Localization in a system of interacting particles diffusing in a regular crystal

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Tunneling diffusion of particles in a crystal with an extremely narrow band, in which the particles begin to interact intensely with each other even at a low concentration, is analyzed. The periodic potential relief of the host has several consequences. On the one hand, it means that a particle must jump a finite distance for a resonant transition to occur, and the number of equivalent sites is limited. On the other, it causes umklapp processes and limits the kinetic energy. The result is the formation of clusters within which both single-particle and many-particle excitations are suppressed. The equivalent bandwidth for the motion of a cluster as a whole falls off exponentially with increasing number of particles in the cluster. At a certain concentration x_∞ an immobile cluster of infinite size forms, and the system of particles breaks up into mobile and immobile subsystems. The immobile subsystem creates an immobile defect structure, and localization begins in the mobile subsystem at a certain concentration x_c. The critical behavior of the diffusion coefficient near x_c is that of classical percolation. The disruption of localization at low temperatures by an interaction with phonons is analyzed. The results are compared with experiments on localization and phonon-induced delocalization in the diffusion of He^3 atoms in solid He^4.

1. INTRODUCTION

Previous studies of the localization problem have essentially always reduced to the analysis of a single-particle problem in a random, inhomogeneous, static field or in a medium with a static distribution of irregularities. This is true of both the quantum-mechanical localization problem[1] and all problems in the classical theory of percolation (see Ref. 2, for example). The interaction between diffusing particles in this case may substantially change the picture near the percolation threshold, but the inhomogeneity of the medium remains the governing factor for localization.

In studying the diffusion of particles which are interacting with each other in a strictly regular crystal we run into the situation, in the case of narrow bands, that at a comparatively low particle concentration x the field configuration which is realized at each instant is such that the field inhomogeneity scale exceeds the critical value required for localization of an individual particle in the static case. A fundamental distinction here, however, is the generally dynamic nature of the random field. We are led to ask whether a localization encompassing the entire subsystem of diffusing particles as a whole can arise under such conditions, so that the diffusion coefficient D would vanish.

A first glance at the homogeneous analog of the problem—diffusion in a liquid— leads to a negative answer. In a liquid without stratification an increase in the concentration of the diffusing particles does not lead to any of the features characteristic of localization. For example, experiments on the diffusion of He^3 atoms in liquid He^4 have demonstrated a continuous increase in D with decreasing temperature T over the entire He^3 concentration range studied (see Ref. 3, for example).

Under certain conditions, however, as the detailed analysis below shows, the interaction between particles as they diffuse through an ideal crystalline host does give rise to a localization. We consider only the case of extremely narrow bands, for which the interaction between particles over an average distance $\bar{r}$, $U(\bar{r})$, and also the value of $a\,|\nabla U|$ at this distance reach the value of the bandwidth, Δ, at a low particle concentration $x \ll 1$, and the condition $T > \Delta$ or even the stronger condition $T > U(\bar{r})$ holds at such low temperatures that the effects of the interaction with phonons are still slight. This is a typical situation, in particular, in the tunneling diffusion of atomic particles in a crystal. It was for this case that the idea of localization in a system of interacting particles was first suggested[4] (see also Ref. 5); this idea has since been developed along with the problem of phonon-induced delocalization.[6,7] The nature of the localization which occurs has not been analyzed comprehensively.

The decisive factor giving rise to this type of localization is the discrete nature of the space, which is a consequence of the crystalline structure of the host. Because of this discrete setting, the system has many properties of fundamental importance which distinguish it from the case of a homogeneous medium:

1. Umklapp processes occur, becoming particularly pronounced at $T \gtrsim \Delta$.

2. Tunneling occurs only over a finite (interatomic) distance a. The number of equivalent sites in the nearest coordination sphere, z, is limited.

3. The kinetic energy of the particles is limited to values on the order of the bandwidth Δ.

The umklapp rules out a nondissipative drift state, even in the complete absence of an inelastic interaction with the host.

In a liquid a diffusing particle may undergo resonant displacements over some arbitrarily small distance, with adiabatic structural adjustments in the surroundings. That this behavior is impossible in principle in a crystal can be seen very clearly in the He^3–He^4 system, for example, where the effective masses of He^3 in liquid and solid solutions at comparable densities (the effective mass in the solid phase can easily be found if the bandwidth is known) differ by four orders of magnitude (cf. Refs. 8, 9, and 3). In a crystal the unavoidable limitation on the amplitude of the resonance transition, Δ_0, to a minimum possible distance a combines with the finite number of possible transition paths (z) to cre-

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ate a situation in which the level shift $\delta\varepsilon$ at neighboring sites caused by the interaction with other particles exceeds $\Delta \approx z\Delta_0$ in order of magnitude, and the motion of the particle under consideration is blocked. It is easy to see that at concentrations $x_{00} \ll 1$, at which a shift of this magnitude on the average occurs throughout the crystal in a statistical manner, clusters in which single-particle motions are suppressed will exist in the system. As is shown in Section 2, the internal many-particle motions are also suppressed, and the displacement amplitude $(\tilde{\Delta}_n)$ of such a cluster as a whole in free space, although not zero, does fall off exponentially with increasing value of n, the number of particles in the cluster. At a certain concentration x_∞, which has the same scale value x_{00}, an immobile infinite cluster forms. Even at a smaller level shift, clusters with $n > 2$ lose the ability to move as a whole that individual particles have; that value of the shift at which clusters lose their mobililty falls off progressively with increasing n. It is easy to show that this effect gives rise to an immobile infinite structure (a more "friable" structure) at a lower concentration. The problem of the formation of an immobile cluster is analyzed in detail in Sections 2 and 3.

At concentrations $x \gtrsim x_\infty$, a significant number of the particles do not belong to an infinite cluster and instead remain as free individuals or members of small clusters. As a result, the system of interacting particles in an ideal crystal breaks up into two subsystems: an immobile subsystem reminiscent of a swarm of bees in winter hibernation and a mobile subsystem whose particles remain able to move. Because of the fundamental limitation on the kinetic energy of the mobile particles, their interaction with an immobile cluster cannot excite the latter (Section 2). An immobile cluster therefore serves as a static defect formation for the mobile particles. It thus becomes clear that at a certain particle concentration x_c the mobile particles lose their ability to move off to infinity, and complete localization occurs in the system.

As in the traditional percolation problem, the value of x_c is related to the size of the free volume in which the particles can move. There is a fundamental distinction here: As the mobile particles undergo collisions they can exchange energy in amounts on the order of their kinetic energy, i.e., Δ. Consequently, these particles kinetically have access to the entire volume in which the level shifts at neighboring sites due to the immobile cluster, $\delta\varepsilon$, do not exceed Δ in order of magnitude. At $T > U(\bar{r})$, there are no special restrictions of any sort on motion anywhere in this volume, and a further temperature increase plays no role in the absence of an interaction with phonons. The subsystem of immobile particles is insensitive to increases in T (the swarm continues to sleep). The concentration x_c corresponds to a definite minimum value of the volume which is free in the kinetic sense.

The overall problem is discussed in Section 3; at this point we wish to examine the nature of the critical behavior of $D(x)$ near x_c. We see that the important role of inelastic processes in the kinetics of the mobile particles leads to a critical exponent which is approximately the same as in the classical percolation theory (see Ref. 2, for example). In Section 4 we use the results of Ref. 6 to examine the role played by the interaction with phonons, primarily the induced delocalization of particles caused by this interaction at $x > x_c$ and the effective increase in the number of allowed paths at $x < x_c$.

The phenomenon of localization in a system of interacting particles in a regular crystal was first observed experimentally by Mikheev *et al.*[10-12] in studies of the diffusion of He^3 atoms in He^4. They established the critical nature of the x dependence of D and simultaneously found an anomalous temperature dependence, which is inherent in a phonon-induced delocalization. The results were found to agree well with the theoretical predictions of Refs. 4, 6, and 7. The system of He^3 atoms in He^4 is a very appropriate one[7] for studying localization of this type.

In the last section of this paper we discuss comparisons of experimental data with theoretical predictions.

2. CLUSTER FORMATIONS AND LOCALIZATION

We consider a subsystem of N particles in an ideal crystal with an extremely narrow band. We assume that in each of the N_0 unit cells a particle can occupy only a single state. The Hamiltonian of the subsystem can then be written in the site representation as

$$\hat{H} = \Delta_0 \sum_{\mathbf{r},\mathbf{g}} \hat{a}^+_{\mathbf{r}+\mathbf{g}} \hat{a}_{\mathbf{r}} + \frac{1}{2} \sum_{\mathbf{r}_1,\mathbf{r}_2} U(\mathbf{r}_1 - \mathbf{r}_2)\, \hat{a}_{\mathbf{r}_1}{}^+ \hat{a}_{\mathbf{r}_2}{}^+ \hat{a}_{\mathbf{r}_2} \hat{a}_{\mathbf{r}_1}. \qquad (2.1)$$

Here $\mathbf{g}(|\mathbf{g}| = a)$ is the translation vector in the first coordination sphere. We assume that the interaction between particles can be described by the simple power law

$$U(r) = U_0 (a_0/r)^\alpha, \quad \alpha \geqslant 3. \qquad (2.2)$$

The parameter a_0 is related to the volume of the unit cell: $v_0 = \frac{4}{3}\pi a_0^3$. For order-of-magnitude estimates we will ignore the distinction between a_0 and a, the lattice constant. For definiteness we assume $U_0 > 0$. The restrictions which arise in the case of attraction and also in the case of a nonspherical interaction (e.g., the interaction caused by a strain field) will be discussed in the last section of the paper.

At a particle concentration $x = N/N_0 \rightarrow 0$ band motion of the particles takes place in the crystal. We assume that the bandwidth Δ satisfies the inequality

$$\Delta \approx z\Delta_0 \ll U_0, \qquad (2.3)$$

where z is the number of nearest neighbors. In this case the potential energy per particle begins to exceed the kinetic energy even at a low particle concentration $x \approx x_0$. The band motion is disrupted, and the particles go into quasiliquid motion. We are interested in the behavior of the subsystem of particles at $x > x_0$, but we retain the condition $x \ll 1$; then at $T \gtrsim \Delta$ there is no degeneracy in the system, and we can ignore the nature of the statistics which the particles obey.

This system has a clearly defined tendency to form clusters in which the relative motion of the particles, even over atomic distances, is suppressed. A cluster forms when the scale value of the level shift $(\delta\varepsilon)$ upon the displacement of a particle into the first coordination sphere exceed $\gamma\Delta$, and the minimum level shift exceeds $\gamma\Delta_0 (\gamma > 1)$. Here there must be at least one more particle within a sphere of radius $R_{00} \gg a$

around each particle of the cluster, where this radius is determined by the condition

$$\delta\varepsilon_{00} \equiv a|\nabla U|_{r=R_{00}} = \gamma\Delta, \tag{2.4}$$

Strictly speaking, the set of sites which are coupled by level shifts exceeding $\gamma\Delta$ actually has a more complicated shape than overlapping spheres of radius R_{00}, but this circumstance will not affect the results of the calculations below.

Even in the example of two particles it is easy to see that, in addition to the suppression of any relative motion in the radial direction by the discrete nature of the lattice, at $\gamma \gg 1$ the motion of each particle in *any* direction will be suppressed in the overwhelming majority of configurations. When a particle is simultaneously in the field of two or more particles, this suppression occurs at a substantially smaller value of the parameter γ.

We will now show that if single-particle motions are suppressed in a cluster then any internal many-particle motions will also be suppressed. To demonstrate this point we begin with two-particle motions in a cluster.

Treating the kinetic energy in (2.1) as a perturbation, we can write the following expression for the amplitude of the two-particle motion:

$$\Delta_2 = \frac{\Delta_0^2}{\delta\varepsilon_1} + \frac{\Delta_0^2}{\delta\varepsilon_2} = \frac{\Delta_0^2}{\delta\varepsilon_1\,\delta\varepsilon_2}\,[\varepsilon_{fi} - (g_1\nabla_1)(g_2\nabla_2)U(\mathbf{r}_1 - \mathbf{r}_2)]. \tag{2.5}$$

Here $\delta\varepsilon_s$ is the change in the energy of the cluster upon a displacement g_s of the sth particle, and ε_{fi} is the difference between the final and initial energies of the cluster. Since the distance (r) between particles is large in comparison with a, we have expanded the potential energy in a/r in calculating $\delta\varepsilon_1 + \delta\varepsilon_2$. After we isolate ε_{fi} in the numerator in (2.5), we are left with only the second derivative of the direct interaction between particles, which is even smaller than $\delta\varepsilon$, since it contains a small factor on the order of a/r. In general, ε_{fi} will be large in comparison with the second term in square brackets in (2.5), and we will have

$$|\Delta_2/\varepsilon_{fi}| \sim (\Delta_0/\delta\varepsilon)^2 \ll 1.$$

A random realization of a resonant situation, $|\varepsilon_{fi}| < |\Delta_2|$, which would be required for an actual transition of two particles at the same time, is substantially less probable than in the case of single-particle motions.

Working in the same way, we can derive an expression for the amplitude of a k-particle excitation in a cluster:

$$\Delta_k = \frac{\Delta_0^k}{\delta\varepsilon_1 \ldots \delta\varepsilon_k}\,(\varepsilon_{fi} + E_k^{(2)}), \tag{2.6}$$

where $E_k^{(2)}$ is another quantity containing an additional factor of the small parameter a/r. A fixed set of k particles actually has a great number (z^k) of paths for motion. The transition with the highest amplitude is obviously that in which each individual particle is displaced in the direction of the minimum level shift. This minimum level shift has a typical value $\delta\varepsilon_{\min} \approx \delta\varepsilon_{00}/z$, so we find the following expression for the maximum value of amplitude (2.6):

$$\Delta_k \approx (z\Delta_0/\delta\varepsilon_{00})^k (\varepsilon_{fi} + E_k^{(2)}) \sim \gamma^{-k}. \tag{2.7}$$

We thus see that in practice the resonant situation cannot arise at $\gamma > 1$, even for the most dangerous path of motion.

Consequently, under the conditions we have assumed here, all collective motions in the cluster are suppressed.

We turn now to the motion of an isolated cluster of n particles as a whole. In this case we can use (2.6), setting $\varepsilon_{fi} = 0$ in it and noting that upon a displacement of all the particles of the cluster by an identical translation vector g the set $\delta\varepsilon_s$ takes on all possible values in the interval $\delta\varepsilon_{00}$. We can then write

$$\tilde{\Delta}_n \approx \Delta_0 (E_n^{(2)}/\Delta_0) \exp[-n \ln(\gamma' z)], \quad \gamma' z \gg 1. \tag{2.8}$$

In this expression we certainly have $\gamma' < \gamma$; at a large value of n, we would have $\gamma' \approx e$.

We write a separate expression for $\tilde{\Delta}_2$ using explicit expressions (2.5) and (2.2):

$$|\tilde{\Delta}_2| \approx \Delta_0 (\alpha + 1)(a/r_{00})(1/\gamma z). \tag{2.9}$$

We see thus that the cluster translation amplitude $\tilde{\Delta}_n$ falls off exponentially with increasing number of particles in the cluster. When we take into account the possibility of internal motions, we conclude that the amplitude of the cluster could in principle be far larger than (2.8). In particular, it could approach the value in (2.7) if we set $k = n$ in it. In this case, however, we would have $\Delta_n \ll \varepsilon_f$, so that such a motion would not actually occur.

It follows from these results that in the limit $n \to \infty$ we obtain a cluster with neither internal motion nor translational motion.

An infinite cluster defintiely exists in our system if the concentration satisfies $x > x_\infty^{(1)}$. If we assume that when the system was prepared the particles were distributed among lattice sites in a purely random fashion, we can use the results of the "random sites problem" in percolation theory (see Ref. 2, for example); we find

$$x_\infty^{(1)} = \zeta x_{00}, \tag{2.10}$$

where we find $\zeta \approx 2.7$ from numerical calculations, and the scale concentration x_{00} is given by

$$x_{00} = (a_0/R_{00})^3. \tag{2.11}$$

At $x > x_\infty^{(1)}$ the crystal thus contains a subsystem of immobile particles in which all the internal motions are suppressed, as is the translational motion of the cluster as a whole. At the same time, the crystal regains a significant number of isolated particles and small clusters. The number of individual particles ("loners"), which do not belong to any of the clusters, for example, is

$$N_1 = Ne^{-y}, \quad y = x/x_{00}. \tag{2.12}$$

To determine the number of isolated "duos," $\tilde{N}_2$, we need to find the probability that two particles will be separated by a distance $b < R_{00}$, while there will be no other particles in a volume $v(b)$ around them (Fig. 1), and then sum over $\mathbf{b}$:

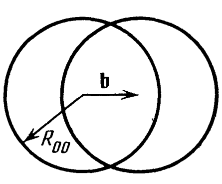

FIG. 1.

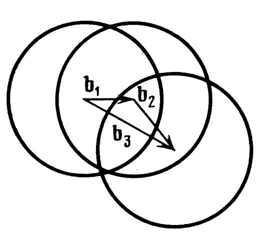

FIG. 2.

$$\tilde{N}_2(x)=\frac{1}{2}N\sum_{|\mathbf{b}|<R_{00}} x\exp[-xv(\mathbf{b})/v_0]=\frac{1}{2}Nye^{-y}F_1(y),$$

$$F_1(y)=\left(\frac{4}{3}\pi R_{00}\right)^{-3}\int d^3b\exp[y-xv(\mathbf{b})/v_0]$$
$$\approx\frac{64}{9y^3}\gamma\left(3,\frac{3}{4}y\right). \qquad (2.13)$$

Here $\gamma(\alpha, x)$ is the incomplete gamma function.

Analogously, summing over all configurations of "trios" (Fig. 2) for which two distances of the three are smaller than R_{00}, we find

$$\tilde{N}_3(x)=\frac{1}{3!}\sum_{b_1b_2b_3}\delta_{b_1+b_2+b_3,0}x^2\exp[-xv(b_1b_2b_3)/v_0]$$
$$=\frac{1}{6}Ny^2e^{-y}F_2(y), \qquad (2.14)$$

where we can use

$$F_2(y)\approx 2[F_1(y)]^2. \qquad (2.15)$$

for an estimate.

Pursuing these arguments we see that at $x \approx x_\infty^{(1)}$ the loners, duos, and trios constitute about 10% (7%, 2%, and 1%, respectively) of the total number of particles.

In principle, the collisions of isolated particles are inelastic. For example, two loners may exchange an energy on the order of Δ in an interaction. For this exchange to occur, it is generally not necessary that the particles execute a motion equivalent to an actual band motion. It is sufficient that the particles be delocalized within one or two coordination spheres.

Can single-particle transitions occur in a cluster as it interacts with loners? The energy of single-particle excitations in a cluster lies in the interval $\gamma\Delta_0 - \gamma z\Delta_0$, as is clear from the discussion above. Accordingly, in an inelastic collision with a cluster a mobile particle, at a distance $r > R_{00}$ from the bound particle with which it interacts, must lose an energy greater than $\gamma\Delta_0$. Let us consider the interval $R_{00} < r < R'$ directly adjacent to the cluster "boundary" [R' is found from (2.4) by setting $\gamma = 1$]. Here the inelastic exchange with the mobile particle will be described by the amplitude Δ_2 in (2.5). For an actual transition, the condition $\varepsilon_{fi} \approx 0$ must hold within a value on the order of Δ_2. We thus have $|\delta\varepsilon_2| \approx |\delta\varepsilon_1|$ and

$$\Delta_2\approx\gamma^{-2}|E^{(2)}|\ll\Delta_0. \qquad (2.16)$$

At $r > R'$ the mobile particle may be quasilocalized at a distance greater than a. In order to describe its state in this case we need to consider the kinetic energy in (2.1) from the outset. The amplitude for the simultaneous transition of this particle and of one cluster particle is determined by the two-particle matrix element of their interaction potential energy, $U(\mathbf{r}_{12})$. Taking into account the large distance (r) between the particles, the limitation on the change in the localization center upon the transition, and the relative shift of the initial and final states, we can write the following expression for the part of the interaction which is responsible for the transition $\mathbf{r}_1 = \mathbf{r} + \boldsymbol{\rho}_1$, $\mathbf{r}_2 = \boldsymbol{\rho}_2$:

$$U(\rho_1,\rho_2)\approx-\frac{\partial^2U(r)}{\partial r_i\,\partial r_k}\rho_{1i}\rho_{2k}. \qquad (2.17)$$

If we consider that during localization in an individual cell the impurity of states at adjacent sites with a relative level shift $\delta\varepsilon$ is proportional to $\Delta_0/\delta\varepsilon$, then we easily see that the matrix element of (2.17) agrees with Δ_2 in (2.5) at $\varepsilon_{fi} \approx 0$.

The decrease in the second derivative of U with increasing r, combined with the circumstance that the matrix element of ρ corresponding to the mobile particle definitely does not increase, means that the amplitude for the inelastic exchange is smaller than (2.16). It is thus clear that inelastic single-particle processes in a cluster are suppressed. It is not difficult to see that many-particle excitations in a cluster upon collisions with loners are suppressed even more strongly.

We see that the interaction between mobile particles and a cluster is essentially always elastic. (The rare random satisfaction of the condition for a real process involving the inelastic excitation of a particle in a cluster and its displacement over an interatomic distance will change nothing in the picture drawn below.)

In principle, a particle could collide with an n-particle cluster as a whole. In such a collision, however, the possible exchange of energy would be on the order of $\tilde{\Delta}_n$, as can be seen by associating with an n-particle cluster an effective mass m_n, whose ratio to the effective mass of a loner, m_1, is

$$m_n/m_1\approx\Delta_0/\tilde{\Delta}_n. \qquad (2.18)$$

In this sense the subsystem of particles forming the infinite cluster actually creates a static defect structure in the crystal.

In summary, once an infinite cluster forms, the system of particles in an ideal crystal breaks up into two fundamentally distinct subsystems. The mobile particles making up one of these subsystems now move in the irregular static field produced by the subsystem of immobile particles, which are distributed over the crystal in a substantially random manner, although there are definite spatial correlations. Clearly, at a sufficiently high density of the infinite cluster ($x > x_\infty$), the immobile subsystem will form a static defect configuration of a type which will block the mobile particles. In other words, the mobile particles will become unable to move from any spatial point off to infinity, even when we take into account the inelastic interaction in the subsystem of mobile particles itself.

In this case we definitely have a localization for the entire system of particles as a whole.

3. LOCALIZATION TRANSITION IN A SYSTEM OF INTERACTING PARTICLES

In analyzing the picture of the transition to localization it is natural to consider the relative size of the "free" volume (the "white" region), i.e., that part of the volume or that subset of the sites which is accessible to the free particles in the course of their motion. It is here that the single-particle and many-particle problems (we mean mobile particles here) are fundamentally different.

In analyzing the single-particle problem in a crystal with static defect we are interested in the relative volume in which the energy of the particles in the potential relief differs from the band value by an amount less than Δ. In the many-particle problem, the exchange of energy between mobile particles (although still limited to a value on the order of Δ in each individual collision event) gives rise to a diffusion in energy space. The effect is to increase the "accessible energy band" and thus the corresponding free volume. With an eye on the kinetic problem, we note that in principle the effective width of this band depends on the temperature. If, however, T exceeds a scale temperature of the potential relief, determined by the interaction of the particles over the average distance, $U(\bar{r})$, this temperature dependence vanishes. In this case the free volume includes essentially all sites which may contain an isolated loner if we pretend that all the mobile particles have been removed.

In the case of an extremely narrow band, the independence from the temperature arises at very low values of T (the corresponding transition temperature tends toward zero in the limit $\Delta_0 \to 0$). In analyzing the problem we can thus ignore the interaction with phonons (see the next section of the paper).

To estimate the relative number of free sites, w, in this case, we note that for "ideally" free sites, within a radius R_{00} of which there are not even any loners, we would have

$$w_0 = e^{-y}, \quad y = x/x_{00}. \tag{3.1}$$

If there is no particle at a particular site, and if there is one isolated particle within a radius R_{00} of it, then this site will also be a free one, and we should add to w_0 a probability [cf. (2.13)]

$$w_1 = {}^1/_2 y e^{-y} F_1(y). \tag{3.2}$$

Analogously, using (2.14), we can calculate the probability (w_2) that there will be two loners or a mobile duo within a radius R_{00} of a free site:

$$w_2 \leqslant {}^1/_2 y^2 e^{-y} F_2(y). \tag{3.3}$$

The reason for the "less than" sign here is that, as will be seen below, the number of truly mobile duos is substantially smaller than $\tilde{N}_2$ in (2.13).

Ignoring the other configurations, we use the sum of (3.1) through (3.3) to estimate the relative size of the free volume. At $x \approx x_\infty^{(1)}$ this sum is about 0.14. In comparing this value with the values from percolation theory (see Ref. 2, for example), we must allow for the possibility that the critical concentration x_c, at which percolation through the free volume ceases, may lie slightly to the left of $x_\infty^{(1)}$ or at any rate in a region in which the strength of the infinite cluster is still low [x_c is clearly greater than the concentration $2x_{00}$, at which the condition $(w_0 + w_1) > 0.2$ holds].

At these concentrations, however, there is already a well-developed subsystem of immobile particles, formed by clusters with $n \geqslant 2$. Up to this point we have ignored the fact that isolated clusters of n particles cease to move even at level shifts $\delta\varepsilon_n \ll \delta\varepsilon_{00}$ because of the exponential decrease in $\tilde{\Delta}_n$ in comparison with Δ_0 [see (2.8)]. If an n-particle cluster is to be able to move in the face of the power-law nature of the interaction, (2.2), there must be no particles near this cluster which belong to other m-particle clusters with $m \geqslant n$ in a region with linear dimensions R_n substantially greater than R_{00}. This dimension is determined by the obvious relation

$$\delta\varepsilon_n = a |\nabla U|_{r=R_n} = \gamma_n z |\bar{\Delta}_n|, \quad \gamma_n > 1. \tag{3.4}$$

It follows immediately that [see (2.4)]

$$(R_n/R_{00})^3 \approx (\Delta_0/\bar{\Delta}_n)^{3/(\alpha+1)} \gg 1. \tag{3.5}$$

The reason for the condition $m \geqslant n$ here is that smaller clusters could in principle leave a region with a level shift on the order of $\delta\varepsilon_n$.

At $x > 2x_{00}$ more than 80% of the particles are in clusters with $n \geqslant 3$. It is easy to see that the probability that a sphere of radius R_3 will not contain at least one of these particles is very small. It follows immediately that the overwhelming majority of the trios will actually be immobile. The label of immobility can be applied even more safely to clusters with $n > 3$. Estimates show that in this concentration interval the overwhelming majority of the duos will also be immobile. In practice this means that at these concentrations there is an infinite immobile cluster of a new type, for which the relative motion of the constituent clusters with $n \geqslant 3$ is suppressed at a lower density. An infinite cluster of this type actually arises even at a substantially lower concentration x_∞, as can be seen by examining the subsystem of trios alone. Ignoring the dimensions of these trios in comparison with R_3, introducing the trio concentration $\tilde{x}^{(3)} = \tilde{N}^{(3)}/N_0$, and working by analogy with (2.10) and (2.11), we find the value of $\tilde{x}_\infty^{(3)}$ at which an infinite cluster of trios appears:

$$\tilde{x}_\infty^{(3)} = \zeta_3 x_{00}^{(3)}, \quad x_{00}^{(3)} = (a_0/R_3)^3. \tag{3.6}$$

Substituting expressions (2.14) and (3.5) into (3.6) we find an equation for the particle concentration $x_\infty^{(3)}$ (the concentration of particles, not clusters):

$$\begin{gathered} {}^1/_6 t^3 e^{-t} F_2(t) = A_3, \\ t = x_\infty^{(3)}/x_{00}, \quad A_3 = \zeta_3 (\gamma_3 \bar{\Delta}_3/\gamma\Delta_0)^{3/(\alpha+1)}. \end{gathered} \tag{3.7}$$

Solving Eq. (3.7) for realistic parameter values and for $\alpha = 3$–4, we find $x_\infty^{(3)} \approx 0.5 x_{00}$. Clearly, the actual value of x_∞ could only be smaller than $x_\infty^{(3)}$, although it certainly looks like the two are fairly close.

At $x \approx x_c$ a substantial fraction of the particles thus belong to an infinite immobile cluster of more complicated structure. Estimates show that at this concentration a substantial fraction of the duos are also immobile. Only the loners actually remain mobile. We wish to emphasize that the interaction of the loners with a cluster of this sort is purely elastic, as can be seen from the arguments in the preceding section, which would be even stronger here because the average level shift for the particles of the constituent clusters would be even greater than $\delta\varepsilon_{00}$.

The critical concentration x_c and the value of x_∞ are significantly different. The localization actually occurs in a region in which the density of the infinite immobile cluster is high. At concentrations $x_\infty < x < x_c$, where the two subsystems of particles coexist, the macroscopic diffusion coefficient can be written

$$D(x) = D_*(x) Q(x). \tag{3.8}$$

Where $D_*(x)$ is the local diffusion coefficient. The factor $Q(x)$, associated with long-range correlations, is given near x_c by

$$Q(x) \sim \left(\frac{x_c - x}{x_c}\right)^\sigma. \tag{3.9}$$

In deriving these results we have tacitly assumed temperatures

$$T > T_* \equiv U(x_c). \tag{3.10}$$

Increasing the temperature further would not change the size of the free volume, so that under condition (3.10) the concentration x_c and the nature of the critical behavior do not depend on the temperature (at least as long as the interaction with the phonons has not come into play).

To analyze the nature of the localization and the critical behavior of D near x_c, we begin with a problem of independent interest: diffusion in a crystal with static impurities. For definiteness we assume that the interaction of the particles with the impurities is again described by law (2.2). Examining the single-particle problem in the absence of any inelastic scattering mechanisms, we can determine the equivalent radius (R_0) for the interaction of the particle with an impurity from the condition

$$U(R_0) = \Delta. \tag{3.11}$$

For a narrow band we would have $R_0 \gg a$. According to the classical theory of percolation, diffusion to infinity disappears at a certain degree of overlap of the spheres of radius R_0, which are actually regions inaccessible to particles (excluded volumes). The corresponding critical concentration x_c^{im} is determined by the scale length x_0 associated with the radius R_0:

$$x_c^{im} = \eta x_0, \quad x_0 = (a/R_0)^3. \tag{3.12}$$

At a lower concentration, however, a quantum localization should set in. Far from the localization point, the quantum correction to the diffusion coefficient, δD, can be estimated by determining the fraction of particles which return as a result of rescattering to a volume of radius λ (the wavelength) around the point which these particles left at the time $t = 0$ (see Ref. 13, for example). It is a simple matter to directly show that

$$\delta D/D \sim -\lambda^2/l_0^2, \tag{3.13}$$

where l_0 is the mean free path of the particles. In the region $x^{im} \sim x_0$ we have $l_0 \sim R_0$; also using $\lambda \sim a$, we find

$$|\delta D|/D \ll 1.$$

It follows from (3.13) that in terms of the local diffusion coefficient the quantum localization condition $|\delta D|/D \sim 1$ is satisfied at $l_0 \sim a$. This condition becomes satisfied at $x^{im} \sim x_{00} > x_0$, x_c^{im} [see (2.11) and (2.4)]. Actually, as x_c^{im} is approached, the decrease in the number of effective paths for long-range diffusion effectively increases the scattering, which is accompanied by a return to the original region. This behavior increases the quantum interference effects in a determination of the macrosopic coefficient D, although the quantum corrections to the local diffusion coefficient remain negligibly small.

Within x_c^{im} the correlation length and the diffusion coefficient D can be written

$$L_c \approx R_0 \left(\frac{x_c^{im}}{x_c^{im} - x^{im}}\right)^\nu, \quad D = D_*^{im} \left(\frac{x_c^{im} - x^{im}}{x_c^{im}}\right)^t. \tag{3.14}$$

The critical indices in (3.14) correspond to classical localization and in the 3-D case have values $\nu \approx 0.8$–0.9 and $t \approx 1.6$–1.7. (see Ref. 2, for example). Over scale lengths smaller than L_c the diffusion is rapid, with a coefficient on the order of D_*^{im}. Consequently, in a volume on the order of L_c^3 around the point which the particles left at $t = 0$ a uniform distribution with a density on the order of L_c^{-3} is established; this distribution slowly dissipates at the diffusion coefficient D given by (3.14). The scale time for the density decay, t', is found from $t' \sim L_c^2/D$.. Over this time, a particle flux density v_g/L_c^3 (v_g is the group velocity) crosses the spherical surface $\sim\lambda^2$, and the fraction of particles which return to the vicinity of the initial point is given in order of magnitude by

$$\lambda^2 (v_g/L_c^3)\, t' \approx v_g \lambda^2 / L_c D\ .$$

This value determines the relative quantum correction to the macroscopic diffusion coefficient describing transport over distances large in comparison with L_c. Working from (3.14) and the fact $D_*^{im} \approx v_g R_0$, we find

$$|\delta D| D \sim \left(\frac{\lambda}{R_0}\right)^2 \left(\frac{x_c^{im}}{x_c^{im} - x^{im}}\right)^{t-\nu}. \tag{3.15}$$

It follows from (3.15) that the transition to the quantum localization regime occurs only after a very pronounced decrease in D in accordance with the classical law (3.14), in the immediate vicinity of x_c^{im} [the corresponding impurity concentration x_q can easily be estimated by equating (3.15) to 1; the critical concentration corresponding to quantum localization lies very close to this transition concentration]. A corresponding result has been derived by Khmel'nitskiĭ[14] in an analysis of another problem.

We thus see that in the case of extremely narrow bands the critical exponents over by far the greatest part of the critical region correspond to the classical percolation problem; only in a very narrow concentration interval near the transition point do the critical indices take on the values characteristic of the quantum localization problem. We might point out that these results are based on the assumption of a purely elastic scattering by defects and may apply to both a monochromatic distribution in energy and a uniform distribution of particles over the bandwidth. Even a comparatively slight inelastic scattering, with a scale time $\tau_{\text{inel}} < t'$, however, will disrupt the quantum correlations, and the behavior $D(x)$ will be determined at all x^{im} by the classical correlation problem.

If there is no interaction with phonons, and the inelastic scattering of particles with each other is important, so that the corresponding mean free path becomes comparable to l_0, the situation may change considerably. In a model in which the impurities are impenetrable spheres of radius R_0, the value of x_c^{im} and the critical behavior in (3.14) remain in force; only the coefficient D_*^{im} changes. If the interaction with impurities is instead a power law (2.2), the energy exchange during inelastic scattering of particles with each other will allow the particles to penetrate into the region $r < R_0$ near an impurity. Since the energy which is exchanged cannot exceed Δ, however, a region $r < R_{00}$ is now inaccessible, where R_{00} is determined by an expression analogous to (2.4). The entire region outside the spheres of radius R_{00}, on the other hand, is kinetically accessible, at least at $T > U(x^{im})$. The substantial increase in the free volume at $x^{im} \sim x_0$ causes delocalization in this concentration region. Now a localization of a new type occurs, at a substantially higher concentration $x_c^{im} \sim x_{00}$ [see (2.11)]. This concentration corresponds to overlapping spheres of radius R_{00}. The critical behavior of the diffusion coefficient here corresponds to the classical percolation problem, and the kinetic nature of the development of the free volume affects only the value of D_*. The position of the new critical point does not depend on T if inequality (3.10) holds.

We can now easily explain the situation which prevails in a crystal without static impurities. At a particle concentration $x \sim x_0$, a transition occurs from a gaseous region to a quasiliquid region (with an interaction on the order of Δ), without any manifestations of localization, of course. The quasiliquid region persists up to $x = x_\infty$, beyond which, as we have already mentioned, an infinite immobile cluster appears in the system and serves as a static defect structure. The strong interaction between the immobile particles at $x > x_\infty \sim x_{00}$ makes the entire kinetically accessible region free for these particles. At $x \approx x_c$, although the density of the immobile cluster is high, the concentration of mobile loners is still significant, and inelastic processes continue to play a governing role in the mobile subsystem. As a consequence, the point x_c is a critical point of the second kind, and the critical index σ in (3.9) must have a value close to that of the index characteristic of classical localization. Generally speaking, we cannot rule out that there will be some small difference between these indices in this case, because the distribution of particles in an infinite cluster will have some correlation, in contrast with the completely random distribution of static defects.

As x changes, there are simultaneous changes in the concentrations of the immobile and mobile subsystems. The only critical change, however, is that in the concentration of the immobile subsystem: The change in the concentration of nearly mobile particles leads to only a change in the local diffusion coefficient, and this change is insensitive to the critical point.

4. TEMPERATURE AND CONCENTRATION DEPENDENCE OF THE DIFFUSION COEFFICIENT; ROLE OF THE INTERACTION WITH PHONONS

We first consider the concentration dependence of D over the broad interval $x < x_c$ in the absence of an interaction with phonons. At $x < x_0$, the motion of the particles is a band motion. The clearly pronounced umklapp processes ($T > \Delta$) cause the rate at which particles collide with each other, $\Omega_p(x)$, to be essentially the same as the rate of collisions with defects. In this case the diffusion coefficient is given by[5,6]

$$D(x) = {}^1/_3 z a^2 \Delta_0^2 / \Omega_p(x), \tag{4.1}$$

where

$$\Omega_p(x) \approx (a_0 \Delta)(x/a_0^3)\sigma_{eff}, \quad \sigma_{eff} \approx \pi R_0^2. \tag{4.2}$$

The value of R_0 in this expression is given by (3.11)

At $x > x_0$ the concentration dependence of the diffusion coefficient changes, because of the transition of the system of interacting particles in the crystal to a quasiliquid regime. This transition can be seen simply from the circumstance that at these concentrations an individual particle is localized in the instantaneous potential relief created by the surrounding particles. The corresponding linear dimension (l) of the virtual localization region can be found from the condition for a shift of the band by an amount on the order of its width:

$$l |\nabla U|_{r=\bar{r}} \approx \Delta, \quad \bar{r} = a_0 x^{-1/3}. \tag{4.3}$$

Using (2.2), (3.11), and (3.12), we find

$$l \approx \alpha^{-1} a_0 x^{-1/3} (x_0/x)^{\alpha/3} \approx a_0 (x_{00}/x)^{(\alpha+1)/3}. \tag{4.4}$$

At $x \gg x_0$ the size of the region in which the particles are localized becomes small in comparison with the average distance between particles, $\bar{r}$.

When two particles interact, each can go into one of the quasilocalized states whose wave functions are nonzero in a volume of radius l. It is not difficult to see that the number of such states is $\sim (l/a)^3$. The matrix element of this transition, which is determined by interaction (2.17), is given by the following expression for particles separated by a distance r:

$$V(r) \approx \alpha(\alpha+1) U_0 (a_0/r)^{\alpha+2} (l_1/a)(l_2/a) I_1 I_2, \tag{4.5}$$

where I_s is the overlap integral corresponding to the sth particle.

As long as the condition $l/a \gg 1$ holds, the number of final states (in an energy interval $\sim \Delta$) is so large, and the distance (ω) between levels so small, that the following condition holds:

$$V(\bar{r})/\omega \gg 1. \tag{4.6}$$

As a result, the interaction with the surrounding particles prevents a state from forming. The energy spectrum essentially becomes a continuum, and the motion of the particles and the exchange of energy in the course of their interactions become classical. Here we have a self-consistent dynamic picture in which a particle is moving in a fluctuating external potential relief.

An individual particle moves a distance on the order of l in a time τ determined by quasiband motion:

$$\tau \approx l/v_g, \quad v_g \approx a\Delta_0. \tag{4.7}$$

It is easy to show that this time is also the scale time for a change in the potential at the given point and thus for a shift of the band by an amount on the order of (we wish to stress this point) Δ. As a result, the effective diffusion coefficient in this unusual liquid is given approximately by

$$D(x) \approx {}^1/_3 l^2/\tau \approx {}^1/_3 z a^2 \Delta_0^2/\Omega_p'(x), \tag{4.8}$$

where

$$\Omega_p'(x) \approx \delta\varepsilon(x) = a|\nabla U|_{r=\bar{r}}. \tag{4.9}$$

At $x \approx x_0$ the rate $\Omega_p'(x)$ is equal within a numerical coefficient to $\Omega_p(x)$ in (4.2).

It follows from (4.8) and (4.9) that at $x \approx x_0$ the diffusion coefficient undergoes a change in concentration dependence from $D \propto x^{-1}$ [see (4.1) and (4.2)] to

$$D \infty x^{-(\alpha+1)/3}. \tag{4.10}$$

The possible appearance of a functional dependence of this type in the case of an interaction through a strain field ($\alpha = 3$) was discussed in Refs. 15 and 16.

In principle, this analysis applies at concentrations up to $x = x_\infty$. At $x > x_\infty$, the diffusion inolves only the particles of the mobile subsystem [the concentration of loners is $x_1(x) < x$], which are now in the irregular static potential field created by the infinite immobile cluster. As long as the concentration of the mobile subsystem is relatively large or comparable in magnitude to that of the immobile subsystem, $x_2 (x_2 = x - x_1)$, the local diffusion coefficient retains the structure in (4.8). It is useful to note here that an analysis of energy diffusion in a static potential relief leads to an expression similar to (4.8). Noting that the particles exchange an energy on the order of Δ in an inelastic collision, we find that the time required to cross an energy interval on the order of $U(x_2)$ is

$$t \approx U^2(x_2)\tau(x_1)/\Delta^2.$$

Here the particle traverses the scale dimension of the potential relief, $\bar{r}$, so that we have

$$D \infty \bar{r}^2/t.$$

It is not difficult to see that when we use (4.3) this expression becomes literally identical to (4.8) at $x_1 \sim x_2$,

When x_1 decreases greatly, inelastic exchange in the mobile subsystem is hindered, and the corresponding value of $\tau(x_1)$ begins to increase rapidly from the value in (4.7). Near the localization point, however, the relative concentration of mobile particles, $x_1(x_c)$, is still significant, and expression (4.8) can be used to find D_* in (3.5) approximately. The actual concentration in this region will of course be determined by the function $Q(x)$.

A point deserving special note is that the interval (x_0, x_{00}) may prove extremely narrow in a real situation. This is generally true if $\alpha \gg 1$ (in the problem of impenetrable spheres we have $x_0 = x_{00}$). However, even at $\alpha = 3$, a typical value for an interaction through a strain field, x_0 and x_{00} are approximately equal if the ratio Δ / U_0 is not small enough. This situation occurs, in particular, in the diffusion of He^3 through a crystalline He^4 host. In this case, concentration dependence (4.1) may give way to the critical behavior (3.8) without any explicit manifestation of the behavior determined by relation (4.10).

Here we have an important comment. As the concentration x_{00} is approached, the ratio l/a decreases, reaching values on the order of unity. At the same time, ω increases, ultimately reaching values on the order of Δ_0. Transition matrix element (4.5) in this case is given approximately by $(I_1, I_2 \sim 1)$

$$V \approx (\alpha+1)\gamma_z x_{00}^{-1/3}(x_1/x_{00})^{(\alpha+2)/3}\Delta_0.$$

The condition $V/\omega > 1$ imposes certain conditions on the parameters in this region. The arguments above regarding the value of the local diffusion coefficient in the concentration interval (x_∞, x_c) implicitly assumed that these conditions hold.

We note in this connection that in our analysis of the kinetics we have used a qualitative picture which would correspond to an effective partitioning of the volume into a "black" region (associated with the immobile cluster) and a "white" region (kinetically accessible to the loners). We cannot rule out the possibility, however, that there may be a "gray" region near spheres of radius R_{00} around particles belonging to a cluster. The nature of the particle motion in a gray region may be sensitive to the value of V. It is not difficult to see that if such a region does exist it will not cause any fundamental changes in the qualitative structure of the results, although it may reduce the value of x_c. In the opposite limit, $V/\omega \ll 1$, however, the volume of the gray region may become large; this case requires special study.

In the entire analysis above we have assumed $T > U(x)$. Under this condition all the characteristic configurations are equiprobable at $x < x_\infty$. In the opposite limit, $\Delta < T \ll U(x)$, some of the configurations may, in contrast, be improbable. In a state with static impurities we would have obtained an ordinary activation law for the diffusion coefficient:

$$D \infty e^{-\xi U(x)/T}, \quad \xi \sim 1.$$

In our case, although the potential relief for an individual particle is not fixed, the contraction of the number of effective paths associated with the decrease in the number of allowed configurations as the temperature is reduced leads to a similar activation-law behavior:

$$D = D'(x)e^{-\eta U(x)/T}. \tag{4.11}$$

The coefficient η in this expression is clearly smaller than ξ because of the lability of the system, which effectively reduces the effective barrier height. The same behavior is found for $D_*(x)$ in the interval (x_∞, x_c), with a coefficient between ξ and η in the exponential function in (4.11).

At $x > x_c$ the diffusion coefficient is nonzero only to the extent that there is an interaction with phonons. As has been shown in previous work,[4,6] the dynamic fluctuations in the relative positions of the levels in the adjacent cells under the influence of the interaction with phonons give rise to a delocalization of the particles. This is true of all the particles, including those belonging to the immobile cluster. At this point the particles begin to move, remaining in the infinite cluster or undergoing a transition to a free volume, which is bounded under these conditions. On the other hand, particles from the free volume may combine with the infinite cluster. A snapshot of the situation will look statistically as before, with a change over time in the configuration of the cluster in absolute space.

A fundamental kinetic characteristic of the interaction with phonons is the decay frequency of the density-matrix elements which are nondiagonal in the site index, $\Omega_{\text{ph}}(T)$; this frequency is also a measure of the relative fluctuations of the levels in the adjacent wells.[4–6] A particle which is a member of a cluster hops to an adjacent cell as a result of the interaction with phonons with a probability given at $T > U(x)$ by[4,6]

$$W_{r,r+g} = \frac{2\Delta_0^2 \Omega_{ph}(T)}{(\varepsilon_{r,r+g})^2 + \Omega_{ph}^2(T)}. \tag{4.12}$$

Here $\varepsilon_{r,r+g}$ is the relative shift of the energy levels in the neighboring cells. In order to determine the contribution of the cluster particles to the macroscopic diffusion, we need a definite procedure for averaging (4.12) over the distribution of level shifts.

If $\Omega_{\text{ph}}(T) \ll |\varepsilon_{r,r+g}|$, this averaging will not depend on T and will lead to the replacement of $\varepsilon_{r,r+g}$ by an effective value

$$\delta\varepsilon_*(x) = \beta U_0 x^{(\alpha+1)/3}, \tag{4.13}$$

where only the numerical factor β depends on the nature of the averaging.

Particles which do not belong to the immobile cluster and which remain small in general as x increases may undergo displacements over distances of order $\bar{r}$ only by overcoming, by virtue of the interaction with phonons, regions with a relative shift greater than Δ, in which the kinetics of the hops is governed by (4.12). Consequently, the contributon of these particles to the long-range diffusion effectively causes a redefinition of β in (4.13), and the general expression for the total macroscopic diffusion coefficient becomes

$$D \approx {}^1/_3 z a^2 \Delta_0^2 \Omega_{ph}(T) / [\delta\varepsilon_*(x)]^2. \tag{4.14}$$

In the opposite case, $\Omega_{\text{ph}} \gg |\varepsilon_{r,r+g}|$, probability (4.12) is completely independent of the static shifts; everything is determined exclusively by the dynamic level shift, and we have

$$D \approx {}^1/_3 z a^2 \Delta_0^2 / \Omega_{ph}(T). \tag{4.15}$$

In either case, the temperature dependence of the diffusion coefficient is universal, independent of the particular features of the potential relief. If $\Delta \ll \Theta_D$ (Θ_D is the Debye temperature), two-phonon processes are governing, and at $T \ll \Theta_D$ we have

$$\Omega_{ph}(T) \propto T^9. \tag{4.16}$$

In metals at low temperatures, dynamic fluctuations due to interactions with electrons may be predominant. In this case we would have

$$\Omega_{ph}(T) \to \Omega_{el}(T) \propto T.$$

If $\Omega_{\text{ph}}(T)$ and the characteristic shifts are comparable in magnitude, the result of the averaging depends on T. For the behavior in (4.16), however, the intermediate temperature interval is narrow, and we can write the following general expression for the diffusion coefficient:

$$D_1 \approx \frac{1}{3} z a^2 \Delta_0^2 \frac{\Omega_{ph}(T)}{[\delta\varepsilon_*(x)]^2 + \Omega_{ph}^2(T)}, \tag{4.17}$$

with the value of β found in the temperature interval in which (4.14) holds.

We turn now to the effect of the interaction with phonons on the diffusion coefficient in the region $x < x_c$. At $x < x_\infty$ the existence of an additional mechanism for the scattering of particles by phonons leads to changes in the expressions for D in (4.1) and (4.8) (see Refs. 5 and 6):

$$D_0 \approx \frac{1}{3} z a^2 \Delta_0^2 \frac{1}{\Omega_p(x) + \Omega_{ph}(T)}. \tag{4.18}$$

At $x_\infty < x < x_c$ the particles belonging to the infinite cluster, whose density remains constant over time, diffuse in accordance with (4.17). Among the particles which do not belong to the infinite cluster, only that fraction $\xi(x)$ which are on infinite percolation paths participates in the development of a large-scale diffusion. We thus have $Q(x) \approx \xi(x) x_1/x$ in (3.5), and the critical behavior is related to $\xi(x) \propto (x_c - x)^\sigma$. The other "free" particles, with a concentration $x_1(1-\xi)$, are on dead-end paths and participate in the large-scale diffusion only by overcoming the regions with a scale shift exceeding Δ by virtue of the interaction with phonons. In this sense the behavior of these particles is analogous to that of the particles of the immobile subsystem at $x > x_c$, but for the same reasons these particles are described by a diffusion coefficient approximately the same as that in (4.17), along with the particles which belong to the infinite cluster. The relative number of these free particles is

$$x_1(1-\xi)/x + (x - x_1)/x = 1 - \xi x_1/x.$$

As a result we can describe the diffusion coefficient at $x > x_\infty$ by an approximate expression similar to that introduced in Ref. 6:

$$D(x, T) = D_0(x, T) Q(x) + D_1(x, T) [1 - Q(x)]. \tag{4.19}$$

This expression actually applies to the entire x and T ranges, giving the correct values at $x < x_\infty$ $[Q(x) \to 1]$ and at $x > x_c$ $[Q(x) = 0]$.

5. CONCLUDING REMARKS

The results found in the preceding sections have been based on the particular particle interaction potential in (2.2), which corresponds to a repulsion, but many of these results are independent of the sign of the interaction. For the formation of an immobile cluster, for example, as for the motion of the particles at $x \sim x_{00}$, what is important is not the values of the potential energy but the level shifts in neighboring cells. As is easily seen, these shifts change sign as the cells in the first coordination sphere adjust, so that the sensitivity to the sign of the interaction itself is lost. In the absence of an interaction with phonons, the particles cannot diffuse into a region in which the shifts exceed Δ. Consequently, under inequality (3.10) the kinetics is the same for the cases of attraction and repulsion. When the interaction with phonons is turned on, however, and there is an attraction, the temperature T must be higher than the depth of the potential well for the binary interaction if the results derived above are to be valid. In the opposite case, a stratification of phases or at least a formation of droplets will occur in the system.

In the case of narrow bands we are always interested in low concentrations and thus the interparticle interaction which falls off most slowly. In a crystal this interaction would usually be the coupling of particles through the strain field, which falls off as r^{-3}. This interaction changes sign as a function of the angle, so that the applicability of the results in this case depends on the satisfaction of the same conditions as for an attractive potential. It should be noted that, by itself, an anisotropy of the interaction which would complicate the geometry of the surrounding volumes on whose basis the clusters are constructed would cause no fundamental changes. The important point is the way in which the modulus of the interaction changes over distance. For estimates we can therefore use the results found for $\alpha = 3$.

In this light it is easy to see that an exceptionally good system for a study of this phenomenon would be a system of interacting He^3 atoms which are diffusing through a crystalline He^4 host. Not only is the band narrow ($\Delta \sim 10^{-4}$ K; Refs. 8 and 9), but also the interaction between the diffusing particles is weak, even when separated by atomic distances ($U_0 \sim 10^{-2}$ K; Ref. 17). On the one hand, the concentration x_{00} is on the order of a few percent in this case, and the condition $x_c \ll 1$ holds, while on the other we have not only $T \gg U(x)$ but also $T \gg U_0$ at very low temperatures. Since it is through a strain field that the He^3 atoms interact with each other, the latter inequality means that the picture will be insensitive to the changes in the sign of this interaction with direction in the crystal, and to the fact that all possible configurations of the diffusing particles will be statistically equiprobable. At concentrations $x \sim x_{00}$, temperatures $T > 0.1$ K are sufficient to prevent stratification. At such temperatures, however, the interaction with phonons (a two-phonon interaction) is still quite weak, so that experiments could reveal the localization pattern to its full extent.

Another important circumstance, found clearly even in the early experiments (see Refs. 18 and 19, for example; see also Refs. 9 and 20), is that the motion of He^3 atoms at a low concentration is a band motion, and despite the small value of Δ the mean free path is determined not by defects but by collisions of particles with each other. These comments apply even more strongly at a high particle concentration. Consequently, in this case we are actually dealing with a system of interacting particles which are diffusing in an essentially ideal crystal.

All these circumstances, taken together, show that it is possible to experimentally detect localization in this system, as was first done by Mikheev *et al.*[10–12] Interestingly, Mikheev *et al.*[11,12] reported that the particular way in which the diffusion coefficient falls off with concentration is approximately as predicted by the classical percolation theory, which corresponds to the results of Section. 3. A point very important for the analysis of the overall picture is the observation in these studies of a phonon-induced delocalization of the particles, with the clearly defined nontrivial temperature dependence in (4.17). This comment applies to that concentration interval in which the scale length for the critical decrease in D is large, so that most of the particles are either in the immobile cluster or on nonpercolation paths (Section 4). The temperature dependence of D was studied over a broad range of x, spanning both the region of purely band motion and the region of a pronounced critical decrease in D. The results found agree well with the theoretical values predicted by a relation of the type in (4.19) over the entire plane of parameters. We might note that for the parameter values of this system we would typically have $x_0 \sim x_{00}$, so that the concentration dependence of the diffusion coefficient in (4.2) probably converts directly into the critical dependence, skipping the region in which (4.10) holds. This would be why interpolation relation (4.19) with Ω_p from (4.2), as proposed in Refs. 6 and 7, has not proved adequate for describing all the results.

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