Phase transitions in an exciton semiconductor and in a low-density superfluid Fermi liquid: the Bose-liquid approach. Dimensionally quantized and layered systems. Crossover between 3D and 2D behavior

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We investigate crossover between the 3D and 2D nature of phase transitions in dimensionally quantized and layered systems that allow a description in terms of an effective Bose liquid. As a specific physical realization of such systems, we consider a semiconductor near the exciton instability and a low-density Fermi liquid with an attractive interaction. We calculate the dependence of the temperature of the phase transition on the thickness of the dimensionally quantized film L (the width of a quantum well in the heterostructure). We show that as L increases, the transition temperature varies continuously from the 3D to the 2D form, successively passing through a series of regimes. The physical reason for the successive changeover of regimes has to do, first of all, with the change in the relative occupancy of the ground and higher subbands of dimensional quantization at the transition point and, secondly, with the change in the nature of the renormalization of the interboson interaction. Values of the critical lengths are found at which one regime replaces another. It is shown that an analogous behavior is demonstrated by layered systems in response to variation of the magnitude of the interlayer coupling (e.g., the thickness of the barriers in a superlattice). For superfluid dimensionally-quantized systems we show that there exists a critical thickness, the Berezinskii–Kosterlitz–Thouless length L_{BKT}, at which the physical mechanism of the superfluid transition changes. For $L<L_{BKT}$ destruction of the superfluid state is due to the formation of unpaired vortices, and for $L>L_{BKT}$, it is due to irrotational fluctuations. The dependence of the superfluid transition temperature on L is found.

1. INTRODUCTION

Modern methods of molecular-beam epitaxy make it possible to artificially create layered semiconductor structures with a prescribed single-electron spectrum. By varying the parameters of such systems (e.g., the width of an isolated quantum well or the thickness of the potential barriers in a superlattice), one can create series of structures whose single-electron spectra successively change over from the 2D to the 3D form. By growing structures from materials possessing one or another instability of an electronic nature leading to phase transformations, it is possible to examine an interesting class of problems associated with the study of crossover between the 3D and 2D nature of the phase transitions. The simplest and for semiconductors the most natural type of such instability is the interband exciton instability, arising when the exciton energy ε_{ex} exceeds the width of the forbidden band ε_g ($\varepsilon_{ex}>\varepsilon_g$).[1] As a system in which it is apparently possible to satisfy this condition, one might suggest a structure based on InAs/GaSb compounds with a smooth variation of the thickness of the layers, thus allowing one to vary the width of the forbidden band over wide limits, successively changing over from a semiconductor spectrum to a semimetallic one.[2] It may also be noted that recently experimental indications have appeared of the appearance of exciton condensation in the GaAs/AlAs system.[3]

Of special interest is the question of the changeover of the phase transition regime from 3D to 2D associated with a smooth modification of the single-particle spectrum (e.g., associated with a change in the thickness of a dimensionally quantized film) for superfluid systems such as superconductors and Bose liquids. As is well known, in these systems, possessing global gauge invariance, the superfluid phase transition in the 2D form takes place by the Berezinskiĭ–Kosterlitz–Thouless (BKT) mechanism and is connected with the pairing below T_{BKT} of specific topological excitations (quantum vortices), which exist above the transition temperature in free form.[4] As the film thickness L increases smoothly and transition to the 3D form occurs, two types of behavior are in principle imaginable. Either the phase transition has a vortex character as before and the superfluidity breakdown temperature is determined by how much vortex threads of length L (for arbitrarily large L) ending on the faces of the film are favored, or at some critical thickness L_{BKT} the regimes change over and destruction of the superfluid state is associated with ordinary irrotational fluctuations. For a Bose liquid the possibility that the phase transition in the 3D case has a vortex nature has been raised by a number of authors,[5,6] but an unambiguous answer to this question, as far as we know, has not yet been found.

The present paper is dedicated to a study of crossover between 2D and 3D collective behavior both in superfluid (degenerate) and in nonsuperfluid (exciton semiconductor) layered and dimensionally quantized systems. For layered systems the character of the single-electron spectrum varies with the strength of the interlayer bond (the width of the transverse band), and for dimensionally quantized systems,

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due to a change in the thickness of a single layer (the width of a quantum well in a semiconductor heterostructure or the film thickness). As an example of a nonsuperfluid system we consider a semiconductor near the exciton instability. Here, specifically we assume that the condition

$$(\varepsilon_{ex}-\varepsilon_g)/\varepsilon_{ex}\ll 1. \tag{1}$$

is fulfilled. This inequality guarantees that the mean distance between excitons is much greater than their radius r_0. As we showed in a previous paper,[7] in this case an asymptotically exact description (in the parameter (1)) of the system in terms of a dilute effective Bose liquid is possible. The partition function in this case is given by the following functional integral:

$$Z=\int D\varphi D\varphi^* e^{-S_{\text{eff}}}, \tag{2}$$

where S_{eff} is the effective low-energy action of a Bose liquid of excitons[7]

$$S_{\text{eff}}=\int d\tau d^D r\left\{\varphi^*(\partial_\tau+\xi(\nabla)-\lambda)\varphi+\frac{1}{2}t_0\varphi^*\varphi\varphi^*\varphi\right\}. \tag{3}$$

In Eq. (3) φ is the Bose field of constituent particles, ξ_k is the corresponding dispersion law, and λ is the boson chemical potential, which is fixed and equal to

$$\lambda=\varepsilon_{ex}-\varepsilon_g. \tag{4}$$

The starting value of the interaction t_0, written in Eq. (3) in local form, has a scale of the order of the boson radius r_0. The invariance of the action (3) with respect to variation of the phase of the field φ in the case of an exciton semiconductor is always violated due to the presence of interactions with the spillage of particles from band to band. This leads to the appearance of a gap in the spectrum of collective excitations, the disappearance of superfluidity, and the appearance of vortex excitations. Usually, in semiconductors the strength of the interactions leading to interband transitions is much smaller than that of the density–density interaction, which preserves phase invariance. We will consider specifically this case in which the phase is weakly fixed. Specifically, we assume that vortex-free fluctuations, as before, are described by the action (3), and the contribution of the vortex configurations is completely suppressed due to a violation of global gauge invariance.

As a superfluid analog of an exciton semiconductor in the limit (1), we may take a dilute Bose liquid or Schafrodt superconductor, where the fermion density is so low that the mean distance between fermions is much greater than the radius of the two-particle bound state. In Ref. 8 it was shown that in this case the effective action has the form (3), where φ is a field describing the two-particle bound state, and the chemical potential λ is equal to twice the electron chemical potential and is determined by the equation for the number of particles

$$\rho=\frac{n}{2}=-T\frac{\partial}{\partial\lambda}\ln Z. \tag{5}$$

Here ρ is the boson density, which is equal in the Schafrodt limit to half the electron density n. In superfluid systems the global gauge symmetry of the action (3) is not violated, which then leads to the possibility of the appearance of superfluidity and rotational phase transitions in 2D systems.

To investigate the change in the nature of the phase transition in systems with the action (3) due to continuous variation of the single-particle spectrum from the 3D to the 2D form, it is necessary to have a description of a Bose liquid that is the same for both limiting cases (3D and 2D systems). A self-consistent approximation at once satisfying this requirement and free from infrared divergences for any dimension D was formulated in our previous paper.[7] The expression for the thermodynamic potential below the transition point T_0 in the case of fixed λ in the low density limit has the form

$$\Omega_<=-\frac{\lambda^2-\Delta^2}{4t}-\frac{\lambda\Delta}{2t}+T\sum_k \ln(1-e^{-E_k/T}), \tag{6}$$

where $E_k=\sqrt{\xi_k(\xi_k+2\Delta)}$ is the Bogoliubov spectrum, and Δ is the anomalous self-energy function, determined by minimizing expression (6)

$$\Delta=\lambda-2t\sum_k\frac{\xi_k}{E_k}n_k. \tag{7}$$

The total boson energy is easy to find by differentiating the thermodynamic potential (6) with respect to the chemical potential λ:

$$\rho=\frac{\lambda}{t}-\sum_k\frac{\xi_k}{E_k}n_k\equiv\frac{\lambda+\Delta}{2t}. \tag{8}$$

In Eqs. (7) and (8), $n_k\equiv n(E_k)$ is the Bose distribution function. The normal (high-temperature) phase has $\Delta=0$, and the thermodynamic potential is given by

$$\Omega_>=-\frac{\Sigma^2}{4t}+T\sum_k\ln\left\{1-\exp\left(-\frac{\xi_k-\lambda+\Sigma}{T}\right)\right\}, \tag{9}$$

where Σ is the self-consistent potential that minimizes Ω given by (9). Finally, the interboson exchange potential t entering into Eqs. (6)–(9) is renormalized to account for interference in (2) in the "fast" variables with momenta in the region $\sqrt{\lambda}<k<r_0^{-1}$:

$$t=\frac{t_0}{1+t_0\Pi},\quad \Pi=\sum_{\sqrt{\lambda}<k<r_0^{-1}}\frac{1}{2\xi_k}. \tag{10}$$

This scheme does not have divergences at small momenta for any spatial dimensionality and allows one in a noncontradictory way to describe phase transitions in a low-density Bose liquid due to irrotational fluctuations.

The subsequent development is constructed in the following way. Section 1 analyzes phase transitions in dimensionally quantized systems. The dependence on the film thickness L of the transition temperature T_0 decreases due to irrotational fluctuations is calculated. It is shown that as L decreases, the temperature $T_0(L)$ varies from the 3D to the 2D form, successively passing through a series of intermediate regimes. The values of the critical thickness are found at

which one regime is replaced by another. It is shown that for any L the phase transition is first-order. In nondegenerate systems (an exciton semiconductor) this transition corresponds to the appearance of true long-range order and an exciton condensate.

The specifics of phase transitions in degenerate dimensionally-quantized systems (a superconductor, a dilute Bose liquid) are considered in Sec. II. Neglecting vortex configurations, the temperature $T_0(L)$ corresponds to the formation of a superfluid density and a change in the way the pairwise correlation function falls off from exponential to power-law. Taking spontaneous creation of vortices into account leads to the possibility of a BKT vortex transition. In our approximation it turns out that for a dilute Bose liquid there exists a critical film thickness L_{BKT} such that for $L>L_{\mathrm{BKT}}$ the superfluid transition is due to irrotational fluctuations and really does take place at $T_0(L)$, while for $L<L_{\mathrm{BKT}}$ the superfluid state arises via the BKT mechanism at the temperature T_{BKT}. The temperature $T_0>T_{\mathrm{BKT}}$ in the latter case corresponds to a transition with the appearance of "rigidity" in the system ρ_s. It is only by virtue of this that vortices and the acoustic branch of the collective excitations carrying the intervortex interaction can exist. The presence of a Nelson–Kosterlitz universal jump[9] during the BKT transition allows one to calculate the superfluid transition temperature for $L<L_{\mathrm{BKT}}$ as a function of L. It is necessary to point out that the problem of the variation of the transition temperature in superfluid films has frequently been treated in connection with helium via the macroscopic and phenomenological ψ-theory of superfluidity,[10,11] but only for thick films, where a macroscopic description is actually justified (see, for example, Ref. 10). Our microscopic approach places no lower bound on L and allows the system to continuously approach the pure 2D case. However, the need for a low density parameter does not allow one to directly apply the results to such systems as, for example, liquid helium.

Section 3, presents an analysis of the crossover between the 2D and 3D character of the phase transition in layered systems as the width of the transverse band increases from zero.

2. PHASE TRANSITIONS IN DIMENSIONALLY QUANTIZED SYSTEMS

Let us consider a system of thickness L, bounded in the z direction and infinite in the other two. We assume the dispersion law ξ_k to be isotropic and quadratic, and we use periodic boundary conditions to allow for the finiteness of the transverse length. Such a treatment does not limit the generality of the results, but somewhat simplifies the calculations. In addition, wherever it is not stated otherwise, we use the system of units in which $2m=1$ (m is the mass of the boson state). If we take into account, all of the above the dispersion law becomes

$$\xi_n(p)=p^2+\left(\frac{2\pi n}{L}\right)^2, \tag{11}$$

where p is the 2D momentum perpendicular to the z axis, and n labels the subbands of dimensional quantization. In the dilute Bose liquid of component particles (excitons or electron pairs) which we consider there are two natural length scales. These are the boson radius r_0, having the same order of magnitude as the interaction radius, and the scale $\xi=\lambda^{-1/2}$, connected with the mean particle density and determining collective effects. These two scales are combined together to give the dimensionless "gaseousness" parameter r_0/ξ, which in our case is much smaller than unity. By decreasing the thickness L, we should make the transition from the 3D to the 2D regime of the phase transition. Obviously, as one decreases L down to r_0 and lower ($L<r_0$) a "trivial" 2D regime arises when the two-particle bound states themselves become two-dimensional, thus forcing two-dimensionality of the phase transition. More interesting is another question: Can effectively 2D-collective behavior arise when the component bosons themselves remain three-dimensional? It is just this situation that we will consider below. That is, we take $L\gg r_0$ and, consequently, the energy and radius of the bound state entering into the self-consistency equation (7) through the strength of the interparticle interaction t are determined by a 3D expression.

For a dimensionally quantized system, we write the self-consistency equation for the anomalous eigenenergy function as follows:

$$\Delta=\lambda-\frac{2t}{L}\sum_{n=-\infty}^{\infty}\int\frac{d^2p}{(2\pi)^2}\frac{\xi_n(p)}{E_n(p)}n(E_n(p)). \tag{12}$$

Formally, the solutions of this equation change with decreasing L.for two reasons. First, the presence of a series in expression (12) is essential. As $L\to\infty$ the series transforms into an integral, which leads to 3D behavior, whereas in the limit $L\to 0$ the dominant role is played by the zeroth term of the series, leading to the purely 2D regime. This part of the self-consistency equation (12) describes the contribution of the low-energy fluctuations. The second reason is the change in the renormalization of the interaction t given by Eq. (10) due to high-energy fluctuations of the field φ. Note that such a division of contributions of fast and slow fluctuations is possible by virtue of the low density condition ($\xi=\lambda^{-1/2}\gg r_0$).

Let us find the dependence $t(L)$ for the case of 3D bound states. The starting value of the interaction t_0 is proportional to the quantity r_0:

$$t_0=ar_0,$$

where a is a constant determined by the details of the fermion–fermion interaction in the initial system (thus, for a point potential it satisfies $a=4\pi$). We write the polarization operator Π in Eq. (10) with allowance for dimensional quantization

$$\Pi=\Pi^{3D}+\delta\Pi,$$

$$\delta\Pi=\frac{1}{2L}\sum_{n=-\infty}^{\infty}\int\frac{d^2p}{(2\pi)^2}\frac{1}{p^2+(2\pi n/L)^2}-\int\frac{d^3k}{(2\pi)^3}\frac{1}{2k^2}. \tag{13}$$

The three-dimensional polarization operator Π^{3D} can be represented in the form

$$\Pi^{3D}=\gamma r_0^{-1}.$$

If the momentum dependence of the interboson interaction potential is a step-function, the numerical coefficient is $\gamma=1/4\pi$. Calculating expression (13) for $L>r_0$ and substituting the result into Eq. (10), we finally obtain

$$t(L)=ar_0\left[1+a\gamma\left(1-\frac{1}{4\pi\gamma}\frac{r_0}{L}\ln(1-e^{-L/\xi})\right)\right]^{-1}. \tag{14}$$

The first (three-dimensional) interaction regime is realized for

$$\frac{1}{4\pi\gamma}\frac{r_0}{L}\ln(1-e^{-L/\xi})\ll 1.$$

Here

$$t(L)=t^{3D}=\frac{ar_0}{1+a\gamma}\equiv\beta r_0. \tag{15}$$

In the opposite limit the vertex t is given by

$$t=\frac{4\pi L}{\ln(\xi/L)}. \tag{16}$$

It is natural to call this regime two-dimensional. The transition from regime (15) to regime (16) takes place at

$$L\ll L_{c2}=r_0\ln\frac{\xi}{r_0}. \tag{17}$$

For the component bosons to remain three-dimensional, the condition $L>r_0$ must be fulfilled. This is entirely possible since, by virtue of the low density, $L_{c2}\gg r_0$ holds. For a model liquid of point bosons with scattering length r_0 L can decrease further without change of the properties of the particles themselves. In this case, for $L<r_0$ the quantity t/L stops decreasing and saturates, taking on purely 2D form (see Ref. 7):

$$\frac{t}{L}=\frac{4\pi}{\ln(\xi/r_0)}. \tag{18}$$

Now let us analyze how Eq. (12) changes when L is decreased and calculate the phase transition temperature $T_0(L)$. First we will consider the case $(2\pi/L)^2\gg 2\Delta$. The latter condition allows us to discard Δ from all terms of the series on the right-hand side of Eq. (12) except $n=0$. Calculating the asymptotic limit of the 2D integral corresponding to the term $n=0$ for $2\Delta/T\ll 1$, we obtain the self-consistency equation near the transition point

$$\Delta=\lambda-\chi(T)-\frac{t}{2\pi L}T\ln\frac{T}{2\Delta}. \tag{19}$$

The function $\chi(T)$ is the sum of all the terms of the series in Eq. (12) except $n=0$:

$$\chi(T)=-\frac{t}{2\pi L}T\sum_{n\neq 0}\ln\left(1-\exp\left(-\frac{4\pi^2}{L^2T}n^2\right)\right). \tag{20}$$

As the temperature increases, the solution with $\Delta\neq 0$ vanishes abruptly when the straight line $\lambda-\chi-\Delta$ touches the function $(tT/2\pi L)\ln T/2\Delta$. Differentiating both the right and left sides of Eq. (19) with respect to Δ, we find that the value $\Delta(T_0)=\Delta_c$ at the transition point is related to T_0 by the formula

$$\Delta_c=\frac{t}{2\pi L}T_0. \tag{21}$$

Substituting Eq. (21) in Eq. (19), we obtain a transcendental equation for $T_0(L)$:

$$T_0=\frac{2\pi L}{t}\frac{\lambda-\chi(T_0)}{\ln(e\pi L/t)}. \tag{22}$$

The form of the solution of this equation is determined by the function $\chi(T_0)$, which depends on the dimensionless parameter $4\pi^2/L^2T_0$. For $4\pi^2/L^2T_0\ll 1$ we have

$$\chi(T_0)\approx 2taT_0^{3/2},\quad a=\zeta(3/2)/(4\pi)^{3/2}. \tag{23}$$

Here the renormalized vertex t is given by the three-dimensional expression (15). As a result, a 3D regime with temperature T_0 develops near the transition temperature in a three-dimensional system (see Ref. 7):

$$T_0(L)=T_B\left\{1-\frac{1}{6\pi a}\frac{\xi}{L}\left(\frac{2a\beta r_0}{\xi}\right)^{1/3}\ln\frac{e\pi L}{\beta r_0}\right\}, \tag{24}$$

$$T_B=\lambda\left(\frac{\xi}{2a\beta r_0}\right)^{2/3}.$$

If the condition

$$4\pi^2/L^2T_0>1, \tag{25}$$

is fulfilled, then $\chi(T_0)$ tends exponentially to zero and becomes much smaller than λ in Eq. (22):

$$\chi(T_0)\approx\frac{t}{2\pi L}T_0\exp\left(-\frac{4\pi^2}{L^2T_0}\right)\ll\lambda. \tag{26}$$

The "intermediate" regime arises when $\chi(T_0)$ has already assumed the asymptotic form (26) and the renormalized potential still preserves the 3D form (15). For the transition temperature in this regime we find

$$T_0=2\pi\lambda\frac{L/\beta r_0}{\ln(e\pi L/\beta r_0)}. \tag{27}$$

Substituting relation (27) into condition (25) , we find the critical length L_{c1} below which the intermediate regime (27) replaces the three-dimensional one (24):

$$L_{c1}=r_0\left[\frac{4\pi\beta}{3}\left(\frac{\xi}{r_0}\right)^2\ln\frac{\xi}{r_0}\right]^{1/3}. \tag{28}$$

When the length L becomes less than L_{c2} given by (17) and the interaction potential is determined by relation (17), the quasi-2D regime with transition temperature

$$T_0=\frac{1}{2}\frac{\lambda\ln(\xi/L)}{\ln\{(e/4)\ln(\xi/L)\}} \tag{29}$$

is realized. Note that Eq. (29) has the characteristic 2D form with a double logarithm (see, for example, Refs. 6, 7, and

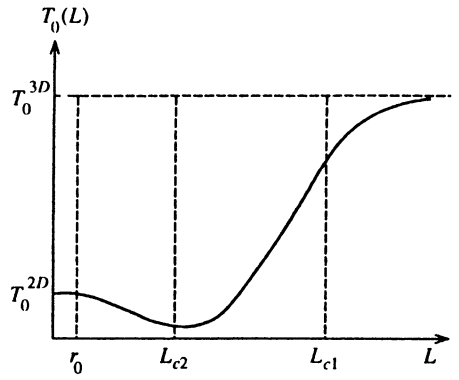

FIG. 1. Qualitative dependence of the temperature of the phase transition on the thickness of the dimensionally quantized system.

12), where instead of the scattering length the sample thickness appears. Thus, as L decreases the solution of Eq. (22) successively passes through three regimes—the 3D (24), the intermediate (27), and the quasi-2D (29). These regimes succeed one another at L equal respectively to L_{c1} (28) and L_{c2} (29). Note that these lengths satisfy the condition

$$r_0 \ll L_{c2} \ll L_{c1}.$$

For a Bose liquid of point particles it is meaningful to speak of a decrease of L down to r_0 and below. In this case ($L<r_0$) T_0 ceases to depend on L and is given by the well-known 2D expression

$$T_0 = T^{2D} = \frac{1}{2}\frac{\lambda \ln(\xi/r_0)}{\ln\{(e/4)\ln(\xi/r_0)\}}. \tag{30}$$

A qualitative picture of the dependence of the transition temperature T_0 on the thickness of the sample L is given in Fig. 1.

For $\Delta(T_0)=\Delta_c$ finite at T_0 the phase transition is first-order. The magnitude of the jump Δ_c is given by (21) and can be easily calculated in each of the three regimes. Figure 2 plots the function $\Delta(T)$ obtained by solving the self-consistency equation (12) at three different points $L_1>L_2>L_3$. For all $T<T_0$ there exist two branches of the solutions of (12). The lower branch (depicted in Fig. 2 by a dashed line) corresponds to the maximum of the thermodynamic potential and, consequently is absolutely unstable. The

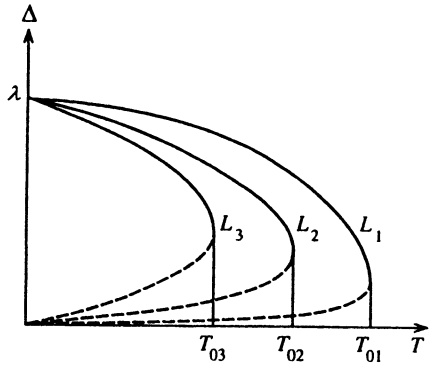

FIG. 2. The dependence $\Delta(T)$ in a dimensionally quantized system for different thicknesses ($L_1>L_2>L_3$).

minimum of the thermodynamic potential, corresponding to the normal phase, exists all the way to $T=0$ (for any finite L), becoming metastable for $T<T_0$. It can be easily shown that T_0 is the transition temperature of a first-order transition (i.e., that at the moment of its appearance the phase with $\Delta \neq 0$ becomes more favored than the normal phase) by calculating the difference $\delta\Omega$ of the thermodynamic potential of the normal (high-temperature) phase $\Omega_>$ given by (9) and the thermodynamic potential $\Omega_<$ of the phase with $\Delta \neq 0$ given by (6) at the point $T=T_0$. Obvious but lengthy calculations lead to the result

$$\delta\Omega = \Omega_> - \Omega_< = \frac{\Delta_c^2}{4t}[(\eta+1)^2-2], \quad \eta = \frac{\Sigma(T_0)-\lambda}{\Delta_c}.$$

The quantity η at the point T_0 does not depend on L and is determined by the condition $e^{-\eta}=e\,\eta/2$ (see Ref. 7). Solution of this equation gives $\eta \approx 0.463$. Consequently, $\delta\Omega>0$ holds, and at the point where the new phase with $\Delta \neq 0$ appears the high-temperature phase immediately finds itself in the supercooled state.

These results correspond to systems with a variable number of particles (fixed chemical potential λ). Now let the total density ρ be given. The existence of a simple relation between λ and ρ makes it easy to eliminate the chemical potential from the self-consistency equation (7) (or (12)). As a result, in place of Eq. (12) we now have

$$\Delta = t\rho - \frac{t}{L}\sum_{n=-\infty}^{\infty}\int \frac{d^2p}{(2\pi)^2}\frac{\xi_n(p)}{E_n(p)}n(E_n(p)). \tag{31}$$

Comparison of Eqs. (12) and (31) shows that the solution of Eq. (31) ($\rho=$const) can be obtained by solving Eq. (12) ($\lambda=$const) via the substitution $2t\to t$ followed by the substitution $\lambda \to t\rho$. Thus, for example, we obtain the following equation (by making the above substitutions in Eq. (22)) for the transition temperature T_0:

$$T_0 = 4\pi L\frac{\rho-\Phi(T_0)}{\ln(2e\pi L/t)}, \tag{32}$$

$$\Phi(T) \equiv \frac{\chi(T)}{2t} = -\frac{T}{4\pi L}\sum_{n\neq 0}\ln\left(1-\exp\left(-\frac{4\pi^2}{L^2T}n^2\right)\right). \tag{33}$$

The case of a fixed number of particles permits a deeper understanding of the physical difference between these regimes. Indeed, the function $\Phi(T_0)$ defined by (33) is the number of particles occupying all the dimensional-quantization subbands with the exception of the ground subband ($n=0$). Consequently, the particle density $\rho_{n=0}$ stands in the numerator in Eq. (32). Thus, the 3D regime differs from the intermediate regime, the quasi-2D regime, and the 2D regime by the relative occupancyo f the ground and higher subbands at the phase transition point. Specifically, the 3D regime has $\rho_{n=0}/\rho_{n>0} \ll 1$, whereas in the other regimes the opposite inequality $\rho_{n=0}/\rho_{n>0} \gg 1$ holds. The "intermediate" regime merges into the quasi-2D regime and then into the 2D regime, in response to the changing character of the renormalization of the interboson interaction.

We give here the expressions for the transition temperature in the case ρ=const in successive intervals of the thickness L:

for $L > L_{c1}$

$$T_0 = T_B\left(1 - \frac{1}{6\pi a}\,\frac{1}{L}\left(\frac{a}{\rho}\right)^{1/3}\ln\frac{2e\pi L}{\beta r_0}\right), \tag{34}$$

for $L_{c1} > L > L_{c2}$

$$T_0 = \frac{4\pi L\rho}{\ln(2e\pi L/\beta r_0)}, \tag{35}$$

for $L_{c2} > L > r_0$

$$T_0 \frac{4\pi L\rho}{\ln\{(e/8)\ln(1/L^3\rho)\}}, \tag{36}$$

for $L < r_0$

$$T_0 = \frac{4\pi L\rho}{\ln\{(e/8)\ln(1/r_0^3 L\rho)\}}. \tag{37}$$

In Eq. (34) $T_B = (\rho/a)^{2/3}$ is the condensation temperature of an ideal Bose gas [$a = \zeta(3/2)/(4\pi)^{3/2}$, see Eq. (23)]. The critical lengths separating regimes (34)–(37) for ρ=const have the form

$$L_{c1} \approx \left(\frac{\pi}{3\rho}\ln\frac{1}{r_0^3\rho}\right)^{1/3}, \tag{38a}$$

$$L_{c2} \approx r_0\ln(1/r_0^3\rho). \tag{38b}$$

The magnitude of the jump of the anomalous eigenenergy function at the transition point is given by

$$\Delta_c(L) = \frac{t(L)}{4\pi L}T_0(L). \tag{39}$$

Recall that so far we have only considered the solution of the self-consistency equations when the quantity Δ can be dropped in all terms of the series with $n \neq 0$ [Eq. (12) or (31)], i.e., we assume the condition

$$(2\pi/L)^2 \gg 2\Delta. \tag{40}$$

holds. Substituting the value of the jump Δ_c in the regime (34) in condition (40), we find that our treatment is valid for

$$L \ll \rho^{-2/3} r_0^{-1} \gg L_{c1}. \tag{41}$$

Thus, condition (40) places an upper bound on the region of validity of Eq. (34), and also Eq. (39) relating Δ_c and T_0. In the limit opposite to (40) the behavior of the system is not substantially different. As before, we obtain a 3D regime with transition temperature near the three-dimensional value, but with a different form of the small L-dependent correction than in formula (34). Fundamental changes in the nature of the transition in the thickness region $L \gg \rho^{-2/3} r_0^{-1}$ arise only in degenerate systems if vortex excitations are taken into account.

3. DEGENERATE DIMENSIONALLY-QUANTIZED SYSTEMS

The temperature T_0 calculated in Sec. 2 corresponds to a phase transition caused by irrotational fluctuations. In systems that violate phase invariance (an exciton semiconductor) a pure condensate appears, together with true long-range order. In degenerate (superfluid) systems for any finite thickness L, long-range order is absent all the way to $T = 0$, the same as in purely 2D systems. The vanishing of the correlation function at infinity is completely natural, since at large distances the main contribution comes from fluctuations in the region of infinitesimal energies, where by virtue of the boundedness of the system in the z direction the spectrum has a two-dimensional character. Let us calculate the case of the pairwide correlation function at low temperature. In this case, as usual

$$\langle\varphi^*(\mathbf{r},\tau)\varphi(\mathbf{r}',\tau)\rangle \propto \exp\left(-\frac{1}{2}\langle[\phi(\mathbf{r},\tau)-\phi(\mathbf{r}',\tau)]^2\rangle\right), \tag{42}$$

where $\phi(\mathbf{r},\tau)$ is the phase of the Bose field. The correlation function (42) looks quite simple when the transverse coordinates coincide ($z = z'$). For the argument of the exponential on the right-hand side of Eq. (42) we obtain

$$\frac{1}{2}\langle[\phi(\mathbf{r},\tau)-(\phi(\mathbf{r}',\tau)]^2\rangle = \frac{T}{L}\sum_{n,\omega}\int\frac{d^2p}{(2\pi)^2}\langle\phi_n(\mathbf{p},\omega)\phi_n \times(-\mathbf{p},-\omega)\rangle(1-e^{-i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')}). \tag{43}$$

The low-energy asymptotic behavior of the correlator of the phase fluctuations is well known (see, for example, Ref. 6). For a dimensionally quantized system we can write

$$\langle\phi_n(\mathbf{p},\omega)\phi_n(-\mathbf{p},-\omega)\rangle \approx \frac{1}{2\rho}\left[\mathbf{p}^2+\left(\frac{2\pi n}{L}\right)^2+\frac{\omega^2}{c^2}\right],$$

where c is the speed of sound. In the limit $|\mathbf{r} - \mathbf{r}'| \to \infty$ the spatial dependence of expression (42) is determined by the term $n = 0, \omega = 0$ in Eq. (43). The remaining terms contribute only to the coefficient of the function defining the spatial dependence. Ordinary calculations lead to a power-law falloff of the correlation function

$$\langle\varphi^*(\mathbf{r})\varphi(\mathbf{r}')\rangle \propto |\mathbf{r}-\mathbf{r}'|^{-a}, \quad a = T/4\pi L\rho. \tag{44}$$

The latter expression shows that pure long-range order at $T > 0$ arises only at $L = \infty$.

If we neglect rotational configurations, the power-law behavior of the correlation function replaces exponential behavior at the temperture T_0. The superfluid density ρ_s appears at the same point. The magnitude of ρ_s is equal to the difference between the total density and the density of the normal component ρ_N:

$$\rho_s = \rho - \rho_N. \tag{45}$$

We will determine the density ρ_N for a dimensionally quantized film by calculating the momentum density $\mathbf{P}$ in a coordinate system moving in the direction perpendicular to the z axis with velocity v

$$\mathbf{P} = \frac{1}{2}\rho_N\mathbf{v} = -\frac{1}{2L}\sum_n\int\frac{d^2p}{(2\pi)^2}\mathbf{p}(\mathbf{p}\cdot\mathbf{v})\frac{\partial n(E_n(p))}{\partial E_n(p)}.$$

As a result, we obtain

$$\rho_N=\frac{1}{L}\sum_n \int \frac{d^2p}{(2\pi)^2}\frac{p^2}{T}$$
$$\times\exp\left\{\frac{E_n(p)}{T}\right\}\Big/\left(\exp\left\{\frac{E_n(p)}{T}\right\}-1\right)^2. \quad (46)$$

Substituting expression (46) into Eq. (45) and expressing the total density in terms of Δ with the help of the self-consistency equation (31), we find for the superfluid density

$$\rho_s=\frac{\Delta}{t}-\frac{1}{L}\sum_n \int \frac{d^2p}{(2\pi)^2}\left\{\frac{\xi_n(p)}{E_n(p)}n(E_n(p))\right.$$
$$\left.-\frac{p^2}{T}\exp\left\{\frac{E_n(p)}{T}\right\}\Big/\left(\exp\left\{\frac{E_n(p)}{T}\right\}-1\right)^2\right\}. \quad (47)$$

The second (integral) term in Eq. (47) tends toward zero for $\Delta/T \ll 1$. Accordingly, near the transition temperature ρ_s is proportional to $\Delta(T)$:

$$\rho_s \approx \Delta/t \quad (48)$$

and, consequently, experiences a jump at T_0 equal to Δ_c/t. Equalities (48) and (39) allow us to calculate the ratio $L\rho_s/T_0$ which defines the scale dimensionality of the field φ at the transition point

$$\frac{L\rho_s(T_0)}{T_0}=\frac{L\Delta_c}{tT_0}=\frac{1}{4\pi}. \quad (49)$$

Taking into account the condition of validity for relation (39) [see condition (41)], it follows that Eq. (49) is valid for $L \ll \rho^{-2/3}r_0^{-1}$.

Taking account of the vortex excitations leads to the possibility of a BKT phase transition. The breakdown temperature of the superfluid state T_{BKT} in this case is determined by the condition of energetic favoredness of the formation of a vortex in the free state.[4] At the BKT transition point, the ratio $L\rho_s/T$ has the universal form[9]

$$\frac{L\rho_s(T_{BKT})}{T_{BKT}}=\frac{1}{\pi}. \quad (50)$$

Comparing Eqs. (50) and (49) shows that in the region of L satisfying condition (41), the temperature at which superfluidity is destroyed due to vortex fluctuations is less than the irrotational phase transition temperature T_0. Consequently, superfluidity arises by way of the BKT mechanism at the temperature T_{BKT}. However, the normal (high-temperature) phase appears only at $T > T_0$. In the region $T_{BKT} < T < T_0$ the quantity ρ_s given by (47) describes the "rigidity" of the system, by virtue of which the appearance of vortices and the acoustic branch of the excitations carrying the intervortex interaction. For $T > T_{BKT}$ the unpaired vortices screen the acoustic branch. A result of this is exponential falloff of the correlation function and absence of superfluidity. In a dilute Bose liquid the transition temperature T_{BKT} lies quite near T_0. This fact allows one to calculate T_{BKT} as a function of L using the Nelson–Kosterlitz relation (50), the relation between ρ_s and Δ (48) and the self-consistency equation (31) which determines the temperature dependence of $\Delta(T)$. As a result, we find for $L < \rho^{-2/3}r_0^{-1}$ that in the 3D regime ($L_{c1} < L < \rho^{-2/3}r_0^{-1}$) the dependence $T_{BKT}(L)$ is given by

$$\frac{T_0}{T_{BKT}}-1\approx\frac{1}{L\rho^{1/3}}\frac{\ln(e^3/4)}{2\pi a^{3/2}}. \quad (51)$$

For the remaining regimes arising for $L < L_{c1}$, we can write down the general expression

$$\frac{T_0}{T_{BKT}}-1\approx\frac{\ln(e^3/4)}{\ln(2e\pi L/t)}. \quad (52)$$

The formulas for $T_{BKT}(L)$ in the intermediate, quasi-2D, and 2D regimes are obtained by substituting expressions (15), (16), and (18), respectively, for the vertex t in relation (52).

As can be seen from relation (51), as L increases the region where free vortices exist rapidly narrows. An interesting phenomenon takes place for L satisfying the inequality opposite to (41):

$$L \gg \rho^{-2/3}r_0^{-1}. \quad (53)$$

In this region the self-consistency equation (31) has in fact a three-dimensional form and, consequently, T_0 is given by the three-dimensional expression (see Ref. 7). As was shown in Ref. 7, in the 3D case the phase transition is also weakly first-order. The jump in Δ, which via formula (48) determines the jump in ρ_s at the transition point, is equal to

$$\Delta_c=\frac{t^2T_0^2}{32\pi^2}\approx\frac{t^2T_B^2}{32\pi^2}. \quad (54)$$

Consequently, for the ratio $L\rho_s/T$ we obtain

$$\frac{L\rho_s(T_0)}{T_0}=\frac{LtT_0}{32\pi^2}\approx\frac{\beta a^{-2/3}}{32\pi^2}L\rho^{2/3}r_0. \quad (55)$$

Thus, the quantity (55) grows without limit as L increases and if condition (53) is fulfilled exceeds the corresponding value at the BKT transition point (50). This latter result means that the phase transition caused by the irrotational fluctuations takes place at a temperature T_0 at which vortex formation is still impossible. Thus, in degenerate systems there is one critical thickness L_{BKT} at which the physical mechanism of destruction of the superfluid state changes. For $L > L_{BKT}$ the superfluid transition takes place by way of the BKT vortex mechanism, and for $L > L_{BKT}$, as a result of irrotational fluctuations. The nature of the transition changes when the ratio $L\rho_s/T$ at the irrotational transition point T_0 becomes equal to this ratio at the BKT transition (50). Consequently, $L = L_{BKT}$ is the solution of the equation

$$\frac{L\rho_s(T_0(L))}{T_0(L)}=\frac{1}{\pi}. \quad (56)$$

The solution of this equation is graphically illustrated by Fig. 3. From the foregoing considerations it is obvious that Eq. (56) is satisfied for

$$L_{BKT}\propto\rho^{-2/3}r_0^{-1}. \quad (57)$$

4. LAYERED AND ANISOTROPIC SYSTEMS

In layered systems the presence of even a weak interlayer bond substantially reduces the probability for the emergence of vortex configurations. Therefore, from a formal point of view the description of thermodynamically spatially-

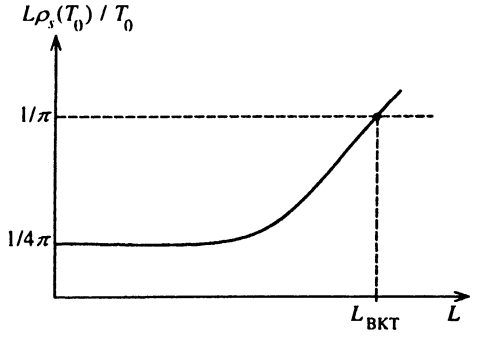

FIG. 3. Dependence on L of the ratio $L\rho_s(T_0)/T_0$, illustrating the solution of equation (56).

homogeneous states is in fact identical for both degenerate and nondegenerate systems. (Here, by nondegenerate we, of course, mean only weak violation of phase symmetry.) The difference consists only in the absence of superfluidity in the last case.

Let us consider a system consisting of two-dimensional layers perpendicular to the z axis. The dispersion law of the two-particle bound states [the effective bosons figuring in the action (3)] ξ_k can be represented in the following quite general form:

$$\xi_k=\frac{p^2}{2m}+\eta(k_z), \tag{58}$$

where p is the 2D momentum, parallel to the layers, and in the z direction the dispersion law $\eta(k_z)$ satisfies the conditions

$$\eta(k_z)=Wf(k_za), \quad f(-x)=f(x),$$
$$f(0)=0, \quad f(\pi)=1. \tag{59}$$

In Eq. (59) W is the width of the transverse band of effective bosons. For example, assume that the description of the dispersion in the z direction for the initial fermions using the tight-binding method and the nearest-neighbor approximation be considered acceptable. Then the fermion dispersion law has the form

$$\varepsilon_k=\frac{p^2}{2m_f}+w(1-\cos k_za).$$

The solution of the two-particle problem with such a spectrum leads to the following boson dispersion law in the z direction (if the energy of the bound state ε_0 is greater than the width of the fermion transverse band w):

$$\eta(k_z)=\frac{w^2}{\varepsilon_0}\sin^2\frac{k_za}{2}. \tag{60}$$

Obviously, the function (60) is a special case of (59) ($W=w^2/\varepsilon_0$; $f(x)=\sin^2x/2$).

Let us investigate the question of the variation of the transition temperature as the width of the transverse band W increases from zero. We pose the question: Is effective 3D behavior possible when the boson states themselves remain two-dimensional? The latter situation obtains if the binding energy of the two-particle state ε_0 is much larger than the width of the fermion band in the z direction and, naturally, much larger than the width of the boson band W (see Eq. (60)). In this limit the product of the polarization operator Π into the starting vertex of the boson–boson interaction t_0 is always much greater than unity. Consequently, as in the purely 2D case, the quantity t_0 falls out of the expression for the renormalized interaction potential t of (10):

$$t\approx 1/\Pi, \tag{61}$$

where according to Eq. (10) Π is defined as follows:

$$\Pi=\int\frac{d^2p}{(2\pi)^2}\int_{-\pi/a}^{\pi/a}\frac{dk_z}{2\pi}\frac{1}{p^2/m+2\eta\,(k_z)}$$
$$=\frac{m}{4\pi a}\left\langle\ln\frac{\varepsilon_0}{\lambda+2Wf(x)}\right\rangle, \tag{62}$$
$$\langle\ldots\rangle=\frac{1}{\pi}\int_0^{\pi}(\ldots)dx.$$

If the condition $\lambda\gg 2W$ holds, the renormalized interaction has the two-dimensional form (see Ref. 7)

$$t\approx t^{2D}a=\frac{4\pi a}{m}\ln^{-1}\frac{\varepsilon_0}{\lambda}. \tag{63}$$

In the opposite limit ($\lambda\ll 2W$) evaluation of the integral in Eq. (62) leads to the following "quasi-two-dimensional" result:

$$t\approx\frac{4\pi a}{m}\ln^{-1}\frac{\varepsilon_0}{2cW}, \quad c=\exp\langle\ln f(x)\rangle. \tag{64}$$

Note that for any relation between λ and W the renormalized vertex can be roughly (with logarithmic accuracy) written in the form

$$t\approx\frac{4\pi a}{m}\ln^{-1}\frac{\varepsilon_0}{\max\{\lambda,W\}},$$

which, by the way, is obvious from Eq. (62).

Let us now find the solution of the self-consistency equation (7) for a layered system when the spectrum (58) differs slightly from two-dimensional. Specifically, let

$$2\Delta_c/W\ll 1. \tag{65}$$

In the temperature region (including the transition temperature) $2\Delta/T\ll 1$ we write the self-consistency equation after integrating with respect to the longitudinal momentum as follows:

$$\Delta=\lambda-\frac{mt}{\pi a}T\left\langle\ln\frac{T}{2\Delta+Wf(x)}\right\rangle. \tag{66}$$

The procedure for calculating the temperature of the jump-like appearance of the nontrivial solution T_0 and the magnitude of the jump Δ_c at the transition point is analogous to that described in Sec. 2. Therefore we present only the final result:

$$T_0=T_0^{2D}\left(1+\frac{W}{2\lambda}\langle f(x)\rangle\right),$$

$$T_0^{2D}=\frac{1}{4}\frac{\lambda\ln(\varepsilon_0/\lambda)}{4\ln\{(e/2)\ln(\varepsilon_0/\lambda)\}}. \tag{67}$$

$$\frac{\Delta_c}{T_0}=\frac{\Delta_c^{2D}}{T_0^{2D}}\left(1-\frac{W}{2\Delta_c^{2D}}\langle f(x)\rangle\right),$$

$$\Delta_c^{2D}=\frac{\lambda}{\ln\{(e/2)\ln(\varepsilon_0/\lambda)\}}. \tag{68}$$

Substituting this value of Δ_c in condition (65), we find the applicability criterion of solutions (67) and (68)

$$\frac{W}{2\lambda}\ln\left(\frac{e}{2}\ln\frac{\varepsilon_0}{\lambda}\right)\ll 1.$$

As one could have expected, the appearance of transverse dispersion causes an increase (in comparison with the 2D case) of the transition temperature T_0 (67) and a decrease of the jump of the anomalous function (meaning the superfluid density in degenerate systems). In addition, the appearance of even weak effects of three-dimensionality leads to the result that, in contrast, to 2D and dimensionally quantized systems (see Sec. 2), there is a finite temperature T_B, below which the normal phase becomes absolutely unstable. This temperature is determined from Eq. (66) [or in the general case from Eq. (7)] at $\Delta=0$ and coincides with the condensation temperature of an ideal Bose gas. With logarithmic accuracy we have

$$\frac{T_0}{T_B}-1=\ln\frac{\lambda}{W}\Big/\ln\ln\frac{\varepsilon_0}{\lambda}. \tag{69}$$

Expression (69) characterizes the width of the two-valued region of the solutions of the self-consistency equation. In the 2D system ($W=0$) $T_B=0$ holds and the self-consistency equation has two solutions for all $T<T_0$; if, on the other hand, we have $W\neq 0$, then the second branch of the solutions exists only for $T_B<T<T_0$.

The regime that can be called "three-dimensional" arises when the ratio $2W/T$ becomes large in comparison with unity ($2W/T\gg 1$). Because of the presence of the distribution function in Eq. (7), only energies less than or of order T are important. Therefore, in this case in the expression for ξ_k (58) it is sufficient to restrict ourselves to the quadratic term in the transverse momentum. In other words, in the limit under consideration the effective mass concept is applicable

$$\xi_k\approx\frac{p^2}{2m}+\frac{k_z^2}{2m_z},\quad \frac{1}{m_z}=Wa^2f''(0). \tag{70}$$

The integral in the self-consistency equation (7) is evaluated in the same way as in the three-dimensional case. Near the transition temperature ($2\Delta/T\ll 1$) we obtain the following expression:

$$\lambda-\Delta=t\frac{(2mT)^{3/2}}{2\pi^2}\sqrt{\frac{m_z}{m}}\left(\frac{1}{2}\sqrt{\pi}\zeta-\pi\sqrt{\frac{2\Delta}{T}}\right), \tag{71}$$

where $\zeta\equiv\zeta(3/2)$ is the Riemann zeta function. The solution with $\Delta\neq 0$ appears with a jump at the T_0:

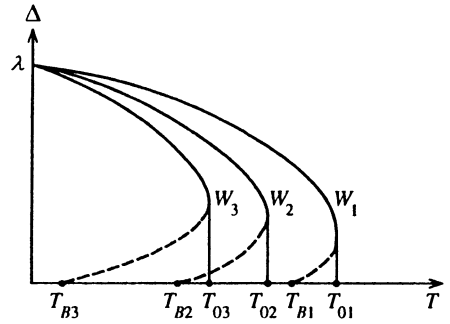

FIG. 4. The dependence $\Delta(T)$ in layered systems for different widths of the transverse zone ($W_1>W_2>W_3$).

$$T_0=T_B\left[1+\frac{4mt}{3\zeta^{4/3}}\left(\frac{m_z}{m}\right)^{1/3}\left(\frac{4\lambda}{t}\right)^{1/3}\right], \tag{72}$$

$$T_B=\frac{\pi}{2m}\left(\frac{m_z}{m}\right)^{1/3}\left(\frac{4\lambda}{t\zeta}\right)^{2/3}. \tag{72a}$$

The normal phase exists all the way to the temperature T_B, becoming metastable below T_0. Substituting the expression for the renormalized vertex (64) and the expression for the transverse mass of the bosons (70), we obtain the transition temperature for layered systems in the 3D regime:

$$\frac{T_0-T_B}{T_B}=\frac{16}{3\zeta^{4/3}}\left(\frac{\pi^2\lambda}{Wf''}\right)^{1/3}\ln^{-2/3}\frac{\varepsilon_0}{2cW}, \tag{73}$$

$$T_B=\frac{W}{2}\left(\frac{\pi f''}{\zeta^2}\right)^{1/3}\left(\frac{\lambda}{W}\ln\frac{\varepsilon_0}{2cW}\right)^{2/3}.$$

These expressions demonstrate the tendency already noted for the 2D regime. Specifically, with increase of the width of the transverse band W the phase transition temperature grows and the region of metastable existence of the normal phase (the two-valued region of the solutions of the self-consistency equation) narrows. The dependence $\Delta(T)$ is shown in Fig. 4 for different values of W. In conclusion, we note that the transition temperature for an anisotropic liquid of the three-dimensional component bosons (the energy of the bound state ε_0 is much smaller than the width of the transverse band w) is also described by formulas (72). In this case, it is necessary to substitute the three-dimensional expression (15) for it as the renormalized vertex t.

5. CONCLUSION

In the present paper we have described crossover between the 3D and 2D phase transitions in systems that can be described as a dilute Bose liquid of component particles (excitons in a semiconductor or electron pairs in a superconductor with low particle density). We have shown that a change in the single-particle spectrum, due to a change in the thickness of the dimensionally quantized system or the width of the transverse band in layered systems, leads to a corresponding change in the phase transition temperature. Specifically, the transition temperature varies gradually from 3D to 2D form, passing through a series of regimes, one superseding the other at the corresponding values of the critical thick-

nesses in dimensionally quantized systems (the critical widths of the transverse band in layered systems). We have shown that the phase transition is first-order for any values of the parameters characterizing the anisotropy of the spectrum. In this regard, note that a first-order transition usually leads to pronounced hysteresis phenomena. In the given case the indicated effects are substantially suppressed since, as was shown in Sec. II, when the new phase appears, the old (high-temperature) phase at once finds itself in the supercooled state. The latter may hinder an experimental determination of the order of the phase transition. And finally, for superfluid dimensionally-quantized films we have demonstrated the existence of a critical thickness at which the physical mechanism of destruction of the superfluid state changes.

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