Quasiparticles in two-dimensional quantum crystals

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(Submitted 20 September 1984)
Zh. Eksp. Teor. Fiz. **88**, 1079-1088 (March 1985)

Using the equation of I. M. Lifshitz we construct a scattering theory for quasiparticles in a two-dimensional lattice space; we use it to study a system such as adsorbed helium on a graphite substrate (two-dimensional quantum lattice systems). For well defined values of the density of the covering the diffusion coefficient of the quasiparticles experiences anomalous drops caused by the suppression of tunnelling processes due to phase transitions in the two-dimensional system of adatoms. We evaluate the correction to the free energy of a two-dimensional quantum crystal which is caused by the binary interactions between the quasiparticles. We show that there is a singularity in the heat capacity at a well defined temperature.

1. INTRODUCTION

It is well known that under certain conditions helium changes into a quantum-crystal state.[1] Quantum crystals are strongly anharmonic even at absolute zero and therefore possess unique properties, in particular, an essentially new motion of the atomic particles is possible in them: quantum diffusion.[1,2]

Experiments show that atoms of the helium isotopes adsorbed on a graphite substrate form different phases—gas, liquid, solid—with sharply expressed quantum properties, and in that case phenomena are observed which have no analogy in the three-dimensional case.[3,4]

The surface of a graphite substrate consists of a network of shallow potential wells with a depth of about 20 K. For a certain value of the density of covering[1)] ($x = 0.58$) and at a temperature of 3 K a rather steep heat capacity anomaly appears which indicates the occurrence of a transition from a two-dimensional gas with a disordered arrangement of the atoms into a regime of epitaxial ordering in the field of the graphite substrate. Due to the repulsion between atoms at small separations this ordered state arises at a density of the covering such that there is one helium atom for three potential wells of the substrate, so that the potential wells on the other side of the neighboring ones are occupied (commensurable phase transition).[3]

Measurements have been performed of the NMR relaxation times $T_{1,2}$ in helium monlayers and their dependence on the density of the covering was obtained.[4] For instance, measurements performed at a frequency of 1 MHz in a constant field showed that there are steep drops in the relaxation times for covering density values of $x_1 = 0.98$ and $x_2 = 0.58$, while in the region $0.58 < x < 0.98$ no anomalies were observed. This indicates that for the values $x_{1,2}$ of the density of the covering a suppression of tunnelling processes occurs which is caused by phase transitions, respectively, into the two-dimensional gas phase and into a two-dimensional classical solid (completely populated monolayer). It thus seems to be established that in the range $0.58 < x < 0.98$ the adatoms are in a quantum-crystal state.

For the calculation of the diffusion coefficient of the quasiparticles we need to know the cross-section for their mutual scattering,[2,5] and there thus arises the necessity to construct a scattering theory of the quasiparticles in a two-dimensional lattice space.

In the present paper we use Lifshitz's equations[6,7] to construct a scattering theory which enables us to obtain the density dependence of the diffusion coefficient (DC) of the quasiparticles. Moreover, this enables us to obtain an expression for the contribution of the interacting quasiparticles to the free energy of a 2*D* quantum crystal and, hence, to evaluate the heat capacity of this system.

2. SCATTERING OF QUASIPARTICLES IN A 2*D* LATTICE SPACE

Due to the delocalization of the atomic particles in quantum crystals it is extraordinarily important to take into account there the quasiparticle short-range repulsion in scattering processes. As in Refs. 7,8 we choose the interaction potential in the form

$$V(\mathbf{R},\ \mathbf{R}') = V_0\delta_{\mathbf{R},\mathbf{R}'}, \tag{1}$$

where $\mathbf{R}$ and $\mathbf{R}'$ are the two-dimensional integer vectors of the lattice sites, $\delta_{\mathbf{R},\mathbf{R}'}$ is the Kronecker symbol, and V_0 a characteristic interaction energy. The case $V_0 \to \infty$ corresponds to the case when two quasiparticles cannot simultaneously be at a single lattice site (the case of the so-called "impenetrable" potential).

Let two quasiparticles with energy $\varepsilon(\mathbf{k}_1)$ and $\varepsilon(\mathbf{k}_2)$ be scattered by the potential (1). Such a scattering process in lattice space is described by the Lifshitz equation which has the form

$$\sum_{\mathbf{R}'} J(\mathbf{R}_1-\mathbf{R}')\psi(\mathbf{R}',\mathbf{R}_2) + \sum_{\mathbf{R}'} J(\mathbf{R}'-\mathbf{R}_2)\psi(\mathbf{R}_1,\mathbf{R}')$$
$$+V_0\sum_{\mathbf{R}'}\delta_{\mathbf{R}_1,\mathbf{R}'}\delta_{\mathbf{R}',\mathbf{R}_2}\psi(\mathbf{R}_1,\mathbf{R}_2-\mathbf{R}') = z\psi(\mathbf{R}_1,\mathbf{R}_2), \tag{2}$$

where $J(\mathbf{R}-\mathbf{R}')$ is the jump integral, $z = E + i0$, E is the scattering energy; $\psi(\mathbf{R},\mathbf{R}')$ is the two-quasiparticle wavefunction.

In the case of a two-dimensional lattice space the solution of Eq.(2) corresponding to the scattered wave has the form

 0038-5646/85/030634-05$04.00

$$\Psi(\mathbf{R})=\tau V_0\int\frac{\exp(i\boldsymbol{\chi}\mathbf{R})\,d^2\chi}{\varepsilon(\boldsymbol{\chi}+\mathbf{q}/2)+\varepsilon(\boldsymbol{\chi}-\mathbf{q}/2)-z},\qquad(3)$$

where $\mathbf{q}$ is the quasimomentum of the center of mass of the two scattered quasiparticles and

$$\tau(\mathbf{q},E)=\left[1-V_0\int\frac{d^2\chi}{\varepsilon(\boldsymbol{\chi}+\mathbf{q}/2)+\varepsilon(\boldsymbol{\chi}-\mathbf{q}/2)-z}\right]^{-1}.\qquad(4)$$

The quantity $|\tau(\mathbf{q},E)|^2$ determines the probability that two quasiparticles hit a single lattice site. It follows from (4) that as $V_0\to\infty$ this probability tends to zero. We note that the jump integral $J(\mathbf{R}-\mathbf{R}')$ and the quasiparticle energy $\varepsilon(\mathbf{k})$ are related through the following equation:

$$\varepsilon(\mathbf{k})=\sum_{\mathbf{R}}J(\mathbf{R})\,e^{i\mathbf{k}\mathbf{R}}.\qquad(5)$$

We consider an approximate method for evaluating the wavefunctions. We note at once that this method enables us to take into account the lattice nature of the problem; the quasimomentum $\mathbf{q}$ of the center of mass which classifies the state of the quasiparticles in the lattice occurs in the wavefunction and in the scattering amplitude as a parameter.

We consider the function

$$\Pi(\boldsymbol{\chi},\mathbf{q})=\varepsilon(\boldsymbol{\chi}+\mathbf{q}/2)+\varepsilon(\boldsymbol{\chi}-\mathbf{q}/2).\qquad(6)$$

Let the minimum of the function $\Pi(\boldsymbol{\chi},\mathbf{q})$ be reached for $\boldsymbol{\chi}=\boldsymbol{\chi}^{(1)}(\mathbf{q})$ and be equal to $\omega^{(1)}(\mathbf{q})$ and the maximum for $\boldsymbol{\chi}=\boldsymbol{\chi}^{(2)}(\mathbf{q})$ and be equal to $\omega^{(2)}(\mathbf{q})$. We expand the function $\Pi(\boldsymbol{\chi},\mathbf{q})$ in series near the extrema, restricting ourselves to the quadratic terms:

$$\Pi(\boldsymbol{\chi},\mathbf{q})-E=\begin{cases}\Delta\sum_{i=1}^{2}\left[A_ia^2(\chi_i-\chi_i^{(1)})^2-\frac{1}{2}\eta_1^2\right]\\ -\Delta\sum_{i=1}^{2}\left[B_ia^2(\chi_i-\chi_i^{(2)})^2-\frac{1}{2}\eta_2^2\right]\end{cases},\qquad(7)$$

where a is the lattice constant and Δ the width of the quasiparticle band,

$$\eta_1^2=\frac{1}{\Delta}[E-\omega^{(1)}(\mathbf{q})],\qquad\eta_2^2=\frac{1}{\Delta}[\omega^{(2)}(\mathbf{q})-E],$$

$$A_i=\frac{1}{2}\nabla^2\Pi(\boldsymbol{\chi},\mathbf{q})\,|_{\chi=\chi_i^{(1)}},\qquad B_i=\frac{1}{2}\nabla^2\Pi(\boldsymbol{\chi},\mathbf{q})\,|_{\chi=\chi_i^{(2)}},$$

$$A_i,\ B_i>0.$$

We note that the quantity $\Omega(\mathbf{q})=\omega^{(1)}(\mathbf{q})-\omega^{(2)}(\mathbf{q})$ is the width of the band of two-quasiparticle states.

Substituting the expansion (7) into Eq. (3) for the wavefunction and integrating over χ we get

$$\Psi(\mathbf{R})=\frac{i\tau_1V_0}{\Delta(A_1A_2)^{1/2}}e^{i\chi^{(1)}\mathbf{R}}\begin{cases}J_0(\eta_1R_1'), & E>\omega^{(1)}(\mathbf{q})\\ K_0(\alpha_1R_1'), & E<\omega^{(1)}(\mathbf{q}),\end{cases}\qquad(8)$$

$$\Psi(\mathbf{R})=-\frac{i\tau_2V_0}{\Delta(B_1B_2)^{1/2}}e^{i\chi^{(2)}\mathbf{R}}\begin{cases}J_0(\eta_2R_2'), & E<\omega^{(2)}(\mathbf{q}),\\ K_0(\alpha_2R_2'), & E>\omega^{(2)}(\mathbf{q})\end{cases}\qquad(9)$$

where

$$\mathbf{R}_1'=\left\{\frac{x_i}{aA_i^{1/2}}\right\},\qquad\mathbf{R}_2'=\left\{\frac{x_i}{aB_i^{1/2}}\right\},\qquad\alpha_i^2=-\eta_i^2,\qquad i=1,2.$$

In Eqs. (8) and (9) the $J_0(z)$ and the $K_0(z)$ are zeroth order modified Bessel functions of the first and second kinds. It follows from (8) and (9) that these wavefunctions correspond to scattering if the scattering energy E lies within the bounds of the two-quasiparticle band, and they correspond to bound states if the scattering energy lies outside the two-quasiparticle band.

The quantities $\tau_i(\mathbf{q},E)$ are evaluated using Eq. (4) and the expansions (7):

$$\tau_i(\mathbf{q},E)=\left\{1-\frac{c_iV_0}{\Delta}\left[\ln\left|\frac{\omega^{(2)}-E}{\omega^{(1)}-E}\right|+i\pi\theta(\pm E\mp\omega^{(i)})\right]\right\}^{-1},$$

$$i=1,\ 2,\ c_1=\pi/(A_1A_2)^{1/2},\ c_2=\pi/(B_1B_2)^{1/2}.\qquad(10)$$

The scattering amplitudes are obtained from the wavefunctions (8) and (9) by the standard method (we give the result for the "impenetrable" potential):

$$f_i(\mathbf{q},E)=\pm\left(\frac{2a}{\pi}\right)^{1/2}\left[\frac{\Delta}{\pm E\mp\omega^{(i)}}\right]^{1/4}\times\frac{\exp i\pi/4}{\ln|(\omega^{(2)}-E)/(\omega^{(1)}-E)|+i\pi\theta(\pm E\mp\omega^{(i)})},\qquad(11)$$

and thus we have from (11) for the scattering cross section

$$\sigma_i(\mathbf{q},E)=\frac{4a\Delta^{1/2}[\pm E\mp\omega^{(i)}]^{-1/2}}{\pi^2+\ln^2|(\omega^{(2)}-E)/(\omega^{(1)}-E)|}.\qquad(12)$$

It follows from (13) that the scattering cross section has singularities near the edges of the two-quasiparticle band. We can easily understand this behavior if we recall that Eq. (12) was obtained using the quadratic expansions (7).

3. BOUND STATES IN 2D QUANTUM CRYSTALS

Pitaevskiĭ[9] has shown that in crystals bound states both of the same and of different excitations can arise for arbitrarily weak interactions between them. In particular, in quantum crystals bound states may be formed even when the interaction between the quasiparticles is repulsive.[2,10] This is explained by the specific motion of the quasiparticles with energy bands of vanishing width.[2] We shall show here that bound states of quasiparticles are formed also in two-dimensional quantum crystals.

The equation for determining the binding energy has the following form:[10]

$$\tau^{-1}(\mathbf{q},\ E)=0,\qquad(13)$$

where $\tau(\mathbf{q},E)$ is given by Eq. (4) and can be evaluated exactly in the case of a square lattice of adatoms with as quasiparticle dispersion law

$$\varepsilon(\mathbf{k})=\varepsilon_0+J(\cos ak_x+\cos ak_y).\qquad(14)$$

Using (14) and integrating in (4) we get the following expression:

$$\tau^{-1}(\mathbf{q},E)=1-\frac{V_0}{2J(\varkappa_1\varkappa_2)^{1/2}}\left[P_{-1/2}(\lambda)+\frac{i}{2\pi}Q_{-1/2}(\lambda)\right],$$

$$\varkappa_i=\cos\frac{aq_i}{2},\qquad\lambda=\frac{1}{8\varkappa_1\varkappa_2}\left[(2\varkappa_1)^2+(2\varkappa_2)^2-\left(\frac{E-2\varepsilon_0}{J}\right)^2\right],\qquad(15)$$

where $P_{-1/2}(\lambda)$ and $Q_{-1/2}(\lambda)$ are Legendre functions of the first and second kind, respectively. After we introduce the notation $g_0 = V_0/J(\varkappa_1\varkappa_2)^{1/2}$ and use (15), Eq. (13) becomes

$$1-g_0P_{-1/2}(\lambda)-i\frac{2g_0}{\pi}Q_{-1/2}(\lambda)=0. \qquad (16)$$

Due to the transcendental nature of Eq. (16) one can study its solutions in the case of the so-called averaged impenetrable potential, i.e., $g_0 \to 0$.[2)]

Taking the asymptotic expressions for the Legendre functions[11] we find the following equation:

$$1+\frac{2g_0}{\pi}\ln(1+\lambda)^{1/2}-ig_0=0. \qquad (17)$$

We introduce the binding energy $\delta(\mathbf{q}) = 2\varepsilon(\mathbf{q}/2) - E$, where $\varepsilon(\mathbf{q}/2) = \varepsilon_0 + J(\varkappa_1\varkappa_2)$; we then have from (17)

$$\delta(\mathbf{q})=-\frac{\varkappa_1\varkappa_2}{\varkappa_1+\varkappa_2}e^{-\pi/g_0}. \qquad (18)$$

The binding energy is thus exponentially small. The stability condition of the bound state consists in requiring that the coefficient of the exponential be negative and have the form

$$\cos(aq_i/2)>0, \quad aq_i<\pi \quad (i=1,\ 2). \qquad (19)$$

In the opposite case the bound state is unstable (in that case one will speak of a *virtual* bound state).

The equation to determine the bound state of quasiparticles within the framework of the approximate scattering theory is obtained from Eq. (10) and has the form

$$1=g_i\ln\left|\frac{\omega^{(2)}-E}{\omega^{(1)}-E}\right|, \qquad (20)$$

where $g_i = c_i V_0/g$, $(i = 1,2)$.

Considering the energy range $E<\omega^{(1)}(\mathbf{q})$ we introduce the binding energy $\delta_1(\mathbf{q}) = E - \omega^{(1)}(\mathbf{q})$; solving Eq. (20) we then get

$$\delta_1(\mathbf{q})=-\Omega(\mathbf{q})e^{-1/g_1}, \quad g_1\to 0. \qquad (21)$$

In the range $E>\omega^{(2)}(\mathbf{q})$ Eq. (20) has no solutions.

In the two cases we thus get results in qualitative agreement: there are regions in quasimomentum space where arbitrarily weak interactions between the quasiparticles lead to the formation of bound states with an exponentially small binding energy.

4. DIFFUSION COEFFICIENT OF QUASIPARTICLES

We shall show in this section that the DC of quasiparticles in a $2D$ quantum crystal for certain well defined values of the covering density shows an anomalous behavior which qualitatively agrees with the behavior of the NMR relaxation times $T_{1,2}(x)$ (see Introduction). We estimate this using the following gas-kinetic formula:

$$D={}^1/_2lv, \qquad (22)$$

where v is the velocity of the motion of the quasiparticles in a band of width Δ, $v\sim a\Delta/\hbar$ and l is the mean free path.

We introduce the scattering cross-section averaged over the two-quasiparticle band by integrating expression (12) over the energy E:

$$\sigma_i(\mathbf{q})=\frac{1}{4\Delta}\int\limits_{\omega^{(1)}(\mathbf{q})}^{\omega^{(2)}(\mathbf{q})}\sigma_i(\mathbf{q},E)\,dE, \quad i=1,2, \qquad (23)$$

where we have used the fact that the scattering energy E as function of the quasimomenta changes within the limits $[-2\Delta,2\Delta]$. As a result of the integration we then get

$$\sigma(\mathbf{q})=\frac{0.37a}{\pi}\left(\frac{\Omega(\mathbf{q})}{\Delta}\right)^{1/2}. \qquad (24)$$

We introduce the quasiparticle mean free path caused by binary collisions with a fixed value of the quasimomentum $\mathbf{q}$:

$$l(\mathbf{q})=a^2/x_k\sigma(\mathbf{q}), \qquad (25)$$

where x_k is the quasiparticle density.

The mean free path calculated taking into account quasiparticle scattering processes with quasimomenta $\mathbf{q}$, varying within the limits of 0 to some value q_0, where q_0 is a characteristic/quasimomentum for the given system (in what follows we change from q_0 to the quasiparticle density) is

$$l=\langle l(\mathbf{q})\rangle=\left(\frac{a}{2\pi}\right)^2\int\limits_0^{q_{0x}}\int\limits_0^{q_{0y}}l(\mathbf{q})\,d^2q, \qquad (26)$$

where $\mathbf{q}_0 = q_0 = (q_{0x}, q_{0y})$.

Using (24), (25), and (26) we get

$$D=\frac{1{,}35}{(2\pi)^2}\frac{a^4\Delta^{1/2}}{\hbar x_k}\int\limits_0^{q_{0x}}\int\limits_0^{q_{0y}}\frac{d^2q}{\Omega^{1/2}(\mathbf{q})}. \qquad (27)$$

We consider the case of a hexagonal plane lattice of adatoms with a quasiparticle dispersion law

$$\varepsilon(\mathbf{k})=\varepsilon_0+J\cos\left(\frac{\sqrt{3}}{2}ak_x\right)\cos\left(\frac{1}{2}ak_y\right). \qquad (28)$$

After elementary calculations we then have

$$\omega^{(i)}(\mathbf{q})=2\varepsilon_0\mp 2J\left|\sin\left(\frac{\sqrt{3}}{4}aq_x\right)\sin\left(\frac{1}{4}aq_y\right)\right|,$$

$$\Omega(\mathbf{q})=4J\left|\sin\left(\frac{\sqrt{3}}{4}aq_x\right)\sin\left(\frac{1}{4}aq_y\right)\right|. \qquad (29)$$

Substituting (29) into (27) and integrating over $\mathbf{q}$ leads to the following result:

$$D=\frac{a^2\Delta}{x_k\hbar}F(\beta_1,1/\sqrt{2})F(\beta_2,1/\sqrt{2}),$$
$$0\leqslant aq_{0i}\leqslant\pi, \qquad (30)$$

where $\Delta = zJ$, $z = 3$, and $F(\beta_i, 1\sqrt{2})$ is an incomplete elliptic integral of the first kind,

$$\beta_i=\arcsin(1-\sin aq_{0i})^{1/2}, \quad aq_{01}=\frac{\sqrt{3}}{4}aq_{0x}, \quad aq_{02}=\frac{1}{4}aq_{0y}.$$

A study of expression (30) as function of the quasimomentum leads to the following results: when $aq_{01} = \pi/2 \pm 0$ (or $aq_{02} = \pi/2 \pm 0$) we have $D = 0$ and at those points there exist single-sided derivatives of the function $D(q_{01}, q_{02})$ which differ in sign.

In the range of quasimomentum values $aq_{0i} > \pi$ the integration leads to the following result:

$$D=\frac{a^2\Delta}{x_k\hbar}[1-F(\beta_3,1/\sqrt{2})][1-F(\beta_4,1/\sqrt{2})], \qquad (31)$$

where $\beta_i = \arcsin(1+\sin aq_{0i})^{1/2}$, $i = 3,4$, $q_{03} = q_{01}$, $q_{04} = q_{02}$.

The study of expression (31) leads to the conclusion that

$D(q_{01},q_{02})$ increases to a well defined value for $aq_{0i} = \pi - 0$ and then falls discontinuously to zero; the signs of the single-sided derivatives are in that case positive.

Bearing in mind that the gas kinetic approximation of the DC and of the scattering cross section are inversely proportional to each other, it follows from Eqs. (30) and (31) that the anomalous behavior of the DC of the quasiparticles arises because the scattering cross section ceases to be analytical in certain regions of quasimomentum space.

For a further study of this problem we change from the characteristic quasimomentum to the densities x_k. We introduce the quasimomentum k_0 of a quasiparticle: $k_0 = (N_k/S)^{1/2}$ where N_k is the number of quasiparticles on the substrate of area S. We rewrite this expression in the following form: $k_0 = x_k^{1/2}(N_0/S)^{1/2}, x_k = N_k/N$, where N_0 is the number of potential wells on the substrate of area S.

Bearing in mind that $(N_0/S)^{1/2} \approx \pi/a'$, where a' is the lattice constants of the $2D$ lattice of the substrate, $a = 2a'$, a is the lattice constant of the $2D$ quantum crystal, we find that $ak_0 \approx 2\pi x_k^{1/2}$ and that the maximum value of the characteristic quasimomentum q_0 will be equal to $4\pi x_k^{1/2}$.

To continue we take into account that the quasimomentum $\mathbf{q}_0$ is defined up to a reciprocal lattice period. In particular, for a hexagonal plane lattice these periods are

$$\mathbf{b}_1 = 4\pi\hat{\mathbf{y}}/\sqrt{3}, \quad \mathbf{b}_2 = 2\pi(\hat{\mathbf{x}} + \hat{\mathbf{y}}/\sqrt{3}),$$

where $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are unit vectors along the appropriate coordinate axes.

Bearing in mind that $(aq_{0x})^2 + (aq_{0y})^2 = (aq_0)^2$ we can obtain values for the quasiparticle density corresponding to values of the quasimomentum $\mathbf{q}_0$ for which $\sigma(\mathbf{q}_0)$ displays a nonanalytic behavior. For instance, when $aq_{01} = aq_{02} = \pi/2$ we have

$$(aq_{0x} - b_{1x})^2 + (aq_{0y} - b_{1y})^2 = 16\pi^2 x_k, \tag{32}$$

whence we find $x_k^{(1)} = 0.08$ and the corresponding value of the density of the covering is $x_1 = 1 - x^{(1)} = 0.92$. Completely analogously we have for $aq_{01} = aq_{02} = \pi$

$$(aq_{0x} - b_{2x})^2 + (aq_{0y} - b_{2y})^2 = 16\pi^2 x_k, \tag{33}$$

from which it follows that $x_k^{(2)} = 0.48, x_2 = 0.52$. The values obtained for the covering densities $x_{1,2}$ agree with adequate accuracy with the values for which drops were observed in the NMR relaxation times $T_{1,2}$ ($x_1 = 0.98, x_2 = 0.58$).

The nonanalytical behavior of the scattering cross section is thus caused by phase transitions in the adatom system: a) into a $2D$ classical solid, namely, a completely populated monolayer ($x_1 = 0.92$), b) into a $2D$ gas state ($x_2 = 0.52$). Moreover, it follows from (32) and (33) that near the phase transition points quasiparticles scattering is accompanied by Umklapp processes and the quasimomentum conservation law takes the following form:

$$\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_1' + \mathbf{k}_2' + \mathbf{b}_1 \tag{34}$$

near the completion of the monolayer, and

$$\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_1' + \mathbf{k}_2' + \mathbf{b}_2 \tag{35}$$

close to the disordered phase (the $2D$ gas).

One obtains the qualitative behavior of the DC as a function of the density from (30) and (31) by substituting

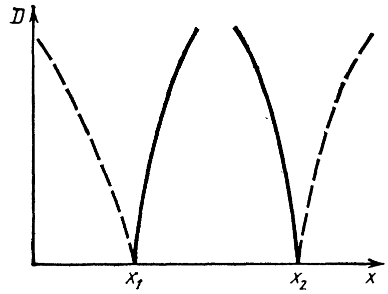

FIG. 1. Qualitative behavior of the DC as function of the covering density x (region where the $2D$ quantum crystal exists is $x_1 < x < x_2$, $x_1 = 0.52$, $x_2 = 0.92$).

$aq_{01} = aq_{02} \sim x_k^{1/2}$. If we use the expression for β_i the density dependence near the values $x_k^{(1,2)}$ then takes the following form:

$$D = \frac{a^2\Delta}{x_k\hbar}\begin{cases}(x_k - x_k^{(1)})^{1/2}, & x_k > x_k^{(1)}\\ (x_k^{(2)} - x_k)^{1/2}, & x_k < x_k^{(2)}\end{cases} \tag{36}$$

or, changing to the covering density x, we have (see Fig. 1):

$$D = \frac{a^2\Delta}{x_k\hbar}\begin{cases}(x_1 - x)^{1/2}, & x \leqslant x_1\\ (x - x_2)^{1/2}, & x \geqslant x_2\end{cases}. \tag{37}$$

The critical index of the DC for a phase transition "in terms of the covering density" in the $2D$ system is thus equal to one half.

5. THERMODYNAMICS OF A TWO-DIMENSIONAL QUANTUM CRYSTAL

The strong interaction between the quasiparticles in quantum crystals (in particular, a short range repulsion which we approximate by the impenetrable potential) does not allow us to apply the virial expansion method when evaluating thermodynamic quantities.

Using the method of I. M. Lifshitz[12] an exact expression was found in Ref. 13 for the contribution to the free energy of strongly interacting quasiparticles:

$$\Delta F = \frac{1}{\pi}\int_{-\infty}^{+\infty} \operatorname{arctg} \frac{\pi V_0 \nu(\varepsilon, \mathbf{q})}{1 + V_0 \displaystyle\int \frac{\nu(\lambda, \mathbf{q})}{\lambda - \varepsilon} d\lambda} \frac{d\varepsilon\, d^d q}{e^{\varepsilon/T} - 1}, \tag{38}$$

where $\nu(\varepsilon,\mathbf{q})$ is the two-quasiparticle density of states given by the expression

$$\nu(\varepsilon, \mathbf{q}) = \int \delta[\varepsilon - \varepsilon(\chi + \mathbf{q}/2) - \varepsilon(\chi - \mathbf{q}/2)]\, d^d\chi. \tag{39}$$

and d is the dimensionality of the problem.

In the impenetrable potential case Eq. (38) simplifies somewhat:

$$\Delta F = \frac{1}{\pi}\int_{-\infty}^{+\infty} \operatorname{arctg} \frac{\pi \nu(\varepsilon, \mathbf{q})}{\displaystyle\int \frac{\nu(\lambda, \mathbf{q})}{\lambda - \varepsilon} d\lambda} \frac{d\varepsilon\, d^d q}{e^{\varepsilon/T} - 1}. \tag{40}$$

From Eq. (39) and the expansions (7) we get for the density of states:

$$\nu(\varepsilon, \mathbf{q}) = \begin{cases} c_1\theta[\varepsilon - \omega^{(1)}(\mathbf{q})], & \varepsilon \geqslant \omega^{(1)}(\mathbf{q})\\ c_2\theta[\omega^{(2)}(\mathbf{q}) - \varepsilon], & \varepsilon \leqslant \omega^{(2)}(\mathbf{q})\end{cases}, \tag{41}$$

where c_1 and c_2 are defined in (10).

To begin with we consider the low temperature region when the excited states are close to the bottom of the two-quasiparticle band: $\varepsilon \approx \omega^{(1)}(\mathbf{q})$. We then have from (40) and (41)

$$\Delta F=\frac{1}{\pi}\int_{\omega^{(1)}}^{\omega^{(2)}}\exp\left[-\frac{\omega^{(1)}(\mathbf{q})}{T}\right]\operatorname{arctg}\left[\pi\ln^{-1}\frac{\Omega(\mathbf{q})}{\varepsilon-\omega^{(1)}(\mathbf{q})}\right]d\varepsilon\, d^2\mathbf{q}. \tag{42}$$

Integrating over the energies in (42) is elementary and thus

$$\Delta F\approx 2\pi\int\Omega(\mathbf{q})\exp\left[-\frac{\omega^{(1)}(\mathbf{q})}{T}\right]d^2\mathbf{q}. \tag{43}$$

In the case of a square lattice of adatoms with a dispersion relation given by Eq. (14) one can integrate the expression in (43) exactly. We then have for $\omega^{(i)}(\mathbf{q})$ and $\Omega(\mathbf{q})$

$$\omega^{(i)}(\mathbf{q})=2\varepsilon_0\mp 2J\left(\cos\frac{aq_x}{2}+\cos\frac{aq_y}{2}\right),\quad \Omega(\mathbf{q})=2J\left(\cos\frac{aq_x}{2}+\cos\frac{aq_x}{2}\right). \tag{44}$$

Substituting this into (43) and integrating over $\mathbf{q}$ leads to the following expression:

$$\Delta F\approx -2\pi e^{-\varepsilon_0/T}I_0(\beta)I_1(\beta),\quad \beta=4J/T, \tag{45}$$

where $I_n(\beta)$ is a modified Bessel function of order n. Using the asymptotic behavior of the Bessel function[11] in the temperature range $T \ll 4J$ we get for the free energy:

$$\Delta F=-2T\exp\left[-(\varepsilon_0-2J)/T\right], \tag{46}$$

and for the heat capacity

$$\Delta C_V=2\left(\frac{\varepsilon_0-2J}{T}\right)^2\exp\left(-\frac{\varepsilon_0-2J}{T}\right), \tag{47}$$

whence it follows that as $T\to 0$ the heat capacity tends to zero exponentially. This is a consequence of the fact that an energy equal to $\varepsilon_0 - 2J$ is necessary to produce a single quasiparticle. We now consider the temperature range $T\sim J$. To do this we write Eq. (42) in the following form:

$$\Delta F=\frac{1}{\pi}\int_{-\infty}^{+\infty}\operatorname{arctg}\left[\pi\ln^{-1}\frac{\omega-z}{\omega+z}\right]\frac{\theta(\omega-z)}{\exp[(z+\lambda)/T]-1}\,dz\,d^2q, \tag{48}$$

where

$$\omega(\mathbf{q})={}^1/_2\Omega(\mathbf{q}),\ \lambda(\mathbf{q})={}^1/_2[\omega^{(1)}(\mathbf{q})+\omega^{(2)}(\mathbf{q})].$$

For planar square and hexagonal lattices $\omega^{(i)} = 2\varepsilon_0 \mp J\varphi(\mathbf{q})$ (see (29) and (45)) so that $\lambda(\mathbf{q}) = 2\varepsilon_0$ and $\varepsilon_0 \gg 2J$; we have thus $\varepsilon_0/T \gg 1$. We substitute $y = z/T$ in (48) and then

$$\Delta F\approx\frac{T}{\pi}\int_{-\infty}^{+\infty}\operatorname{arcctg}\left\{\frac{1}{\pi}\ln\frac{\omega/T-y}{\omega/T+y}\right\}\theta\left(\frac{\omega}{T}-y\right)e^{-2\varepsilon_0/T}d^2q\,dy. \tag{49}$$

By introducing the θ-function in the integrands in (48) and (49) we have taken into account that they are defined in the region $|z|\leqslant\omega$, while in the range $|z|\geqslant\omega$ they must be put equal to zero as follows from the form (41) of the density of states. The integrand in (49) is a slowly varying function of the quasimomentum $\mathbf{q}$ and can thus be replaced by its value at some q_0 such that $\omega(q_0)\sim J$, $q_0^{-1}\equiv\Lambda^{-1}\sim r_0$ is the average distance between the quasiparticles. Hence in what follows we shall put $\omega = \omega(\Lambda)$.

Differentiating expression (49) twice with respect to the temperature and retaining terms with a nonintegrable singularity we find

$$\Delta F_T''\sim\frac{\omega}{\pi T^2}e^{-2\varepsilon_0/T}\int_{-\infty}^{+\infty}\left[\varphi''_{\omega/T}\left(\frac{\omega}{T},y\right)\theta\left(\frac{\omega}{T}-y\right)+\varphi'_{\omega/T}\left(\frac{\omega}{T},y\right)\delta\left(\frac{\omega}{T}-y\right)\right]dy, \tag{50}$$

where for ease of writing we introduced the notation $\varphi(\omega/T, y)$ for the integrand in (49).

To explain the nature of the singularity in (5) for $T\sim J$ we put in the arguments of the θ- and δ-functions $\omega(\Lambda)/T\sim 1$. Further taking into account that both terms in (50) are of the same order of magnitude we get for the heat capacity the following expression:

$$\Delta C_V\approx\frac{\omega(\Lambda)e^{-2\varepsilon_0/\omega(\Lambda)}}{|T-\omega(\Lambda)|\ln^2|\omega(\Lambda)-T|}. \tag{51}$$

The heat capacity of interacting quasiparticles thus shows for $T\sim\omega(\Lambda)$ an anomalous behavior given by Eq. (51). Such a behavior of the heat capacity is characteristic for a phase transition from the quantum crystal phase to a phase where tunnelling processes are suppressed.

The authors consider it a pleasant duty to express their gratitude to A. F. Andreev for discussing this work and for valuable advice.

1)We must take for the covering density the ratio $x = N/N_0$ where N_0 is the number of potential wells on a substrate of a certain area and N the number of adatoms on it.

2)Notwithstanding the condition $V_0\to\infty$, since the impenetrable potential (1) is a function of a discrete variable, we can consider it a small quantity when averaged over the volume of the crystal.

[1]A. F. Andreev and I. M. Lifshitz, Zh. Eksp. Teor. Fiz. **56**, 2057 (1969) [Sov. Phys. JETP **29**, 1107 (1969)].

[2]A. F. Andreev, Usp. Fiz. Nauk **118**, 251 (1976) [Sov. Phys. Usp. **19**, 137 (1976)].

[3]B. Cowen, M. Richards, and A. Thompson, Phys. Rev. Lett. **38**, 165 (1977).

[4]M. Bretz, J. G. Dash, D. C. Hickernell, E. O. McLean, and O. E. Vilches, Phys. Rev. **A8**, 1589 (1973).

[5]I. N. Piradashvili, Zh. Eksp. Teor. Fiz. **84**, 124 (1983) [Sov.Phys. JETP **57**, 72 (1983)].

[6]I. M. Lifshitz, Zh. Eksp. Teor. Fiz. **18**, 293 (1948).

[7]I. M. Lifshitz and G. A. Vardanyan, Dokl. Akad, Nauk Armenian SSR, VIII, 80 (1975).

[8]G. A. Vardanyan and A. S. Saakyan, Fiz. Tverd. Tela (Leningrad) **25**, 1490 (1983) [Sov. Phys. Solid State **25**, 856 (1983)].

[9]L. P. Pitaevskiĭ, Zh. Eksp. Teor. Fiz. **70**, 738 (1976) [Sov. Phys. JETP **43**, 382 (1976)].

[10]G. A. Vardanyan and S. A. Saakyan, Fiz. Tverd. Tela (Leningrad) **23**, 2881 (1981) [Sov.Phys. Solid State **23**, 1681 (1981)].

[11]M. Abramovitz and I. A. Stegun, Handbook of Mathematical Functions, Dover, 1965.

[12]I. M. Lifshitz, Usp. Mat. Nauk **7**, 170 (1952).

[13]G. A. Vardanian, J. Low Temp. Phys. **50**, 427 (1983).

Translated by D. ter Haar