where

$$F(q) = \int_0^{\pi/2} \left(1 - \frac{\sin^2 qs}{q^2 \sin^2 s}\right) \frac{ds}{\sin^2 s},$$

$$\chi_1 = \frac{[x^2+1]^{1/2}}{q} \sin\left[q\left(\frac{\pi}{2} - \tan^{-1} x\right)\right], \quad x = \frac{r}{R}$$

is the solution of the equation

$$\chi'' - U\chi = 0$$

normalized by the condition $\chi_1(\infty) = 1$.

According to Eq. (5), the condition for existence of the level is given by the inequality

$$p(a_0/R)^2 > 3/2. \tag{7}$$

Assuming as in [3] that R is approximately equal to the kinetic theory radius of the particle, and using the tabulated values of polarizability, we find that this inequality is not fulfilled in the case of argon (in agreement with the results of Paul and Saint-Pierre[1] where it is shown that for argon $\sigma_a/\sigma_D = 3$); i.e., the resonance effect is absent in argon. The condition (7), however, is fulfilled for xenon. Therefore we can assume the existence of the resonance effect in xenon.

For all the other molecules investigated by Paul and Saint-Pierre, the inequality (7) is fulfilled; i.e., the resonance effect exists for these molecules. For methane the value of the level given by formula (5) is $\epsilon = 0.05$ eV. Assuming for methane this value of the level, $\epsilon_0 = 0.6$ eV (for $F(q) = 1.5$), the experimental value $\sigma_a/\sigma_D = 20$, $Z_V = 8$, and $E = 0$, we find from (3) the annihilation time τ_a of the bound state in methane: $\tau_a = 3.6 \times 10^{-9}$ sec.

In conclusion it should be noted that a verification of the interpretations suggested would be the observation of elastic scattering of slow positrons ($E \sim 0.1$ eV) in the gases for which the increased annihilation rates have been observed. According to our suggestion, the cross section σ_e of the scattering process should considerably exceed the geometrical cross section of the molecule and should be given by the Wigner formula;

$$\sigma_e = (2\pi\hbar^2/m)/(E + \varepsilon).$$

The weakly bound state of the positron should be easily destroyed in a collision of the positron-molecule ion with another molecule. Therefore the scheme proposed could also be verified by observation of the pressure effect, i.e., the disappearance of the Paul–Saint-Pierre effect on increasing the gas pressure or on dilution by a gas which does not form a bound state with a positron (for example, argon).

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ON THE NATURE OF THE "TAIL" IN THE INCOHERENT INELASTIC SCATTERING CROSS-SECTION OF SLOW NEUTRONS IN CRYSTALS

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1. In investigating the incoherent inelastic scattering cross-section of slow neutrons in crystals a number of authors have observed the differential cross-section to have a noticeable "tail" in a wide region of energy, which without any doubt lies above the upper end of the harmonic-approximation phonon spectrum $\omega_{\max}$. This was established with particular reliability in the case of vanadium by the work of Egelstaff and Turberfield[1], who specifically investigated the temperature dependence of the cross-section in this energy region. At first glance it would seem that "tails" of this kind must be connected with two- or many-phonon processes accompanying the scattering of the neutron from the crystal; however, even the most optimistic estimates (made, in particular, in [1]) show that the calculated values lie well below the experimentally observed values of the cross section. Thus, the question of the origin of the tail in the incoherent inelastic cross-section has remained open.

In this note we show that anharmonic effects in the crystal must necessarily produce a tail in the energy dependence of the cross section. Thus, to all appearances, the observed results are largely connected with anharmonicity.

2. To first order in the ratio of the recoil energy R from an individual nucleus to the characteristic energy ω_0 of the phonon spectrum, the expression for the differential scattering cross-section for scattering from an arbitrary crystal

has the form:

$$\frac{d^2\sigma(\Delta E, \mathbf{x})}{d\varepsilon\,\Delta\Omega} = \frac{m^2 k' \mathbf{x}^2}{8\pi^2\hbar^2 k_0} \frac{1}{N} \sum_j \frac{C_j}{M_j} e^{-W_j}$$

$$\times \sum_{\mathbf{f},\alpha\alpha'} \frac{(\mathbf{q}\mathbf{v}^j(\mathbf{f},\alpha))(\mathbf{q}\mathbf{v}^j(\mathbf{f},\alpha'))}{[\omega(\mathbf{f},\alpha)\,\omega(\mathbf{f},\alpha')]^{1/2}} \frac{\operatorname{Im} G^R_{\mathbf{f},\alpha\alpha'}(\Delta E)}{e^{-\beta\Delta E} - 1},$$

$$C_j = \frac{1}{4}\overline{K_j(K_j+1)B_j^2} + \overline{(A_j^2)} - (\overline{A}_j)^2, \tag{1}$$

where $G^R_{\mathbf{f},\alpha\alpha'}(\Delta E)$ is the Fourier component of the retarded Green function corresponding to the operators $A_{\mathbf{f},\alpha}(t)$ and $A_{-\mathbf{f},\alpha'}(t)$ $(A_{\mathbf{f},\alpha} = a_{\mathbf{f},\alpha} + a^+_{-\mathbf{f},\alpha})$. In formula (1) the notation is the following: $\omega(\mathbf{f},\alpha)$ is the frequency of a phonon with wave vector $\mathbf{f}$ and branch index α; $\mathbf{v}_j(\mathbf{f},\alpha)$ is the polarization vector corresponding to the j-th atom in the unit cell (with mass M_j); A_j and B_j are the constants in the expression $v_j(\mathbf{r}) = (A_j\hat{I} + B_j\hat{\mathbf{s}}\cdot\mathbf{K}_j)\times\delta(\mathbf{r} - \mathbf{R}_j)$ for the energy of interaction of the neutron with the j-th nucleus (which has spin $\mathbf{K}_j$); W_j is the Debye-Waller factor for the j-th nucleus in the unit cell; $k_0(k')$ is the wave vector of the neutron before (after) scattering; $\mathbf{x} = \mathbf{k}' - \mathbf{k}_0 = \mathbf{q}x$; $\beta = 1/kT$.

For simplicity we shall only consider a crystal with cubic symmetry and one atom per unit cell. It is easy to show that in this case the only contribution to (1) comes from the Green functions diagonal in the branch indices (i.e., with $\alpha = \alpha'$). In view of the summation in (1) over the whole volume in phase space, the effects of degeneracy are in practice negligible, and we can use for $G^R_{\mathbf{f},\alpha\alpha}$ the usual form of solution (see, e.g., [2,3]). The result is (for $\Delta E > 0$):

$$\frac{d^2\sigma(\Delta E, \mathbf{x})}{d\varepsilon\, d\Omega} = \frac{m^2 k' \mathbf{x}^2}{8\pi^2\hbar^2 k_0 M} C e^{-W} \frac{1}{N} \sum_{\mathbf{f},\alpha} \frac{n(\Delta E)+1}{\omega(\mathbf{f},\alpha)} \frac{(2\omega(\mathbf{f},\alpha))^2\,\Gamma_{\mathbf{f},\alpha\alpha}(\Delta E)}{[\Delta E^2 - \omega^2(\mathbf{f},\alpha) - 2\omega(\mathbf{f},\alpha)\,\Pi_{\mathbf{f},\alpha\alpha}(\Delta E)]^2 + [2\omega(\mathbf{f},\alpha)\,\Gamma_{\mathbf{f},\alpha\alpha}(\Delta E)]^2}. \tag{2}$$

where $\Gamma_{\mathbf{f},\alpha\alpha}$ and $\Pi_{\mathbf{f},\alpha\alpha}$ are respectively the imaginary and real parts of the polarization operator.

If $\Gamma_{\mathbf{f},\alpha\alpha}$ and $\Pi_{\mathbf{f},\alpha\alpha}$ tend to zero, (2) coincides with the usual expression for incoherent one-phonon scattering in a harmonic crystal. In this case the cross section is proportional to the frequency distribution function of the phonon spectrum and has a sharp cut-off at $\Delta E = \omega_{\max}$.

However, if the anharmonicity constant is finite, we are immediately struck by the fact that the cross-section (2) has a tail for $\Delta E > \omega_{\max}$: if we consider only the cubic anharmonic terms, this tail should in principle extend to $2\omega_{\max}$. We can see this directly by using the explicit expression for $\Gamma_{\mathbf{f},\alpha\alpha}(\Delta E)$:

$$\Gamma_{\mathbf{f},\alpha\alpha}(\Delta E) = \frac{\pi}{2\hbar^2} \sum_{\mathbf{f}_1,\alpha_1;\mathbf{f}_2,\alpha_2} |B_{-\mathbf{f}\alpha,\mathbf{f}_1\alpha_1,\mathbf{f}_2\alpha_2}|^2 \{(n_{\mathbf{f}_1\alpha_1} + n_{\mathbf{f}_2\alpha_2} + 1)$$

$$\times [\delta(\Delta E - \omega(\mathbf{f}_1,\alpha_1) - \omega(\mathbf{f}_2,\alpha_2)) - \delta(\Delta E + \omega(\mathbf{f}_1,\alpha_1)$$

$$+ \omega(\mathbf{f}_2,\alpha_2))] + 2(n_{\mathbf{f}_1\alpha_1} - n_{\mathbf{f}_2\alpha_2})\,\delta(\Delta E + \omega(\mathbf{f}_1,\alpha_1)$$

$$- \omega(\mathbf{f}_2,\alpha_2))\}. \tag{3}$$

The scattering cross-section in the region $\Delta E > \omega_{\max}$ is of order

$$\left(\frac{2\omega_0}{\Delta E}\right)^2 \frac{\omega_0}{\Delta E} \frac{\Gamma}{\Delta E} \sim \frac{\Gamma}{\Delta E}$$

relative to its value in the main region of energy. For $T \sim \omega_0$ this ratio may be ~ 10%.

From equations (2) and (3) it follows that in the classical (high-temperature) limit $\Gamma \sim T$ and $d^2\sigma(\Delta E > \omega_{\max})/d\varepsilon d\Omega \sim T^2$. To this extent the cross-section (2) varies with temperature in the same way as that derived by taking two-phonon terms into account. However, it is important to notice that the cross section corresponding to two-phonon processes is proportional to $(R/\omega_0)^2$ and thus contains the parameter (m/M) squared, whereas expression (2) contains only one power of this parameter. Thus in crystals where $m/M \ll 1$, anharmonic effects will evidently effectively outweigh the contribution from two-phonon processes in the formation of the tail of the cross-section.

We should note that as formula (2) contains the factor $n(\Delta E) + 1$, the transition to the classical limit takes place at a higher temperature for the tail than for the phonons in the main energy region and hence for the two-phonon processes. The observed temperature dependence[1] conforms to this general pattern.

In conclusion we observe that once anharmonic effects are present the incoherent inelastic scattering cross section is unfortunately no longer equivalent to the spectral density which defines uniquely the thermodynamic properties of the crystal.

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