Comment on "Universal Decoherence in Solids"

In a recent Letter [1], Chudnovsky studied the oscillations of a quantum particle in the double-well potential coupled to a solid. He derived the universal lower bound on the decoherence due to phonons for the case that the oscillation frequency ω_0 is small compared to the Debye frequency ω_D . In this Comment, we show that his formula for the decoherence rate Γ has a limited range of validity and is not applicable to evaluation of the width of a low-energy optical mode considered in Ref. [1] as an example. This is due to unjustified use of the Fermi golden rule for calculation of Γ . We present a more general expression for the probability of the phonon-induced transition. For clarity, we restrict ourselves to the case of zero temperature and assume isotropic acoustic phonons with the linear dispersion law $\omega_{\mathbf{k}\lambda} = ck$, where **k** is the wave vector, λ is the polarization, and c is the speed of

To calculate the decoherence rate for the case of a symmetric double-well potential $U(\mathbf{R})$, Chudnovsky makes use of the Fermi golden rule and obtains

$$\Gamma = \frac{\pi m^2 X_0^2 \omega_0^2}{3\hbar \rho V} \sum_{\mathbf{k},\lambda} \omega_{\mathbf{k}\lambda} \delta(\omega_{\mathbf{k}\lambda} - \omega_0) = \frac{m^2 X_0^2 \omega_0^5}{2\pi \hbar \rho c^3}, \quad (1)$$

where m is the particle mass, X_0 is the half of the distance between the degenerate minima of $U(\mathbf{R})$, ρ is the density of the crystal, and V is the normalizing volume. The value of $\hbar\omega_0$ equals the gap between the ground and the first excited state of the particle. Let us recall that Eq. (1) follows from the approximation [2]

$$W_{if}(\omega, t) = |F_{if}|^2 \frac{4\sin^2(\frac{\omega - \omega_0}{2}t)}{\hbar^2(\omega - \omega_0)^2}$$
$$\approx \frac{2\pi}{\hbar} |F_{if}|^2 \delta(\hbar\omega - \hbar\omega_0)t \tag{2}$$

for the probability $W_{if}(\omega,t)$ to find a particle in the state $|f\rangle$ at a time t if it is in the state $|i\rangle$ at t=0 and interacts with the harmonic field $\hat{V}(t)=\hat{F}e^{-i\omega t}+\text{H.c.}$ Here $\hbar\omega_0=E_i-E_f$. The approximation (2) for $W_{if}(\omega,t)$ results from the first-order perturbation theory and is valid if (i) $W_{if}(\omega,t)\ll 1$ and (ii) the time t is sufficiently long, so that one can make use of the relation [2] $\sin^2(\varepsilon t)/\pi t \varepsilon^2 \approx \delta(\varepsilon)$.

If the harmonic field $\hat{V}(t)$ is associated with a phonon having the frequency $\omega_{\mathbf{k}\lambda}$, then, taking into account that the displacements produced by the phonons with different wave vectors are not correlated, one has for the total transition probability

$$W_{if}(t) = \frac{4}{\hbar^2} \sum_{\mathbf{k}, \lambda} |F_{if}(\mathbf{k}, \lambda)|^2 \frac{\sin^2(\frac{\omega_{\mathbf{k}\lambda} - \omega_0}{2} t)}{(\omega_{\mathbf{k}\lambda} - \omega_0)^2}, \tag{3}$$

where $F_{if}(\mathbf{k}, \lambda)$ is the matrix element for the transition $|i\rangle \rightarrow |f\rangle$ due to the emission of a phonon (\mathbf{k}, λ) . The form

of $F_{if}(\mathbf{k}, \lambda)$ depends on the specific nature of the states $|i\rangle$ and $|f\rangle$. For the problem studied in Ref. [1] it is

$$F_{if}(\mathbf{k},\lambda) = mX_0\omega_0\sqrt{\frac{\hbar\omega_{\mathbf{k}\lambda}}{2\rho V}}e_{\lambda}^{x},\tag{4}$$

where \mathbf{e}_{λ} are the unit polarization vectors. Then, making use of the approximation (2), one has

$$W_{if}^{(1)}(t) \approx \frac{2\pi}{\hbar} \sum_{\mathbf{k},\lambda} |F_{if}(\mathbf{k},\lambda)|^2 \delta(\hbar\omega_{\mathbf{k}\lambda} - \hbar\omega_0)t = \Gamma t, \quad (5)$$

where Γ is given by Eq. (1).

To quantify the applicability of the approximation (5), let us analyze the expression (3) for $W_{if}(t)$. One can roughly distinguish two contributions to $W_{if}(t)$. The first comes from the "resonant component," i.e., from the δ -function-like peak of $\sin^2(\frac{\omega_{\mathbf{k}\lambda}-\omega_0}{2}t)/(\omega_{\mathbf{k}\lambda}-\omega_0)^2$ as a function of k at $k_0=\omega_0/c$, with the height $t^2/4$ and the width $\sim 1/ct$. It leads to Eq. (5). The second is from the "nonresonant background" of the phonon spectrum. At $\omega_0\ll\omega_D$ and $t\gg\omega_D^{-1}$ it is

$$W_{if}^{(2)}(t) \approx \frac{m^2 X_0^2 \omega_0^2 \omega_D^2}{4\pi^2 \hbar \rho c^3}.$$
 (6)

The Fermi golden rule (5) for evaluation of the decoherence rate is justified if $W_{if}^{(2)}(t) \ll W_{if}^{(1)}(t) \ll 1$, i.e., if the resonant component prevails over the nonresonant one, and the transition probability is much less than unity. However, this is not always the case. In the example considered in Ref. [1], where an atom of mass $m \sim 3 \times$ 10^{-23} g oscillates at $\omega_0 \sim 10^{12}$ s⁻¹ in a double well with $X_0 \sim 2 \times 10^{-8}$ cm in a crystal with $\rho \sim 5$ g/cm³ and $c \sim$ 10^5 cm/s, one has $W_{if}^{(2)}(t) \sim 10$ for $\omega_D \sim 5 \times 10^{13}$ s⁻¹; i.e., the standard perturbation theory, in general, and the Fermi golden rule, in particular, break down. Strictly speaking, in this case the notion of a "decoherence rate" is misleading, and one has to make use of other approaches to study the decoherence effects. On the other hand, in the case of electron tunneling, one has $W_{if}^{(2)}(t) \sim$ 3×10^{-4} and $\Gamma \sim 3 \times 10^5 \, \mathrm{s}^{-1}$ for the same set of parameters; i.e., the Fermi golden rule is valid at $t > 10^{-9}$ s.

Finally, it is straightforward to generalize our consideration to include the case of an asymmetric double well and finite temperature.

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