Instability zone of point defects in quantum crystals

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It is shown that one of the linear dimensions which govern the nature of the interaction between point defects in quantum crystals [A.F. Andreev and I. M. Lifshitz, Sov. Phys. JETP **29**, 1107 (1969); A.F. Andreev, Sov. Phys. Usp. **19**, 137 (1976)] is r_0, which is the size of the instability zone [V. M. Koshkin and Yu.R. Zavodskiĭ, Sov. Phys. Dokl. **21**, 203 (1976); V. M. Koshkin and Yu.R. Zabrodskiĭ, Sov. Phys. Solid State **16**, 2256 (1975)]. For example, the inelastic cross section of defects for $r_0 > R_0$ is $(\Theta_D/\Delta)^2$ times greater than for $r_0 < R_0$. It is shown that discrete levels should exist in the instability zone and, consequently, there should be microwave absorption due to transitions of an ion between the levels; there should also be quasiparticles formed from two defects but different from those discussed by A.F. Andreev [Sov. Phys. JETP **41**, 1170 (1975)] and A.É. Meĭerovich [Sov. Phys. JETP **42**, 676 (1975)].

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The example of a vacancy and an interstitial atom has been used by us already[1,2] to show that, if the interaction potential of two defects, A and B, is attractive, then around the defect A (assumed to be less mobile) there is a region with a characteristic radius r_0, which can be called an instability zone because there are no minima of the potential energy for B inside this zone. The value of r_0 can be found from[1,2]

$$a\frac{dV}{dr}\bigg|_{r=r_0} = E_m^B, \quad (1)$$

where a is the interatomic distance in the lattice, E_m^B is the migration energy of B in an ideal lattice, and $V(r)$ is the energy of the interaction between A and B. We shall consider the scattering and annihilation of defects in quantum crystals[3,4] in the presence of an instability zone. We shall consider a vacancy v and an interstitial atom i. The results obtained can also be applied to the interaction of other defects, for example, a vacancy and an impurity.[4]

The migration energy v can be estimated from the tunneling probability:

$$\frac{\Delta}{\Theta_D} \sim \exp\left[-\frac{2a}{\hbar}(2mE_m^v)^{1/2}\right],$$

from which we find that $E_m^v \sim 10^{-3}$–10^{-4} eV ($\Delta \sim 1$°K is the width of the energy band of vacancyons and $\Theta_D \sim 20$°K is the Debye temperature of a ^{4}He crystal[4]). The migration energy of i, E_m^i, or—which is equivalent—the width of the energy band i in ^{4}He is not known. Since, in all the familiar cases (see, for example, the book by Boltaks[7]), we have $E_m^i/E_m^v \sim 10^{-1}$–10^{-2}, we shall assume that $E_m^i \sim 10^{-4}$–10^{-6} eV. We shall also assume that i and v attract each other elastically, in accordance with the law[4]

$$V(r) = -V_0(r/a)^3,$$

where $V_0 \sim 10^{-1}$ eV, i.e., this energy is of the same order as the interaction potential of two vacancies. Then, according to Eq. (1), an instability zone forms around v and the radius of this zone is

$$r_0 \approx a(V_0/E_m)^{1/4} \geqslant 10a.$$

We can see that instability zones in a quantum crystal should be quite large.

In a classical crystal, an atom which is within the instability zone of its vacancy, can return in an activation-free manner to its own site,[1,2] whereas, in a quantum crystal, there are stationary levels for an interstitial atom in the potential well created by a vacancy. The number of levels in such an atom can easily be estimated using the quasiclassical Bohr–Sommerfeld quantization condition:

$$N \approx \frac{2}{\pi\hbar}\int_0^{r_0} (2m|U(r)|)^{1/2}\,dr. \quad (2)$$

If $r > a$, the potential is $U(r) \sim V(r)$, but, if $r \lesssim a$, the value of $U(r)$ is governed by the Lennard–Jones potential [the result depends weakly on the actual form of the potential $U(r)$ in the $r < a$ case]. Estimates based on Eq. (2) give $N \sim 10$–10^2.

We shall not assume that the distance between the levels is $\Delta U \approx z\epsilon/N \approx 10^{-3}$–$10^{-4}$ eV, where z is the number of nearest neighbors and ϵ is the interaction between two atoms in the Lennard-Jones potential. The lifetime of an unstable pari will be governed by the probability of phonon scattering in the $\Delta U \ll T$ case[8]:

$$\tau \sim N\frac{\Theta_D}{\Delta U}\left(\frac{\Theta_D}{T}\right)^6 \omega_D^{-1},$$

but, if $\Delta U \gg T$, it is governed by the probability of spontaneous emission of a phonon[9]:

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$$\tau \sim N\left(\frac{\Theta_D}{\Delta U}\right)^3 \omega_D^{-1} \sim 10^{-8}-10^{-9} \text{ sec}.$$

Thus, we can see that, at temperatures $T > T_0 = (\Delta U \Theta_D)^{1/3} \sim 2\,^\circ K$, the lifetime of an unstable pair in a quantum crystal is a function of temperature, in contrast to the case of classical crystals.[10] At temperatures $T < T_0$, the lifetime of an unstable pair in He is independent of temperature but two orders of magnitude greater than for that of ordinary crystal.

We shall now consider the process of annihilation of i and v, which are initially an infinite distance apart. Inside an instability zone, an interstitial atom i should not tunnel across a potential barrier when going over from one interstice to another because its potential energy in such a zone varies monotonically as a function of the $v-i$ distance. According to Andreev and Lifshits,[3,4] i and v cannot approach each other to a distance shorter than $R_0 \sim a(V_0/\Delta)^{1/3}$, so that, for $r_0 > R_0$, we have

$$E_m < (\Delta^4/V_0)^{1/3} \tag{3}$$

and the annihilation probability is governed by the probability of phonon scattering on transition from one level to another:

$$W_1 \sim \frac{\Delta U}{N\Theta_D}\left(\frac{T}{\Theta_D}\right)^6.$$

For the opposite inequality $R_0 > r_0$ [and, consequently, for the opposite inequality of Eq. (3)], the annihilation probability is governed mainly by the probability that i and v approach each other from a distance R_0 to r_0, i.e., by the probability of the tunneling of i accompanied by simultaneous phonon scattering:

$$W_2 \sim \frac{a}{R_0 - r_0}\frac{V_0}{\Theta_D}\left(\frac{a}{R_0}\right)^4\left(\frac{T}{\Theta_D}\right)^6\left(\frac{\Delta}{\Theta_D}\right)^2$$

where $W_1 \gg W_2$, i.e., the cross section for the inelastic scattering of defects (in this case, the annihilation of i and v) is considerably greater for $r_0 > R_0$ than in the opposite case.

An analysis completely analogous to that given above can also be made in the case of two dislocation kinks in the same trough. The potential interaction between these kinks[4,5] is $V'(r) = -\mu a^4/r$, where μ is the shear modulus. The radius of an instability zone for kinks is then $r_0' \approx (\mu a^5/\mathfrak{U}_m)^{1/2}$, where $\mathfrak{U}_m$ is the energy of a Peierls barrier in the case of climb of a dislocation kink. By analogy with Eq. (3), the critical value of the Peierls barrier for the annihilation of kinks is $\mathfrak{U}_m^c = \Delta^2/\mu a^3$ (Δ is the width of the kink band).

Thus, when the condition $R_0 < r_0$ is satisfied, the symmetry of the behavior of defects relative to the sign of the potential of their interaction[4] may be violated quite strongly. For example, the cross section for the inelastic scattering of defects in, for example, diffusion between vacancyons in the case of an attractive interaction potential is (Θ_D/Δ^2) times greater than for the same potential with the opposite sign. The experimentally observed small value of the inelastic scattering cross section of ^3He impurities on vacancyons in ^4He[4] may be due to the fact that ^3He and v repel one another, whereas the absence of interstitial atoms in He may be associated with a large cross section of the annihilation of i and v in the $r_0 > R_0$ case. The interaction of defects in quantum crystals within an instability zone may have a number of features distinguishing it from a classical crystal, including the temperature dependence of the lifetime of a nonequilibrium pair and the existence of stationary levels for one defect in the field of another. According to Eq. (2), at low temperatures T in the wavelength range 0.1–1 cm, there should be absorption associated with ion transitions between levels in an instability zone of another defect. Therefore, it would be of interest to investigate the absorption of a quantum crystal in the rf range. For two- and one-dimensional cases,[5,6] allowance for the influence of an instability zone results in a strong rise in the lifetime of the corresponding quasiparticles on increase in r_0, and it facilitates the formation of complex quasiparticles which are not associated, in contrast to the quasiparticles considered by Andreev and Meĭerovich,[5,6] directly with lattice sites; these particles can be formed, for example, from a ^3He impurity and an interstitial atom located at one of the levels in the instability zone of ^3He.

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