0=3.1K$. To complete the note, we summarize basic results. We have considered the nonideal rarefied Bose-Einstein gas in which only binary collisions are taken into account. Gas atoms occupy quantum states of atoms only with the discrete spectrum of momenta which contains the condensate state. For the condensate being not destroyed, it is assumed that only transition of atoms from the above-condensate state to the condensate state strongly dominate when two atoms are colliding. It is shown that the chemical potential in this model equals zero. Using the Landau postulate, we have determined the energy of interaction between two atoms as an oscillating function of the distance between the two atoms. Here it is assumed that there exists the boundary momentum for atoms occupying the quantum state that is the boundary between quantum states filled with atoms participating in collisions and free atoms. The boundary momentum is connected with the characteristic length of interaction. If the distance between two atoms is smaller than the characteristic length, these atoms are free. Also we have obtain the model Hamiltonian, quasiparticle energy and the condensate density as functions of the temperature of liquid $He-4$ at temperatures $T\leq T_0$.

References

1. N.N.Bogoliubov, Jour. of Phys. (USSR), **11**, 23 (1947).
2. Miller A., Pines D., Nozieres P.,Phys.Rev. **127**, 1452 (1962).
3. L. Landau , Phys.Rev., **75**, 884, 1949.

Received by Publishing Department on April 19, 1996.