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VACANCIES IN QUANTUM CRYSTALS

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Vacancies in ^{3}He crystals (body-centered cubic lattice) and ^{4}He crystals (hexagonal close-packed lattice) are considered. It is shown that throughout the temperature range of existence of the crystals and at not too high pressures the vacancies are quasiparticles (vacancions). The energy gap and band width of the quasiparticles are calculated. The calculations are compared with experimental results.

1. INTRODUCTION

THE crystal lattice of a solid always has a certain number of point defects such as vacancies, and interstitial or substitution atoms. Point defects can move over the crystal lattice, jumping from site to site (from interstice to interstice). At a sufficiently high temperature, the moves from site to site are effected by thermally activated above-barrier transitions. Lowering the temperature leads to a quenching of the thermal effects, and at a certain temperature quantum below-barrier tunneling becomes the decisive mechanism of defect mobility. Since the quantum lifetime of the defect on the site is long enough, the defect has time to enter in thermal equlibrium during its stay at one site, i.e., it can be regarded as a well-localized object. With further drop in temperature, the thermal motion of the atoms ceases and the defect no longer has time to enter in thermal equilibrium with the lattice during its lifetime on the site. The defect thus turns into a delocalized object, a quasiparticle of defecton, which moves over the crystal and collides with phonons and other defectons from time to time.

This paper deals with vacancies in quantum ^{3}He and ^{4}He crystals. A quantum crystal is defined as one in which the energy of the zero-point oscillations of each atom is not small in comparison with the depth of the potential well in which the atom is located.

We shall show that in the entire temperature interval in which solid ^{3}He and ^{4}He exist, i.e., from zero to several degrees, the vacancies are vacancions (we have in mind throughout pressures that are not too high).

It is shown in[1] that at low temperatures the time in which a moving defect can enter in thermal equilibrium with the lattice is $\tau \sim \Theta^{-1}(\Theta/T)^9$; $T \ll \Theta$, where Θ is the Debye temperature, i.e., τ is very large.

The three temperature intervals indicated above can be described by the inequalities $\tau < w_c^{-1} < w_q^{-1}$; $\tau < w_q^{-1} < w_c^{-1}$, and $w_q^{-1} < \tau$, where w_c and w_q are respectively the classical and quantum probabilities that the defect will go from site to site in a unit time. These relations usually hold by virtue of the very low values of the probabilities w_x and w_q. In solid He, however, as will be shown below (see Sec. 3), w_q is of the order of several degrees, and $w_c < w_q$, so that the inequality $w_q^{-1} < w_c^{-1} < \tau \sim \Theta^{-1}(\Theta/T)^9$ holds. To establish this inequality, it is necessary to compare the classical probability with which the atom located in a site next to the vacancy has an energy equal to the height of the barrier, $w_c \sim \exp(-V/T)$, where V is the height of the barrier reckoned from the ground state energy, and the quantum probability of tunneling form the ground state at the given site to the ground state in the neighboring one is

$$w_q \sim \exp\{-(2mV)^{1/2} b/\hbar\},$$

where b is the length of the below-barrier path.

The pre-exponential factors of w_q and w_c are of the same order of magnitude; we therefore compare only the exponentials. To get $w_q > w_c$ we must have $T < (V\hbar^2/2mb^2)^{1/2}$. In solid He, the rms deviation d from the equilibrium position is ~3/10 of the interatomic distance a, i.e., $b \sim 7a/10 \sim 7d/3$ and $\hbar^2/2mb^2 \sim (3/7)^2\hbar^2/2md^2 \sim \hbar\omega/5$, where ω is the frequency of the oscillations of the atom in the potential well,

$$V = \frac{m\omega^2}{2}\left(\frac{a}{2}\right)^2 - \frac{\hbar\omega}{2}.$$

Using again $a \sim 10d/3$ and $\hbar^2/2md^2 \sim \hbar\omega$, we obtain $V \sim \hbar\omega/5$. The result is $T \lesssim \hbar\omega/5$; $\hbar\omega \sim \Theta \gtrsim 20^\circ$K and $T \lesssim 4^\circ$K. Of course, the foregoing is only an estimate, but it is seen that in the temperature interval in which solid He exists it is reasonable to assume that the quantum mechanism of defect mobility is decisive. In addition, as shown above, the defects are strongly delocalized. Thus, the vacancies in quantum crystals should be regarded as quasiparticles or vacancions.

Many experimental data on the deviation of the specific heat from the T^3 law and on the measurements of the relaxation times in NMR in solid ^{3}He (see the review[2]) can be interpreted in terms of the quantum mobility of the vacancies.

In the tight-binding approximation, the dispersion law for vacancions in the case of a primitive cubic lattice is given by

$$\varepsilon(\mathbf{k}) = E_l + 2t(\cos k_x a + \cos k_y a + \cos k_z a).$$

The width of the vacancion band is therefore 2zt, where z is the number of neighbors nearest to the given atom. The energy gap, or the minimum energy necessary for vacancion production, is $\Delta E = E_l - zt$.

Let us examine ΔE, the change of the crystal energy when one vacancy appears in it. Two cases can occur here. First, a Schottky vacancy, when the extra atom that appears as a result of vacancy production goes off to the surface, or the vacancy is simply produced from the surface of the crystal. The second is a Frenkel vacancy, where the extra atom travels over the interstices forming an interstitial impurity. If the crystal is under the influence of external pressure P at T = 0, we have in the first case

$$\Delta E_1 = -\varepsilon + \varepsilon_1 + \Delta + PV_0 - zt. \tag{1.1}$$

Here ϵ is the binding energy per atom inside the crystal, ϵ_1 is the binding energy per atom in the surface layer of the crystal, Δ is the energy connected with the distortion of the lattice around the vacancy, PV_0 is the work necessary to expand the crystal by the volume V_0 per atom, and zt is half the width of the vacancion band. The first four terms in (1.1) constitute the change in the crystal energy following the appearance of a localized vacancy, while the last term represents the decrease of this energy as a result delocalization of the vacancy. In classical crystals, the last three terms of (1.1) are negligibly small in comparison with the first two. Since the energy of the zero-point vibrations is small in classical crystals, and the number of bonds per atom on the surface is half as large, it follows that $\epsilon_1 \sim \epsilon/2$ and $\Delta E_1 \sim -\epsilon/2$. In quantum crystals, on the other hand, all five terms of (1.1) can be of the same order of magnitude.

Unfortunately, it is impossible to estimate ϵ_1, but certain qualitative considerations can be advanced in favor the assumption that $\epsilon_1 \sim \epsilon$. First, by virtue of the high energy of the zero-point vibrations, the difference between ϵ_1 and ϵ is distributed over several atomic layers, and does not affect merely the layer closest to the surface. Second, if the crystal surface is rough enough, then the extra atom that appears as a result of the vacancy production finds it more convenient to stay in a hollow on such a rough surface, where the difference between ϵ_1 and ϵ is minimal. Thus,

$$\Delta E_{1\,min} = \Delta + PV_0 - zt, \tag{1.2}$$

$$\Delta E_{1\,max} = |\varepsilon| + \Delta + PV_0 - zt. \tag{1.3}$$

In the second case, that of Frenkel vacancies, we have

$$\Delta E_2 = -\varepsilon + \varepsilon_2 + \Delta - zt, \tag{1.4}$$

where ϵ_2 is the energy due to the appearance of the delocalized interstitial atom. It is impossible to compare the values of ΔE_1 and ΔE_2 on the basis of qualitative considerations alone.

We shall determine the energy gap ΔE_1 for Schottky vacancy production and the width of the vacancion band. Heatherington[3] performed analogous calculations, using the Nosanov model[4]. This model, however, results in poor agreement with experiment for the energy of the ground state of solid He, and in addition it is very cumbersome from the computational point of view. Notice should also be taken of an attempt to estimate the width of the band in[5], which, however, did not extend far enough to obtain numerical results for quantum crystals.

2. GAP AND WIDTH OF VACANCION BAND

When finding the energy of the ground state of quantum crystals, it is necessary to take into account two circumstances. First, by virtue of the large amplitude of the zero-point vibrations, each atom fluctuates in the self-consistent field of the others. Second, the pair-interaction potential of the helium atoms has at small distances a "hard core" and it is therefore important to take into account the correlation between the particles as they come close together. The helium atoms in the crystal can be regarded as Boltzmann particles, owing to the small overlap of their wave functions. Allowance for the exchange-interaction energy in solid ^{3}He leads to corrections amounting to one-thousandths of the binding energy (see[6]). Ignoring the correlations of order higher than second and assuming that each of the crystal-lattice points is occupied only once, we obtain the following system of equations[7-9]:

$$\left\{-\frac{\hbar^2}{2m}\Delta + U(\mathbf{r}-\mathbf{R}_i)\right\}\varphi_i(\mathbf{r}) = H_i(\mathbf{p},\mathbf{r})\varphi_i(\mathbf{r}) = \Omega\varphi_i(\mathbf{r}), \tag{2.1}$$

$$U(\mathbf{r}-\mathbf{R}_i)\varphi_i(\mathbf{r}) = \sum_{j\neq i} I_{ij}^{-1} v_{ij}, \tag{2.2}$$

$$\begin{gathered} v_{ij} = \int \varphi_j^*(\mathbf{r}')\, v(\mathbf{r}-\mathbf{r}')\, \psi_{ij}(\mathbf{r},\mathbf{r}')\, d\mathbf{r}', \\ I_{ij} = \int \varphi_i^*(\mathbf{r})\, \varphi_j(\mathbf{r}')\, \psi_{ij}(\mathbf{r},\mathbf{r}')\, d\mathbf{r}\, d\mathbf{r}', \end{gathered} \tag{2.3}$$

$$\{H_i(\mathbf{p},\mathbf{r}) + H_j(\mathbf{p}',\mathbf{r}') + v(\mathbf{r}-\mathbf{r}')\}\psi_{ij}(\mathbf{r},\mathbf{r}') = e_{ij}\psi_{ij}(\mathbf{r},\mathbf{r}'), \tag{2.4}$$

$$E = N(\Omega - {}^1\!/\!_2\overline{U}) = N\varepsilon, \tag{2.5}$$

$$\overline{U} = \int \varphi_i^*(\mathbf{r})\, U(\mathbf{r}-\mathbf{R}_i)\, \varphi_i(\mathbf{r})\, d\mathbf{r}. \tag{2.6}$$

Here $\varphi_i(r)$ and $\psi_{ij}(r, r')$ are respectively the single-particle and two-particle wave functions; Ω and e_{ij} are the eigenvalues of the corresponding Schrödinger equations;

$$v(r) = v_0\left[\left(\frac{r_0}{r}\right)^{12} - 2\left(\frac{r_0}{r}\right)^{6}\right]$$

is the potential of the pair interaction of the atoms ($v_0 = 0.498$°K, $r_0 = 2.87$ Å), and ϵ is the energy per atom. The functions φ_i are normalized to unity. Equations (2.1)–(2.6) form a self-consistent system. In[7] they used for $U(r - \mathbf{R}_i)$ the harmonic approximation

$$U(\mathbf{r}-\mathbf{R}_i) = U_0 + \frac{m\omega^2}{2}(\mathbf{r}-\mathbf{R}_i)^2, \tag{2.7}$$

where $3\hbar\omega/2 = \Omega - U_0$. In this approximation, $\varphi_i(r)$ are Gaussian functions and

$$\varepsilon = {}^9\!/\!_8\hbar\omega + U_0/2. \tag{2.8}$$

In a real crystal the potential $U(r - \mathbf{R}_i)$ is not spherically symmetrical, but a spherical approximation is used here, i.e., (2.7) is equated to Eq. (2.2), which is expanded in $q_{i\lambda}$ up to second order ($q_{i\lambda}$ are the projections of the vector $r - \mathbf{R}_i$ on the coordinate axes, $\lambda = 1, 2, 3$) and is then averaged over the angles. The summation in (2.2) is extended to the third coordination sphere. Specifying the mass m of the isotope and the structure and the period of its crystal lattice, and solving the system (2.1)–(2.6), we can obtain in the approximation (2.7) the crystal energy as a function of the crystal value. This procedure was used in[7] for ^{4}He with a hexagonal close-packed lattice and for ^{3}He with a body centered cubic lattice. From the data given in[7] one can obtain the values of ϵ and $\hbar\omega$ as functions of the volume. The pressure is calculated from the same data by the formula $P = -\partial\epsilon/\partial V$. Unfortunately, there are no tabulated data in[7] and the values of ϵ and $\hbar\omega$ were reconstructed from diagrams, so that our results are obviously of low accuracy. In what follows, we shall need the radii of the coordination spheres and the number of atoms on them in the HCP and BCC lattices. In the HCP lattice there are 12 atoms on the first sphere of radius a, six on the second sphere of radius $a\sqrt{2}$, and two on the third of radius $a\sqrt{8/3}$, while in the BCC lattice there are respectively eight atoms on the first sphere of radius a, six on the second of radius $2a/\sqrt{3}$, and 12 on the third of radius $a\sqrt{8/3}$.

Assume that one atom is missing from the lattice of an ideal crystal. We label it by a zero subscript. We shall henceforth omit the complex-conjugation symbol from the definitions (2.3), since all the functions are real. Then Eq. (2.2) can be rewritten in the form

$$U'\varphi_i' = \sum_{j\neq i} \frac{v_{ij}'}{I_{ij}'} - \frac{v_{i0}'}{I_{i0}'},$$

$$\begin{aligned} v_{ij}' &= \int \varphi_j'(\mathbf{r}')\,v(\mathbf{r}-\mathbf{r}')\,\psi_{ij}(\mathbf{r},\mathbf{r}')\,d\mathbf{r}', \\ I_{ij}' &= \int \varphi_i'(\mathbf{r})\,\varphi_j'(\mathbf{r}')\,\psi_{ij}'(\mathbf{r},\mathbf{r}')\,d\mathbf{r}\,d\mathbf{r}', \\ v_{i0}' &= \int \varphi_0'(\mathbf{r}')\,v(\mathbf{r}-\mathbf{r}')\,\psi_{i0}'(\mathbf{r},\mathbf{r}')\,d\mathbf{r}', \\ I_{i0}' &= \int \varphi_i'(\mathbf{r})\,\varphi_0'(\mathbf{r}')\,\psi_{i0}'(\mathbf{r},\mathbf{r}')\,d\mathbf{r}\,d\mathbf{r}'. \end{aligned} \tag{2.9}$$

Unlike in an ideal crystal, here all the wave functions φ and ψ, as well as the quantities v and I in (2.3), are primed. If we put as a first approximation in (2.9) $\varphi_i' = \varphi_i$ and $\psi_{ij}' = \psi_{ij}$, i.e., if the single-particle potential of the given atom remains the same as in the ideal crystal but allowance is made for the appearance of the vacancy (the last term in (2.9)), then

$$U\varphi_i = (U + f_i)\varphi_i = U\varphi_i - v_{i0}/I_{i0}. \tag{2.10}$$

It can be shown (see[7]) that

$$f_i(\mathbf{q}) = -\sqrt{2}\,v_0 \frac{f(|\mathbf{q}+\mathbf{R}_{i0}|, m\omega/\hbar)}{I(R_{i0}, m\omega/2\hbar)}. \tag{2.11}$$

Here

$$f(x,b) = \frac{1}{x}\int_0^\infty g(y,x,b)\,v(y)\,u_0(y)\,dy, \tag{2.12}$$

$$I(x,b) = \frac{1}{x}\int_0^\infty g(y,x,b)\,u_0(y)\,dy, \tag{2.13}$$

$$g(y,x,b) = \exp\{-b(x-y)^2\} - \exp\{-b(x+y)^2\}, \tag{2.14}$$

$$u_0(y) = \exp\{-r_0^5/\sqrt{50}\lambda y^5\}, \tag{2.15}$$

$$v(y) = r_0^{12}/y^{12} - 2r_0^6/y^6.$$

The parameter $\lambda = \hbar/(2mr_0^2 v_0)^{1/2}$ takes on the values 0.310 for ^{3}He and 0.269 for ^{4}He.

Calculating $f_i(q)$ from (2.10) and solving (2.1) and (2.2) with $U + f_i$ instead of U, we can obtain the new φ_i and ψ_{ij} and, substituting them in (2.9), find a new U' etc. This procedure can be carried out only by solving the equations numerically. We therefore stop to discuss the first step, i.e., we determine f_i from (2.11) and then find the changes in φ_i and ϵ.

Since the main change of the single-particle potential of a given atom occurs in the vacancy direction, it is reasonable to assume

$$f_i(\mathbf{q}) = f_i(\zeta) = -\sqrt{2}\,v_0 \frac{f(\zeta, m\omega/\hbar)}{I(R_{i0}, m\omega/2\hbar)}, \tag{2.16}$$

where ζ is the coordinate in the direction from the lattice point at which the vacancy is located to the lattice point at which the i-th atom is located. The origin is at the point with the vacancy. We thus have

$$\left\{-\frac{\hbar^2}{2m}\Delta + U_0 + \frac{m\omega^2}{2}(\mathbf{r}-\mathbf{R}_i)^2 + f_i(\zeta)\right\}\varphi_i' = \Omega_i'\varphi_i',$$

$$\mathbf{r} = (\rho, \zeta) = \{\xi, \eta, \zeta\},\ \mathbf{R}_i = \{0, 0, R_{i0}\}.$$

Here ρ is a two-dimensional vector in a plane perpendicular to the ζ direction. As a result we get

$$U_0 + \frac{m\omega^2}{2}(r-R_i)^2 + f_i(\zeta) = U_0 + \frac{m\omega^2}{2}(\zeta_{i0}-R_{i0})^2 + f_i(\zeta_{i0}) + \frac{m\omega^2\rho^2}{2} + \left[\frac{m\omega^2}{2} + \frac{\ddot{f}_i(\zeta_{i0})}{2}\right](\zeta-\zeta_{i0})^2 + \ldots,$$

where ζ_{i0} is the root of the equation

$$m\omega^2(\zeta - R_{i0}) + f_i(\zeta) = 0,$$

whence

$$\zeta_{i0} = R_{i0} - f_i(\zeta_{i0})/m\omega^2.$$

It can be verified that $\dot{f}_i(\zeta_{i0})/m\omega^2$ is a small quantity and allowance for it leads to corrections of the order of several percent to the sought quantities. For simplicity we put $\zeta_{i0} = R_{i0}$. We introduce the notation

$$m\omega_i'^2 = m\omega^2 + \ddot{f}_i(R_{i0}). \tag{2.17}$$

Now the index i of the function f can be omitted:

$$m\omega_i'^2 = m\omega^2 + \ddot{f}(R_{i0}). \tag{2.18}$$

We obtain, accurate to terms of order $(\zeta - R_{i0})^3$:

$$\left[-\frac{\hbar^2}{2m}\Delta + \frac{m\omega^2}{2}\rho^2 + \frac{m\omega_i'^2}{2}(\zeta-R_{i0})^2\right]\varphi_i'(\mathbf{r}) = [\Omega_i' - U_0 - f(R_{i0})]\varphi_i'(\mathbf{r}),$$

$$\varphi_i'(\mathbf{r}) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\left(\frac{m\omega_i'}{\pi\hbar}\right)^{1/4}\exp\left\{-\frac{m\omega\rho^2}{2\hbar} - \frac{m\omega_i'(\zeta-R_{i0})^2}{2\hbar}\right\}, \tag{2.19}$$

$$\Omega_i' = U_0 + f(R_{i0}) + \hbar\omega + \frac{\hbar\omega_i'}{2},$$

$$\varepsilon_i = \Omega_i' - \overline{{}^1/_2(U + f_i(\zeta))} = \varepsilon + \Delta_i.$$

The superior bar denotes here averaging in the sense of (2.6), and

$$\Delta_i \equiv \varepsilon_i - \varepsilon = {}^1/_2 f(R_{i0}) + {}^3/_8\hbar\omega(\omega_i'/\omega - 1). \tag{2.21}$$

The total change in the lattice energy around the vacancy is

$$\Delta = \sum_{i=1}^{3} n_i\Delta_i. \tag{2.22}$$

Here n_i is the number of atoms in the coordination sphere around a vacancy. The summation in (2.22) extends to the third coordination sphere, since the main contribution to Δ is made precisely by the small distances. This can be verified, for example, by solving the elasticity-theory problem of determining the energy connected with the appearance of a spherical cavity of radius R in an elastic medium. Inclusion of the contributions from the remote coordination spheres would be an exaggeration of the accuracy, since in our method we do not take into account the influence of the lattice restructuring around the vacancy at the given

V, $\frac{\text{cm}^3}{\text{mole}}$	a, Å	ϵ_{theor}, °K	ϵ_{exp}, °K	$(PV_0)_{\text{theor}}$ °K	$(PV_0)_{\text{exp}}$, °K	Δ, °K	(zt) °K	ΔE_{1min} °K	ΔE_{1max} °K	ΔE_{theor} °K
HCC ^{4}He										
20.23	3.62	−4.4	−5.7	6.6	8.9	19.4	1.5	24.5	28.9	—
19.23	3.56	−4.0	−5.1	8.6	13.3	20.4	1.2	27.8	31.8	—
18.23	3.50	−3.5	−4.2	10.8	18.6	21.2	1.0	31.0	34.5	—
BCC ^{3}He										
23.7	3.71	−0.4	−0.9	4.7	6.7	11.8	4.4	12.1	12.5	6.9
22.7	3.66	0	−0.4	6.0	8.6	12.1	4.2	13.9	13.9	8.3
21.7	3.61	+0.4	+0.2	7.9	10.5	12.6	3.9	16.6	17.0	10.0

atom. As will be seen from the numerical results, Δ is a positive quantity. Allowance for the influence exerted on the given atom not only by the presence of the vacancy, as was done here, but also for the restructuring of the entire lattice, should decrease Δ. Thus, the calculated value of Δ is the upper bound of the change of the lattice energy around the vacancy.

We now determine the width of the vacancion band. Each atom from among the nearest neighbors surrounding the vacancy z is in a potential well and its energy level is determined from formula (2.20). Owing to the possible tunneling of the atom into an empty lattice site, this level splits into two and the value of the splitting multiplied by the number of nearest neighbors z, is of the order of the vacancion-band width. Such an approach is equivalent to the well-known tight-binding approximation.

The magnitude of the level splitting is calculated in analogy with the procedure used in the problem of the molecular hydrogen ion (see[10])[1]. Locating the origin at the middle of the segment between the empty and filled sites among the neighbors nearest to the empty site, and using the wave functions (2.19), we have

$$t=\frac{\hbar^2}{2m}\iint\limits_{\zeta=0}d\rho\left\{\varphi'\left(\rho,\zeta-\frac{a}{2}\right)\frac{\partial\varphi'(\rho,\zeta+a/2)}{\partial\zeta}-\varphi'\left(\rho,\zeta+\frac{a}{2}\right)\frac{\partial\varphi'(\rho,\zeta-a/2)}{\partial\zeta}\right\}.$$

The integration is carried out here over the plane $\zeta = 0$, and a is the distance between the nearest neighbors. The calculations yield

$$t=\frac{\hbar\omega'}{2}\left(\frac{m\omega'a^2}{\pi\hbar}\right)^{1/2}\exp\left\{-\frac{m\omega'a^2}{4\hbar}\right\}. \qquad (2.23)$$

ω' is determined from the formula

$$m\omega'^2=m\omega^2+\ddot{f}(a). \qquad (2.24)$$

The necessary values of $f(R_{i0})$ and $\ddot{f}(R_{i0})$, given by formulas (2.12)—(2.16), were obtained by computer calculation, after which Δ and t were determined from (2.22) and (2.23), using formulas (2.21), (2.18), and (2.24). We thus have all the components: ϵ, $PV_0 = -(\partial\epsilon/\partial V)_{V=V_0}V_0$, Δ, and t to determine the energy gap from formulas (1.2) and (1.3) and the width 2zt of the vacancion band.

3. NUMERICAL DATA AND COMPARISON WITH EXPERIMENT

The table lists the numerical results of the calculations for HCC ^{4}He and BCC ^{3}He. The theoretical values of ϵ and $PV_0 = -(\partial\epsilon/\partial V)_{V=V_0}V_0$ are given in accordance with[7], and the experimental values of ϵ and PV_0 were taken from[11,12]. There are no experimental data for the gap and for the width of the band in pure HCC ^{4}He, since no NMR experiments are possible on ^{4}He,[2] and the vacancion contribution to the specific heat is small in comparison with ^{3}He, owing to the larger value of the energy gap. We list the experimental values of the gap E taken from[2] for BCC ^{3}He. The obtained values are in qualitative agreement with the experimental data. We note that the model of[7], which was used for the calculations, underestimates ϵ and PV_0 in comparison with the experimental values, and in all probability results in a highly overestimated Δ. The experimental data on half the bandwidth zt for BCC ^{3}He, also given in[2], have a large spread from 2 to 5°K and do not fit any smooth curve. We can therefore speak only of an order-of-magnitude agreement with the calculated values. As seen from the results, the agreement is quite good.

For more details on the experimental data we refer the reader to the review[2]. Owing to the large value of the gap, the vacancion gas is a Boltzmann gas and the number of vacancions decreases exponentially with temperature like exp (−ΔE/T). It is interesting to note that with increasing (decreasing volume), the vacancion gap increases, and the width of the band decreases, i.e., the vacancion gas becomes more and more classical. This result shows that quantum crystals have no tendency to a phase transition to a crystalline modification in which the number of lattice sites does not coincide with the number of atoms (see[1]).

In conclusion, the author is grateful to V. L. Pokrovskiĭ for useful discussions, and also to A. N. Ivanova and N. S. Nazemets for performing the numerical calculations.

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[1] Allowance for the appearance of an additional slow dependence of the wave function on the coordinate along the tunneling direction, in a manner similar to that used in [10], would mean an exaggeration of the accuracy in this case, since the single-particle potential itself is determined by us in the harmonic approximation, i.e., it is accurate only near its bottom.

[2] It follows from NMR experiments on ^{4}He with small admixture of ^{3}He atoms (see [2]), however, that the width of the vacancion band in ^{4}He is of the same order as in ^{3}He.

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201