Quantum diffusion in deformed crystals

G. E. Gurgenishvili, A. A. Nersesyan, and G. A. Kharadze

Physics Institute, Georgian Academy of Sciences
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We consider the character of quantum transport of light nuclei in a deformed lattice. It is shown that the diffusion coefficient should exhibit a nonmonotonic behavior at low temperatures.

Interest in low-temperature mobility (quantum diffusion) of light atoms in solids has noticeably increased of late. Suitable objects for the observation of the quantum character of the transport of matter at low temperatures are impurity He^3 atoms in solid He^4, and also impurity hydrogen atoms introduced into a crystal lattice. There already exist reliable data (obtained with the aid of pulsed NMR methods) indicating that at 1 °K the mobility of He^3 in solid He^4 has essentially a quantum character.[1,2]

The general laws governing the temperature variation of the diffusion coefficient D on going from the classical regime to the quantum regime are described in[3]. At low temperatures, where above-the-barrier processes are suppressed, an important role is assumed by tunnel transitions with participation of a small number of phonons, and the exponential temperature dependence of D is replaced by a power law. In the extreme low-temperature regime, the coherent character of the motion of impurity atoms will predominate, and D should increase in this region with decreasing temperature.

In the presence of a noticeable amount of impurities, the growth of D with decreasing temperature is limited by the effects of scattering of impuritons by one another. As a result, a low-temperature plateau appears on the plot of $D = D(T)$.

In the present paper we wish to point out that in a deformed lattice containing an extremely small amount of light impurities, the diffusion coefficient should exhibit in the low-temperature coherent regime a nonmonotonic behavior: Growth of D will slow down gradually with decreasing temperature and, after passing through a maximum, the diffusion coefficient begins to decrease with further decrease of temperature.

To demonstrate the character of the low-temperature mobility of the impurity in a deformed crystal, we start from the following general expression for the diffusion coefficient (we consider for simplicity the one-dimensional problem):

$$D = {}^1/_2 \lim_{t\to\infty} \sum_n x_n^2 \dot{\rho}_{nn}(t), \tag{1}$$

where x_n are the coordinates of the equilibrium positions of the impurity, and $\rho_{nn'}(t)$ is the single-particle density matrix in the node representation. The equation of motion for $\rho(t)$ can be represented in the form

$$\dot{\rho}_{nn'}(t) + i[\mathcal{H};\rho(t)]_{nn'} = -\{(1-\delta_{nn'})\Gamma_{nn'}\rho_{nn'} + \delta_{nn'}\sum_{n''}\gamma_{nn''}(\rho_{nn}-\rho_{n''n''})\}. \tag{2}$$

Here $\mathcal{H}$ is the Hamiltonian that specifies the behavior of the impurity in a rigid lattice, and the right-hand (collision) part describes the damping effects due to the interaction with the phonons. An equation similar to (2) was recently used to describe the motion of particles in narrow bands.[5,6]

The Hamiltonian $\mathcal{H}$ can be written in the node representation in the form

$$\mathcal{H} = \sum_n \epsilon_n c_n^+ c_n + \sum_{nn'} h_{nn'} c_n^+ c_{n'}, \tag{3}$$

where ϵ_n is the energy of the ground state of the impurity localized in the n-th site, and the matrix element $a_{nn'}$ describes the corresponding tunnel transitions. We consider below the simplest case of deformation, when an homogeneous collapse of the local levels takes place, i.e., $\epsilon_{n+1} - \epsilon_n = \Delta$. In this situation, starting from (2), it is easy to obtain an expression for the rms displacement of the diffusing particle $\overline{x^2(t)} = \sum_n x_n^2 \rho_{nn}(t)$. Solving the corresponding system of equations with initial condition $\rho_{nn'}(0) = \delta_{n0}\delta_{n'0}$, we can show that

$$\overline{x^2(t)} = 2a^2\left\{\left(\frac{2h^2}{\Gamma^2+\Delta^2}\Gamma + \gamma\right)t + \frac{2h^2}{\Gamma^2+\Delta^2}\left(e^{-\Gamma t} - 1\right) + \frac{2h^2\Delta^2}{(\Gamma^2+\Delta^2)^2}\left(1 - \cos(\Delta t)e^{-\Gamma t}\right) - \frac{2h^2\Gamma\Delta}{(\Gamma^2+\Delta^2)^2}\sin(\Delta t)\, e^{-\Gamma t}\right\}. \tag{4}$$

Using the result (4), it is easy to verify that in the case of a homogeneous collapse of the local levels, the diffusion coefficient is

$$D = a^2\left(\frac{2h^2}{\Gamma^2+\Delta^2}\Gamma + \gamma\right) = D_{coh} + D_{in\,coh}. \tag{5}$$

The physical meaning of this formula is quite clear. At sufficiently low temperatures ($\Gamma \ll \Delta$) the coherent transport is suppressed because of the tendency to impurity localization (effect of collapse of local levels). Raising the temperature leads to a gradual "unfreezing" of the blocked impurities, and D_{coh} increases initially. At $\Gamma \approx \Delta$, a more favorable regime sets in for coherent diffusion. With further rise of temperatures (in the region $\Gamma > \Delta$), the value of D_{coh} begins to decrease, since scattering processes that limit the coherent motion become effective. Thus, in a deformed lattice with collapsed levels one should expect the presence of a low-temperature maximum (in the region $\Gamma \approx \Delta$) on the plot of $D = D(T)$. Of course, such a picture can be observed in case of sufficiently low impurity densities, when their mutual scattering does not mask the temperature dependence of D.

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