STUDY OF THE λ-TRANSITION TEMPERATURE OF He^4 INSIDE CARBON NANOTUBES

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UDC 538

The results of numerical calculations of the temperature dependence of the λ-transition point of He^4 absorbed in narrow single-walled carbon nanotubes are reported. The calculations were carried out for various amplitudes of the bare interaction V_0. A reduction of the λ-transition temperature of He^4 inside nanotubes has been demonstrated, and the relevant "temperature shift" has been determined.

The properties of superfluid helium in thin films and narrow channels are known to differ from those of helium that fills a volume of macroscopic dimensions [1, 2]. Provided the space is confined, a temperature shift of the λ-transition point is observed, as well as variations of the density distribution of the superfluid component and of its heat capacity. This work aims at studying the properties of superfluid helium-4 (He^4) adsorbed in narrow single-walled carbon nanotubes with a diameter $d = 7 \div 15$ Å, namely, the shift of the transition temperature of helium into a superfluid state.

In work [3], by measuring the speed of the fourth sound, the influence of a confined geometry upon the superfluid properties of He II was investigated in a wide range of temperature both at the pressure of saturated vapors and above. The fourth sound propagated in a system of narrow irregular channels. These channels had been formed in a pressed finely divided powder and, as a result, had the irregular form.

In this work, we study the properties of superfluid He^4 in capillaries of a certain form. Owing to this, the method of our researches has a basis different from that of work [3]. We studied the dependences of the λ-transition temperature of helium on the nanotube diameter d and on the amplitude of bare interactions V_0. It is known [4] that, for the description of a helium behavior in the vicinity of its λ-point, it is convenient to choose the "effective wave function" of the superfluid portion of helium, $\Psi(x, y, z) = \eta e^{i\varphi}$, as an order parameter. Then, the superfluid density ρ_s and the superfluid component velocity $\mathbf{V}_s$ are defined as follows:

$$\rho_s = m|\Psi|^2 = m\eta^2, \tag{1}$$

$$\mathbf{V}_{\mathrm{s}} = \frac{\hbar}{\mathrm{m}}\nabla\varphi, \tag{2}$$

where m is the mass of a helium atom ($m = 6.68 \times 10^{-24}$ g) and $\hbar$ is Planck's constant.

The effective wave function is macroscopic. Therefore, we may use it only for dimensions which considerably exceed atomic ones $a \approx 3 \times 10^8$ cm. At the same time, for He II, the temperature of which is far from the λ-point, the density ρ_s near the wall (in our case, the wall of a carbon nanotube) changes at distances of about atomic ones. The presence of confining walls and external fields results in that the order parameter module $|\Psi| = \eta = \sqrt{\rho_s/m}$ of helium at rest becomes non-uniform. In this case, external fields change both the distribution of the liquid density ρ and the λ-transition temperature $T_\lambda \equiv T_\lambda(\rho)$. Therefore, as was shown in work [2], if the potential of the force field $V(\mathbf{r})$ varies in space, the phase transition into the superfluid state does not occur simultaneously in the whole volume. First, as the temperature decreases, those regions of a liquid become superfluid, where the density is the lowest. The regions that are in a superfluid state are separated from neighbor "normal" regions by smeared phase interfaces, whose width and the form (the character of the ρ_s distribution in an interphase layer) depend on the gradient of the external field and on correlation effects.

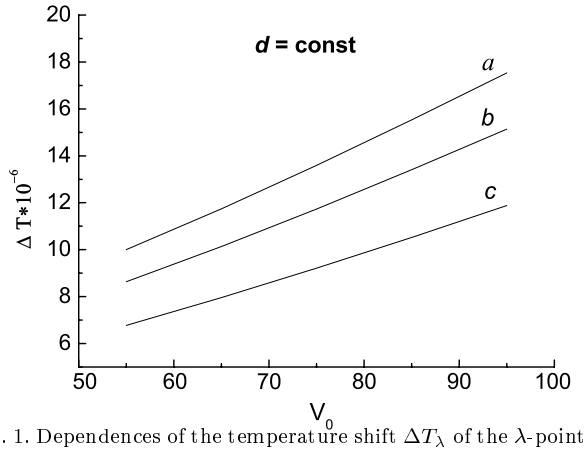

Fig. 1. Dependences of the temperature shift ΔT_λ of the λ-point on the bare interaction amplitude V_0 for various nanotube diameters d: 7 (a), 11 (b), and 15 Å (c)

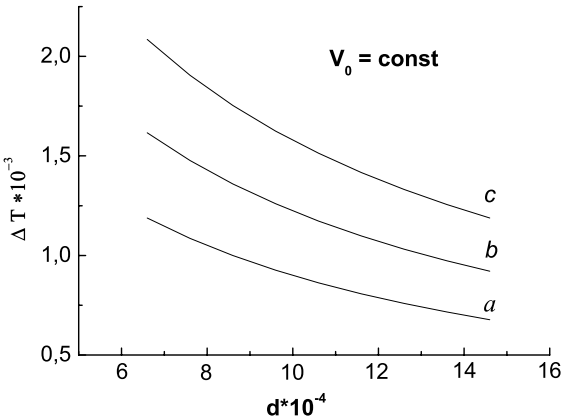

Fig. 2. Dependences of ΔT_λ on d for various V_0: 53 (a), 63 (b), and 73 K (c)

Let us consider the "temperature shift" $\Delta T_\lambda = T_\lambda - T_\lambda(d, V_0)$ induced by boundaries (nanotube walls) and an external field in the vicinity $\varepsilon = (T_\lambda - T)/T_\lambda \ll 1$ of the λ-point with $T_\lambda = 2.17$ K [2]. Below, we assume $\varepsilon \leq 0.1$, i.e. we examine temperatures that are away by no more than 0.1—0.2 K from the λ-point.

As was shown in work [4], if one consider spatially non-uniform problems, where the density ρ changes substantially, it is convenient to use the thermodynamic potential

$$\widetilde{\Omega}_{II}(\mu, T; \Psi, \rho) = \int \Big[F_{II0}(\rho, T, |\Psi|^2) + \frac{\hbar^2}{2m} |\nabla \Psi|^2 - \\ -\rho(\mu + V(\mathbf{r}) + \frac{\delta}{2}(\nabla\rho)^2) \Big] \mathbf{V}. \quad (3)$$

Here, μ is the chemical potential of helium, T is temperature, $F_{II0}(\rho, T, |\Psi|^2)$ is the density of free energy, the component $\rho V(\mathbf{r})$ describes the potential energy of helium in external fields, and the component $\frac{\delta}{2}(\nabla\rho)^2$ takes into account the density correlation. An explicit expression for the potential $V(\mathbf{r})$ will be given later.

After minimizing the thermodynamic potential $\widetilde{\Omega}_{II}(\mu, T; \Psi, \rho)$ with respect to $\Psi^*(\mathbf{r})$ and $\rho(\mathbf{r})$ and renormalizing variables, we obtained, in a conventional manner [5], the equation

$$\triangle_{yy}\widetilde{\psi} = \frac{3}{3+M}\Big(y|y|^{1/3} + (1-M)y^{2/3}|\widetilde{\psi}|^2 + M|\widetilde{\psi}|^4 \Big)\widetilde{\psi}, \quad (4)$$

where

$$y = T - T_\lambda - \frac{dT_\lambda}{d\mu}(\mu - \mu_\lambda - V(\mathbf{r})), \quad (5)$$

$M = 0$ or 1 is the dimensionless parameter, $V(\mathbf{r}) = V_0 f(\mathbf{r})$, V_0 is the approximated value of the bare interaction, and $f(\mathbf{r})$ is the approximate interaction function.

Thus, we have to solve the nonlinear differential equation (4), where V_0 is a free parameter, which is determined by the diameter of a nanotube d. This equation has no exact solution; therefore, we used approximate methods. Since the boundary condition

$$\rho_s(0) = m|\Psi(0)|^2 = 0$$

is satisfied at the wall [1], the function $\tilde{\psi}$ obeys the condition $\tilde{\psi}_{y=d/2} = 0$. Further researches were based on a choice of the interaction between helium atoms. Since we consider this interaction to be averaged over the cross-section, the potential depends only on y. The nanotube is supposed to be a smooth cylinder. Therefore, the potential of the particle field depends only on the distance from the particle to the center of this cylinder. In the calculations presented below, we took advantage of the Carlos and Cole potential [6]

$$V(y_i) = \left(\frac{4\pi V_0 \sigma^4}{a_s d^4} \right) \left[\frac{2}{5} \left(\frac{\sigma}{d} \right)^6 \xi(10, \frac{y_i}{d}) - \xi(4, \frac{y_i}{d}) \right], \quad (6)$$

where $\sigma = 2.74$ Å, $a_s = 2.74$ Å^2, and $\xi(n, y)$ is the generalized Riemann zeta-function [7].

Starting from the fact that an increase of the average value of the superfluid density results in a reduction of the temperature of λ-transition and using our previous results [5], we were able to determine the corresponding

"temperature shift" $\Delta T_\lambda = T_\lambda - T_\lambda(d, V_0)$. For this purpose, we used the relation [5]

$$\triangle T_\lambda = T_\lambda - T_\lambda(d, V_0) =$$

$$= -\frac{V(\mathbf{r})}{T_\lambda}\frac{dT_\lambda}{d\mu}\frac{(\pi\xi_{00})^{3/2}[(3+M)/3]^{3/4}}{d^{3/2}} =$$

$$= -\frac{V(\mathbf{r})}{T_\lambda}\frac{dT_\lambda}{d\mu}\frac{2.12\cdot 10^{-11}[(3+M)/3]^{3/4}}{d^{3/2}}, \qquad (7)$$

where $\xi_{00} = \sqrt{\frac{\hbar^2 T_\lambda 1.43\rho_\lambda}{2m^2\Delta C_p}}$ cm grad $^{2/3}$ is the coefficient in the temperature dependence of the coherence length, $\rho_\lambda \equiv \rho(T_\lambda) = 0.146 \times 10^{-6}$ g/m^3, and $\Delta C_p = 0.76 \times 10^7$erg cm^{-3} grad^{-1}.

The results of calculations according to relation (7) are presented graphically in Figs. 1 and 2. The dependences of the temperature shift ΔT_λ of the λ-point on the bare interaction amplitude V_0 for various nanotube diameters d are shown in Fig. 1, while Fig. 2 displays the dependences of ΔT_λ on d for various V_0.

Thus, we have established the dependences of the temperature T_λ of the λ-transition of superfluid He^4 inside carbon nanotubes on the diameter d of those nanotubes and on the amplitude of the bare interaction V_0. It has been shown that

1. If the diameter of a nanotube is constant, an increase of the interaction between superfluid helium and carbon atoms results in a linear increase of the "temperature shift".

2. If the interaction between helium and carbon atoms is constant, an increase of the nanotube diameter results in a nonlinear decrease of the λ-transition temperature.

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Received 12.08.04.
Translated from Ukrainian by O.I.Voitenko

ДОСЛІДЖЕННЯ ТЕМПЕРАТУРИ λ-ПЕРЕХОДУ He^4 ВСЕРЕДИНІ НАНОТРУБОК

О.М. Ткаченко

Р е з ю м е

Наведено результати чисельних обчислень температурної залежності λ-переходу у He^4, адсорбованому у вузьких одностінних вуглецевих нанотрубках. Обчислення проведено для різних амплітуд затравкової взаємодії V_0. Показано зниження температури λ-переходу в He^4 всередині нанотрубок і знайдено відповідний "температурний зсув".