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Anomalous Transmission of Particles through Perfect Crystals

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A formalism for the transmission of particles through perfect crystals at low temperatures is presented, assuming a Debye model for the lattice vibrations. The results are compared with a similar calculation by DeWames *et al.* in which the Einstein model is used to depict lattice vibrations. It is shown that the requirements of high particle energy and localization of the interaction potential for producing anomalous transmission are justified in the present model. The temperature dependence of the process and its dependence on the energy of the incident particles are established. A comparison is made between the relative effects of the atomic mean-square displacement and the range of the interaction potential.

I. INTRODUCTION

In recent years, several authors have investigated the theoretical[1–3] and experimental[3,4] aspects of the anomalous transmission of particles through perfect crystals. The classisal theory of Lindhard,[1] which is based on the concept of particle trajectory and critical channeling angle, has been very successful in explaining the experimental results for the transmission of heavy particles. However, it is well known[5] that this theory must fail in the case of the channeling of light particles, for which the quantum-mechanical interference effects are not negligible. Also, since the potential governing the particle trajectory is assumed to be independent of depth in this theory, no thickness dependence of the effect is predicted, although experimentally the number of channeled particles has been shown[6] to depend upon the thickness of the crystal. In the quantum-mechanical formulation of DeWames *et al.*[2] (to be referred to as DHL throughout this work), the Einstein model has been used to describe the lattice vibrations. Such an approach is adequate for a qualitative description of the quantum theory of the phenomena, and simplifies the mathematics involved in the lattice-vibration part of the theory. It also clearly shows the vital role played by the interaction potential between the particle and the lattice ions. However, because of the inherent simplicity of the Einstein model, it is difficult to expect quantitative results and the correct energy and temperature dependence of the process. In this paper, which closely follows the formulation of DHL, the results of a study of the anomalous transmission of particles is presented in which the Debye model has been used for the lattice vibrations.

It is well known that the Debye model represents a very reasonable approximation to the realistic situations existing in the crystals and quantitative results derived from it are in good agreement with experiments. In particular there exists a well-developed theory[7] for neutron scattering from the Debye crystals which utilizes the Fermi pseudopotential in the Born approximation. The quantitative results from this theory have been found to agree fairly well with the experimental results. Therefore a Debye-model calculation for the anomalous transmission of particles may be expected to yield good quantitative results besides reproducing the qualitative features of the Einstein-model calculation. In addition it is expected to lead to the correct temperature dependence and energy dependence for the process.

The crystal symmetry plays a crucial role in producing the anomalous transmission effects. It has been customary in the theory of anomalous transmission effects for particles to draw analogies from the corresponding effect for x rays, which is known experimentally as the Borrmann effect.[8] This effect is known theoretically[9] to be a consequence of crystal periodicity which leads to the formation of standing waves in the crystal when the Bragg condition is satisfied. Those waves which have their antinodes at the atomic sites are attenuated at an enhanced rate, while those having nodes at the atomic sites are negligibly attenuated and hence anomalously transmitted. The same physical picture regarding the crystal periodicity is also true for the anomalous transmission of particles. Therefore every attempt to understand the effect theoretically must necessarily assume the existence of the crystal periodicity and any deviations from it must be treated in the perturbation approximation. This feature is present in the Lindhard's theory,[1] in which regular chains of close-packed atoms are assumed to exist in the crystal and also in the formalism of DHL where a ground state having the exact periodicity of the lattice is assumed. In the present work, a very-low-lying crystal state $|n\rangle$ will be assumed to play the role of the ground state in DHL. The following section is devoted to the evaluation of the elements of renormalization matrix C_{hg} of DHL. Assuming the Debye model in Sec. III, this has been used to determine the anomalous transmission condition using two potential models of DHL, obtaining thereby the temperature and energy dependence of the process. The temperature dependence is expected also in analogy with the Borrmann effect, which is known to be temperature dependent. Finally the conclusions are summarized in Sec. IV.

II. RENORMALIZATION MATRIX ELEMENTS

We consider a perfect crystal to be initially in a very-low-lying state $|n\rangle$ at low temperature. A beam of particles of sufficiently high energy is incident upon it. Following the formalism of DHL, the total wave function can be expanded as

$$\Psi(\mathbf{r},\{\mathbf{R}_\sigma\})=\sum_m |m\rangle\varphi_m(\mathbf{r}),\tag{1}$$

where now $\varphi_n(\mathbf{r})$ is the major deriving term, $\mathbf{r}$ being the position of the particle and $\mathbf{R}_\sigma$ the actual position of the $\boldsymbol{\sigma}$th nucleus. We assume that $\varphi_n(\mathbf{r})$ plays the role of $\varphi_0(\mathbf{r})$ in DHL, and using the Born-approximation result for the other coefficients $\varphi_m(\mathbf{r})$, the first-order perturbation equation for $\varphi_n(\mathbf{r})$ is obtained. Now introducing

$$\varphi_n(\mathbf{r})=\sum_{\mathrm{h}} u_{\mathrm{h}}(n)\exp[i(\mathbf{k}_M+\mathbf{K}_{\mathrm{h}})\cdot\mathbf{r}],\qquad V_{nn}(\mathbf{r})=\sum_{\mathrm{h}} V_{\mathrm{h}}(n)\exp(i\mathbf{K}_{\mathrm{h}}\cdot\mathbf{r}),\tag{2}$$

with the assumed symmetry of the initial state (which in fact is very close to the ground state), Eq. (5) of DHL is obtained for $u_{\mathrm{h}}(n)$ in the form

$$(\hbar^2/2m_0)[(\mathbf{K}_{\mathrm{h}}+\mathbf{k}_M)^2-k_n^2]u_{\mathrm{h}}(n)+\sum_{\mathrm{g}}[V_{\mathrm{h-g}}(n)+C_{\mathrm{hg}}(n)]u_{\mathrm{g}}(n)=0,\tag{3}$$

where m_0 is the mass of the incident particle whose energy is E_p, $k_n^2=(2m_0/\hbar^2)E_p$, and the effect of the renormalization of $\varphi_n(\mathbf{r})$ is given by $C_{\mathrm{hg}}(n)$, as in DHL,

$$C_{\mathrm{hg}}(n)=-(2m_0/V'\hbar^2)\int d\mathbf{r}\int d\mathbf{r}'\exp[-i(\mathbf{K}_{\mathrm{h}}+\mathbf{k}_n)\cdot\mathbf{r}+i(\mathbf{K}_{\mathrm{g}}+\mathbf{k}_n)\cdot\mathbf{r}']\sum_{n'\neq n}V_{nn'}(\mathbf{r})V_{n'n}(\mathbf{r}')\times[\exp(ik_{n'}|\mathbf{r}-\mathbf{r}'|)/4\pi|\mathbf{r}-\mathbf{r}'|],\tag{4}$$

where V' is the volume of the crystal. The two-wave solution will be important when a Bragg condition $|\mathbf{K}_{\mathrm{h}}+\mathbf{k}_n|=|\mathbf{k}_n|$ is satisfied and attenuation of the two waves φ_n^+ and φ_n^- will be governed by the complex quantity

$$\eta_\pm=(k_n/2\gamma_nE_p)[\pm(V_{\mathrm{h}}(n)+C_{\mathrm{h0}}(n))-(V_0(n)+C_{00}(n))],\tag{5}$$

where $\gamma_n=\hat{k}_n\cdot\hat{n}$, $\hat{n}$ being the unit normal to the entrance surface pointing inward. Indeed, one has

$$\varphi_n^\pm\simeq\exp[i(\mathbf{k}_n+\eta_\pm\hat{n})\cdot\mathbf{r}][1\mp\exp(i\mathbf{K}_{\mathrm{h}}\cdot\mathbf{r})].\tag{6}$$

It is clear that the $\mathrm{Im}\eta_\pm$ govern the attenuations and since $\mathrm{Im}\eta_+$ has the possibility of being zero, φ_n^+ is the wave which could produce anomalous transmission. However,

$$\mathrm{Im}\eta_\pm=(k_n/2\gamma_nE_p)[\pm\,\mathrm{Im}C_{\mathrm{h0}}(n)-\mathrm{Im}C_{00}(n)]\tag{7}$$

and therefore the anomalous transmission is governed essentially by the imaginary part of the renormalization matrix element,

$$\mathrm{Im}C_{\mathrm{hg}}(n)=-[2m_0\pi/V'\hbar^2(2\pi)^3]\int d\mathbf{k}\int d\mathbf{r}\int d\mathbf{r}'\exp[i(\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{h}})\cdot\mathbf{r}-i(\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{g}})\cdot\mathbf{r}']\times\sum_{n'\neq n}V_{nn'}(\mathbf{r})V_{n'n}(\mathbf{r}')\delta(k^2-k_{n'}^2).\tag{8}$$

Here $k_{n'}$ is the wave vector of the particle if the initial state were $|n'\rangle$. Thus far the formalism of DHL has been adapted in the present case and the Debye-model calculation will now manifest itself in the evaluation of $\mathrm{Im}C_{\mathrm{hg}}(n)$. A general interaction potential $V(\mathbf{r})$ can be written in the form of $V(\mathbf{r})=\sum_\sigma V_\sigma(\mathbf{r}-\mathbf{R}_\sigma)$, where $V_\sigma(\mathbf{r}-\mathbf{R}_\sigma)$ is the interaction potential between the incident particle and the lattice ion whose equilibrium position vector is $\boldsymbol{\sigma}$. Then the expression (8) becomes

$$\mathrm{Im}C_{\mathrm{hg}}(n)=-\frac{2m_0\pi}{V'\hbar^2(2\pi)^3}\int d\mathbf{k}\sum_{n'\neq n}\sum_{\sigma,\sigma'}V_\sigma(\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{h}})\exp[i(\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{h}})\cdot\boldsymbol{\sigma}]\times V_{\sigma'}(\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{g}})\exp[-i(\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{g}})\cdot\boldsymbol{\sigma}']\delta(k^2-k_{n'}^2)\times\langle n|\exp[i(\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{h}})\cdot\mathbf{u}_\sigma]|n'\rangle\langle n'|\exp[-i(\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{g}})\cdot\mathbf{u}_{\sigma'}]|n\rangle,\tag{9}$$

where $V_\sigma(\mathbf{K})=\int V_\sigma(\mathbf{r})\exp(i\mathbf{K}\cdot\mathbf{r})d\mathbf{r}$, and $\mathbf{u}_\sigma$ is the displacement of the corresponding lattice ion from its equilibrium position $\boldsymbol{\sigma}$.

Expressions of the type $\langle n'|\exp(i\mathbf{K}\cdot\mathbf{u}_\sigma)|n\rangle$ for $n'\neq n$ correspond to the exchange of phonons. The procedure to evaluate these is to expand $\mathbf{u}_\sigma$ as,

$$\mathbf{u}_\sigma=(\hbar^2/2MN)^{1/2}\sum_{j,s}(\boldsymbol{\varepsilon}_s/\xi_j^{1/2})[a_j\exp(i\mathbf{f}_j\cdot\boldsymbol{\sigma})+a_j^\dagger\exp(-i\mathbf{f}_j\cdot\boldsymbol{\sigma})],\tag{10}$$

where $\mathbf{f}_j$ and ξ_j are the wave vector and energy of the phonons and $\boldsymbol{\varepsilon}_s$ ($s=1, 2, 3$) are their polarization vectors. The lattice is supposed to be monoatomic and M denotes the mass of each atom. There are N atoms in the crystal and a_j and $a_j^\dagger$ are the well-known phonon creation and annihilation operators. Now since, for a multiphonon exchange, the probability of any two phonons having same wave vector is negligibly small compared to the probability for all the phonons having different wave vectors,[7] one can write for an l-phonon-exchange process

$$\langle n' \mid \exp(i\mathbf{K}\cdot\mathbf{u}_\sigma) \mid n\rangle = \prod_{j=1}^{l} \langle n_j \pm 1 \mid \exp[i(Q_{j\sigma}a_j + Q_{j\sigma}^* a_j^\dagger)] \mid n_j\rangle \prod_{j=l+1}^{N} \langle n_j \mid \exp[i(a_{j\sigma}a_j + Q_{j\sigma}^* a_j^\dagger)] \mid n_j\rangle, \quad (11)$$

where

$$Q_{j\sigma} = (\hbar^2/2MN\xi_j)^{1/2} \sum_s (\mathbf{K}\cdot\boldsymbol{\varepsilon}_s) \exp(i\mathbf{f}_j\cdot\boldsymbol{\sigma}). \quad (12)$$

However, at any finite temperature T, since the exact n_j corresponding to a given state $\mid n\rangle$ is never known, one should replace[10] the operator of the form $\exp(U)$ by $(U^l/l!)\exp(\frac{1}{2}\langle U^2\rangle_T)$ corresponding to the l-phonon process. Thus for the emission of l phonons we get

$$\langle n' \mid \exp(i\mathbf{K}\cdot\mathbf{u}_\sigma) \mid n\rangle = \prod_{j=1}^{l} \frac{[iQ_{j\sigma}^*(n_j+1)^{1/2}]^l}{l!} e^{-W}, \quad (13)$$

where the Debye-Waller factor $2W$ is given by[7]

$$2W = 2DK^2, \quad (14)$$

where

$$2D = (\hbar^2/2MN) \sum_j (1/\xi_j) \coth(\xi_j/2k_BT). \quad (15)$$

Note here that Eq. (13) gives the matrix element for the exchange of l phonons, each having different frequency. But since it has been shown[11] that the exchange of two phonons of the same type is N^{-1} times less probable compared to the one-phonon process, Eq. (13) gives the matrix element for a general l-phonon process within the approximation of neglecting terms of order N^{-1} compared to unity.

Now it is clear from Eq. (13) that an l-phonon process involves the lth power of $Q_{j\sigma} \simeq (\text{energy transfer}/N\xi_j)^{1/2}$, so that the corresponding matrix element decreases rapidly as l increases. On the other hand, the multiphonon processes do not permit even approximate symmetry, which is so crucial for the anomalous transmission. Therefore, as a first approximation we take only the one-phonon-process contributions in Eq. (13) and write it as

$$\langle n' \mid \exp(-i\mathbf{K}\cdot\mathbf{u}_{\sigma'}) \mid n\rangle = -iQ_{\sigma'}^*(n_1+1)^{1/2} \exp(-DK^2), \quad (16)$$

where the subscript $j=1$ has been dropped from $Q_{1\sigma}^*$, $\mathbf{f}_1$, and ξ_1.

After substituting such matrix elements in Eq. (9), one has to average over n_1 because of the finite temperature of the crystal to get

$$\langle (n_1+1) \rangle = [1-\exp(-\xi/k_BT)]^{-1}, \quad (17)$$

where k_B is the Boltzmann constant. Thus finally one gets

$$\begin{aligned}\mathrm{Im}C_{\mathrm{hg}}(n) = &-\frac{2m_0\pi}{V'\hbar^2(2\pi)^3} \int d\mathbf{k} \sum_{\sigma,\sigma'} V_\sigma(\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{h}}) V_{\sigma'}(\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{g}}) \exp[i(\mathbf{k}-\mathbf{k}_n)\cdot(\boldsymbol{\sigma}-\boldsymbol{\sigma}')] \\ &\times \frac{1}{N}\sum_{\mathrm{f}} \left(\frac{\hbar^2}{2MN\xi}\right)\left[\frac{\delta(k^2-k_{n+1}{}^2)}{1-\exp(-\xi/k_BT)} \exp[i\mathbf{f}\cdot(\boldsymbol{\sigma}-\boldsymbol{\sigma}')] + \frac{\delta(k^2-k_{n-1}{}^2)}{\exp(\xi/k_BT)-1} \exp[-i\mathbf{f}\cdot(\boldsymbol{\sigma}-\boldsymbol{\sigma}')]\right] \\ &\times (\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{h}})\cdot(\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{g}}) \exp\{-D[(\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{h}})^2+(\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{g}})^2]\}. \quad (18)\end{aligned}$$

Here we have summed over the processes in which the phonons of various frequencies are exchanged.

If there are no isotopes and the lattice ions are assumed to have zero nuclear spin, then $V_\sigma(\mathbf{K})$ is independent of $\boldsymbol{\sigma}$. Hence setting $V_\sigma(\mathbf{K}) = V(\mathbf{K})$ for simplicity, one gets

$$\begin{aligned}\mathrm{Im}C_{\mathrm{hg}}(n) = &-\frac{2m_0\pi}{V'\hbar^2(2\pi)^3} \int d\mathbf{k}\, V(\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{h}}) V(\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{g}}) \sum_{\sigma,\sigma'} \exp[i(\mathbf{k}-\mathbf{k}_n)\cdot(\boldsymbol{\sigma}-\boldsymbol{\sigma}')] \\ &\times \frac{1}{N}\sum_{\mathrm{f}} \left(\frac{\hbar^2}{2MN\xi}\right)\left[\frac{\delta(k^2-k_n{}^2+2m_0\xi/\hbar^2)}{1-\exp(-\xi/k_BT)} \exp[i\mathbf{f}\cdot(\boldsymbol{\sigma}-\boldsymbol{\sigma}')] + \frac{\delta(k^2-k_n{}^2-2m_0\xi/\hbar^2)}{\exp(\xi/k_BT)-1} \exp[-i\mathbf{f}\cdot(\boldsymbol{\sigma}-\boldsymbol{\sigma}')]\right] \\ &\times (\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{h}})\cdot(\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{g}}) \exp\{-D[(\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{h}})^2+(\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{g}})^2]\}. \quad (19a)\end{aligned}$$

If there are isotopes, however, additional terms will appear in Eq. (19a). For example, an isotope sitting at the origin whose interaction potential is δV (in addition to that of normal atom) will contribute terms involving integrations over the products of V and δV in Eq. (19a).

The $\boldsymbol{\sigma}$ and $\boldsymbol{\sigma}'$ summations in Eq. (19a) can be performed easily[7] to yield $[(2\pi)^3N/v_c]\sum_{\mathrm{h}'}\delta(\mathbf{k}-\mathbf{k}_n\pm\mathbf{f}+\mathbf{K}_{\mathrm{h}'})$, where v_c is the volume of the unit cell. Now Eq. (19a) can be written as

$$\mathrm{Im}C_{\mathrm{hg}}(n)=-[2m_0\pi/V'\hbar^2(2\pi)^3]\int d\mathbf{k}\, V(\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{h}})V(\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{g}})(\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{h}})\cdot(\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{g}})$$
$$\times\exp\{-D[(\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{h}})^2+(\mathbf{k}-\mathbf{k}_n-\mathbf{K}_{\mathrm{g}})^2]\}[(2\pi)^3N/v_c]$$
$$\times\frac{1}{N}\sum_{\mathbf{f}}[G_1(\mathbf{f})\sum_{\mathrm{h}'}\delta(\mathbf{k}-\mathbf{k}_n+\mathbf{f}+\mathbf{K}_{\mathrm{h}'})+G_2(\mathbf{f})\sum_{\mathrm{h}''}\delta(\mathbf{k}-\mathbf{k}_n-\mathbf{f}+\mathbf{K}_{\mathrm{h}''})], \quad (19\mathrm{b})$$

where

$$G_1(\mathbf{f})=\frac{\hbar^2}{2MN\xi}\frac{\delta(k^2-k_n^2+2m_0\xi/\hbar^2)}{1-\exp(-\xi/k_BT)},$$

$$G_2(\mathbf{f})=\frac{\hbar^2}{2MN\xi}\frac{\delta(k^2-k_n^2-2m_0\xi/\hbar^2)}{\exp(\xi/k_BT)-1}.$$

Now since energy $\xi(\mathbf{f})$ is periodic in the reciprocal space $\xi(\mathbf{f})=\xi(\mathbf{f}+\mathbf{K}_{\mathrm{h}'})$ and the $\mathbf{f}$ dependence of $G_1(\mathbf{f})$ and $G_2(\mathbf{f})$ is only through $\xi(\mathbf{f})$, we have $G_1(\mathbf{f})=G_1(\mathbf{f}+\mathbf{K}_{\mathrm{h}'})$ for all $\mathbf{K}_{\mathrm{h}'}$ and $G_2(\mathbf{f})=G_2(\mathbf{f}-\mathbf{K}_{\mathrm{h}''})$ for all $\mathbf{K}_{\mathrm{h}''}$. Therefore the terms in the square brackets in Eq. (19b) can be written as

$$\sum_{\mathbf{f}}[\sum_{\mathrm{h}'}G_1(\mathbf{f}+\mathbf{K}_{\mathrm{h}'})\delta(\mathbf{k}-\mathbf{k}_n+\mathbf{f}+\mathbf{K}_{\mathrm{h}'})+\sum_{\mathrm{h}'}G_2(\mathbf{f}-\mathbf{K}_{\mathrm{h}'})\delta(\mathbf{k}-\mathbf{k}_n-\mathbf{f}+\mathbf{K}_{\mathrm{h}'})]$$
$$=\sum_{\mathrm{h}'}\sum_{\mathbf{f}}G_1(\mathbf{f}+\mathbf{K}_{\mathrm{h}'})\delta(\mathbf{k}-\mathbf{k}_n+\mathbf{f}+\mathbf{K}_{\mathrm{h}'})+G_2(\mathbf{f}-\mathbf{K}_{\mathrm{h}'})\delta(\mathbf{k}-\mathbf{k}_n-\mathbf{f}+\mathbf{K}_{\mathrm{h}'})$$
$$=\sum_{\mathrm{h}'}\sum_{\mathbf{f}'}[G_1(\mathbf{f}')\delta(\mathbf{k}-\mathbf{k}_n+\mathbf{f}')+G_2(\mathbf{f}')\delta(\mathbf{k}-\mathbf{k}_n-\mathbf{f}')]$$
$$=N\sum_{\mathbf{f}}[G_1(\mathbf{f})\delta(\mathbf{k}-\mathbf{k}_n+\mathbf{f})+G_2(\mathbf{f})\delta(\mathbf{k}-\mathbf{k}_n-\mathbf{f})],$$

where $\mathbf{f}$ is restricted to the first Brillouin zone.

Now using the δ functions $\delta(\mathbf{k}-\mathbf{k}_n\pm\mathbf{f})$ for $\mathbf{k}$ integration, we get

$$\mathrm{Im}C_{\mathrm{hg}}(n)=-\frac{m_0}{2Mv_c(2\pi)^2}\int\frac{d\mathbf{f}}{\xi}\left\{\frac{V(\mathbf{f}+\mathbf{K}_{\mathrm{h}})V(\mathbf{f}+\mathbf{K}_{\mathrm{g}})}{1-\exp(-\xi/k_BT)}(\mathbf{f}+\mathbf{K}_{\mathrm{h}})\cdot(\mathbf{f}+\mathbf{K}_{\mathrm{g}})\exp\{-D[(\mathbf{f}+\mathbf{K}_h)^2+(\mathbf{f}+\mathbf{K}_{\mathrm{g}})^2]\}\right.$$
$$\times\delta\left(f^2-2\mathbf{f}\cdot\mathbf{k}_n+\frac{2m_0\xi}{\hbar^2}\right)+\frac{V(\mathbf{f}-\mathbf{K}_{\mathrm{h}})V(\mathbf{f}-\mathbf{K}_{\mathrm{g}})}{\exp(\xi/k_BT)-1}(\mathbf{f}-\mathbf{K}_{\mathrm{h}})\cdot(\mathbf{f}-\mathbf{K}_{\mathrm{g}})\exp\{-D[(\mathbf{f}-\mathbf{K}_{\mathrm{h}})^2+(\mathbf{f}-\mathbf{K}_{\mathrm{g}})^2]\}$$
$$\left.\times\delta\left(f^2+2\mathbf{f}\cdot\mathbf{k}_n-\frac{2m_0\xi}{\hbar^2}\right)\right\}, \quad (20)$$

where $\sum_{\mathbf{f}}$ has been replaced by $[V'/(2\pi)^3]\int d\mathbf{f}$.

Now in order to proceed further with the calculation of $\mathrm{Im}C_{\mathrm{hg}}$, one must choose a model for the interaction potential and also for the lattice vibrations.

III. RESULTS FOR DEBYE CRYSTAL WITH SPECIFIC POTENTIAL MODELS

As already mentioned, an important approximation for the phonon dispersion is to use the Debye model which corresponds to the low-frequency part of any actual dispersion. Thus we set $\xi=\hbar cf$, where c is the velocity of acoustic vibrations in the crystal, and the maximum value of f can be f_0.

Now for neutrons, one can choose the interaction as in DHL,

$$V_\sigma(\mathbf{r}-\mathbf{R}_\sigma)=-(2\pi\hbar^2/m_0)[\beta^3/(\pi)^{3/2}]a_\sigma\exp[-\beta^2(\mathbf{r}-\mathbf{R}_\sigma)^2], \quad (21)$$

which passes on exactly to the Fermi pseudopotential as the width of the potential $\beta^{-1}\to 0$. Here a_σ has the dimension of length and becomes the scattering length (of a bound atom at the site $\boldsymbol{\sigma}$) in the case of Fermi pseudopotential.

With this $V_\sigma(\mathbf{r}-\mathbf{R}_\sigma)$, we get

$$V_\sigma(\mathbf{K})=-(2\pi\hbar^2/m_0)a_\sigma\exp(-K^2/4\beta^2), \quad (22)$$

so that for a perfect crystal we have

$$\mathrm{Im}C_{\mathrm{hg}}(n)=-\frac{\hbar^3a^2}{2Mm_0cv_c}\int\frac{d\mathbf{f}}{f}\left\{\frac{(\mathbf{f}+\mathbf{K}_\mathrm{h})\cdot(\mathbf{f}+\mathbf{K}_\mathrm{g})}{1-\exp(-\hbar cf/k_BT)}\,\delta\left(f^2-2\mathbf{f}\cdot\mathbf{k}_n+\frac{2m_0cf}{\hbar}\right)\right.$$

$$\left.\times\exp\{-D'[(\mathbf{f}+\mathbf{K}_\mathrm{h})^2+(\mathbf{f}+\mathbf{K}_\mathrm{g})^2]\}+\frac{(\mathbf{f}-\mathbf{K}_\mathrm{h})\cdot(\mathbf{f}-\mathbf{K}_\mathrm{g})}{\exp(\hbar cf/k_BT)-1}\,\delta\left(f^2+2\mathbf{f}\cdot\mathbf{k}_n-\frac{2m_0cf}{\hbar}\right)\exp\{-D'[(\mathbf{f}-\mathbf{K}_\mathrm{h})^2+(\mathbf{f}-\mathbf{K}_\mathrm{g})^2]\}\right\}. \tag{23}$$

where

$$D'=D+1/4\beta^2. \tag{24}$$

From Eq. (23) we can easily write the expressions for $\mathrm{Im}C_{\mathrm{h}0}$ and $\mathrm{Im}C_{00}$. In particular we have

$$\mathrm{Im}C_{\mathrm{h}0}(n)=-\frac{\hbar^3a^2}{2Mm_0cv_c}\int\frac{d\mathbf{f}}{f}\left\{\frac{(\mathbf{f}+\mathbf{K}_\mathrm{h})\cdot\mathbf{f}}{1-\exp(-\hbar cf/k_BT)}\exp\{-D'[(\mathbf{K}_\mathrm{h}+\mathbf{f})^2+f^2]\}\delta\left(f^2-2\mathbf{f}\cdot\mathbf{k}_n+\frac{2m_0cf}{\hbar}\right)\right.$$

$$\left.+\frac{(\mathbf{f}-\mathbf{K}_\mathrm{h})\cdot\mathbf{f}}{\exp(\hbar cf/k_BT)-1}\exp\{-D'[(\mathbf{K}_\mathrm{h}-\mathbf{f})^2+f^2]\}\delta\left(f^2+2\mathbf{f}\cdot\mathbf{k}_n-\frac{2m_0cf}{\hbar}\right)\right\}. \tag{25}$$

Since in the Debye model even the maximum allowed phonon wave vector $\mathbf{f}_0$ is small compared to a reciprocal-lattice vector, we neglect $\mathbf{f}$ compared to $\mathbf{K}_\mathrm{h}$ in the Debye-Waller factor, as has been usually done[7] without introducing any significant error. Now we carry out the angular integration, choosing $\mathbf{k}_n$ as the z axis, to get

$$\mathrm{Im}C_{\mathrm{h}0}(n)=-\frac{\pi\hbar^3a^2\exp(-D'K_h^2)}{2Mm_0cv_ck_n}\left[\left(1+\frac{K_h\cos\alpha}{2k_n}\right)\int_0^{f_0}f^2\coth\left(\frac{\hbar cf}{2k_BT}\right)df+\frac{m_0cK_h\cos\alpha}{2\hbar k_n}f_0^2\right]. \tag{26}$$

In the low-temperature limit, $\coth(\hbar cf/2k_BT)\simeq1+2\exp(-\hbar cf/k_BT)$, so that in this limit D becomes

$$D_l=(3\hbar^2/8k_B\Theta_DM)[1+4(T/\Theta_D)^2] \tag{27}$$

and

$$\mathrm{Im}C_{\mathrm{h}0}(n)=-\frac{\pi\hbar^3a^2\exp(-D_l'K_h^2)}{2Mm_0cv_ck_n}\left[\tfrac{1}{3}f_0^3\left(1+\frac{K_h\cos\alpha}{2k_n}\right)\left(1+\frac{6T^3}{\Theta_D^3}\right)+\frac{m_0cK_h\cos\alpha}{2\hbar k_n}f_0^2\right], \tag{28}$$

with $D_l'=D_l+1/4\beta^2$. Here Θ_D is the Debye temperature, and we have neglected terms of order higher than $(T/\Theta_D)^3$. In these equations α is the angle between $\mathbf{K}_\mathrm{h}$ and $\mathbf{k}_n$, and the step function involved in the angular integration of the δ function, occurring in Eq. (25), becomes unity because for high particle energies f_0 is always smaller than $(2k_n\pm2m_0c/h)$.

Now from Eq. (28), it is easy to write

$$\mathrm{Im}C_{\mathrm{h}0}(n)=\mathrm{Im}C_{00}(n)\exp(-D_l'K_h^2)\left[1+\frac{K_h\cos\alpha}{2k_n}+\frac{3m_0cK_h\cos\alpha}{2\hbar k_nf_0(1+6T^3/\Theta_D^3)}\right]. \tag{29}$$

Therefore the wave φ_n^+ will experience no attenuation when $\mathrm{Im}C_{\mathrm{h}0}=\mathrm{Im}C_{00}$, which leads to

$$\frac{K_h\cos\alpha}{2k_n}\left[1+\frac{3m_0c}{\hbar f_0(1+6T^3/\Theta_D^3)}\right]=[\exp(D_l'K_h^2)-1] \tag{30}$$

This is the condition that must be satisfied for complete anomalous transmission. However, even when this is not exactly satisfied, the attenuation of the beam along the direction of anomalous transmission will be governed by

$$|\varphi_n^+|^2\simeq\exp\left[-\frac{\pi\hbar^3a^2f_0^3}{4Mm_0cv_c\gamma_nE_p}\frac{1}{3}\left(1+\frac{6T^3}{\Theta_D^3}\right)(1-\epsilon)\hat{n}\cdot\boldsymbol{\gamma}\right], \tag{31}$$

where

$$\epsilon=\exp(-D_l'K_h^2)\left[1+\frac{K_h\cos\alpha}{2k_n}+\frac{3m_0cK_h\cos\alpha}{2\hbar k_nf_0(1+6T^3/\Theta_D^3)}\right], \tag{32}$$

Noting that D is just half of the mean-square displacement, we conclude from the above equations that for an interaction potential narrow compared to the mean-square displacement, the attenuation at short wavelength is independent of the potential width, because in that case $1/4\beta^2$ can be neglected compared to D_l, so that $D_l'=D_l$.

The attenuation of the other wave φ_n^- at the condition (30) of anomalous transmission is maximum and is determined by 2 $\mathrm{Im}C_{00}$. This can be calculated accurately from Eq. (25). Thus

$$\mathrm{Im}C_{00}(n)=-\frac{\pi\hbar^3a^2}{2Mm_0cv_ck_n}\int_0^{f_0}f^2\exp(-D'f^2)\coth\left(\frac{\hbar cf}{2k_BT}\right)df \tag{33}$$

after the angular integration has been done. In the low-temperature limit, Eq. (33) gives

$$\mathrm{Im}C_{00}(n)=-\frac{\pi\hbar^3a^2}{2Mm_0cv_ck_n}\left[\frac{\hbar c}{8k_BTD_l'^2}\left(\exp\left(-\frac{\Theta_D}{T}-2D_l'f_0^2\right)-1\right)-f_0\frac{\exp(-2D_l'f_0^2)}{4D_l'}[1+2\exp(-\Theta_D/T)]\right.$$
$$+\frac{1}{4D_l'}\left(\frac{\pi}{8D_l'}\right)^{1/2}\left\{\mathrm{erf}[f_0(2D_l')^{1/2}]+\exp\left(\frac{\hbar^2c^2}{8k_B{}^2T^2D_l'}\right)\left(2+\frac{\hbar^2c^2}{2k_B{}^2T^2D_l'}\right)\right.$$
$$\left.\left.\times\left(\mathrm{erf}\left(f_0(2D_l')^{1/2}+\frac{\hbar c}{2k_BT(2D_l')^{1/2}}\right)-\mathrm{erf}\left(\frac{\hbar c}{2k_BT(2D_l')^{1/2}}\right)\right)\right\}\right], \tag{34}$$

where

$$\mathrm{erf}(z)=\frac{2}{\pi^{1/2}}\int_0^z\exp(-t^2)\,dt.$$

The limit of contact pseudopotential is obtained by replacing D_l' by D_l in the above expressions. The limit of wide interaction potentials (β^{-1} large) can be obtained by putting $D_l'=1/4\beta^2$, but in this limit it is difficult to satisfy Eq. (30). This is because the left-hand side of Eq. (30) being less than 10^{-2} for typical values of $\mathbf{k}_n$ and $\mathbf{K}_h$, the right-hand side cannot be anywhere close to that if $1/4\beta^2$ is so large compared to D_l that $D_l'=1/4\beta^2$. This is clearly seen from Table I, where $(1-\epsilon)$ becomes 10^{-1} for $1/4\beta^2=100D_l$.

For the case of charged particles, the excitation of electron cloud surrounding the lattice ions and the vibrational transition of the lattice ion will lead to anomalous behavior because of their localization. The effect can be illustrated as in DHL, by choosing a screened Coulomb interaction of appropriate range, as the interaction between incident charged particles and the lattice atoms,

$$V_\sigma(\mathbf{r}-\mathbf{R}_\sigma)=z_1z_2e^2[\exp(-\Lambda\,|\,\mathbf{r}-\mathbf{R}_\sigma\,|)/|\,\mathbf{r}-\mathbf{R}_\sigma\,|], \tag{35}$$

where Λ is the screening parameter and z_1 and z_2 are the charges of incident particle and the lattice atoms in the units of e, respectively. For this interaction we get

$$V_\sigma(\mathbf{K})=4\pi z_1z_2e^2/(\Lambda^2+K^2), \tag{36}$$

so that using Eq. (20), we get

$$\mathrm{Im}C_{\mathrm{hg}}(n)=-\frac{2m_0(z_1z_2e^2)^2}{M\hbar cv_c}\int\frac{d\mathbf{f}}{f}\left\{\frac{(\mathbf{f}+\mathbf{K}_\mathrm{h})\cdot(\mathbf{f}+\mathbf{K}_\mathrm{g})}{1-\exp(-\hbar cf/k_BT)}\delta\left(f^2-2\mathbf{f}\cdot\mathbf{k}_n+\frac{2m_0cf}{\hbar}\right)\frac{\exp\{-D[(\mathbf{f}+\mathbf{K}_\mathrm{h})^2+(\mathbf{f}+\mathbf{K}_\mathrm{g})^2]\}}{[\Lambda^2+(\mathbf{f}+\mathbf{K}_\mathrm{h})^2][\Lambda^2+(\mathbf{f}+\mathbf{K}_\mathrm{g})^2]}\right.$$
$$\left.+\frac{(\mathbf{f}-\mathbf{K}_\mathrm{h})\cdot(\mathbf{f}-\mathbf{K}_\mathrm{g})}{\exp(\hbar cf/k_BT)-1}\delta\left(f^2+2\mathbf{f}\cdot\mathbf{k}_n-\frac{2m_0cf}{\hbar}\right)\frac{\exp\{-D[(\mathbf{f}-\mathbf{K}_\mathrm{h})^2+(\mathbf{f}-\mathbf{K}_\mathrm{g})^2]\}}{[\Lambda^2+(\mathbf{f}-\mathbf{K}_\mathrm{h})^2][\Lambda^2+(\mathbf{f}-\mathbf{K}_\mathrm{g})^2]}\right\}. \tag{37}$$

To calculate $\mathrm{Im}C_{\mathrm{h}0}$, we again neglect $\mathbf{f}$ compared to $\mathbf{K}_\mathrm{h}$ in the exponential and in the denominator, and get

$$\mathrm{Im}C_{\mathrm{h}0}(n)=-\left(\frac{2\pi m_0(z_1z_2e^2)^2\exp(-DK_h^2)}{M\hbar cv_ck_n(\Lambda^2+K_h^2)}\right)\left[\frac{m_0cK_h\cos\alpha}{2\hbar k_n}\ln\left(1+\frac{f_0^2}{\Lambda^2}\right)+\left(1+\frac{K_h\cos\alpha}{2k_n}\right)\int_0^{f_0}\frac{f^2\coth(\hbar cf/2k_BT)}{\Lambda^2+f^2}df\right], \tag{38}$$

whose low-temperature limit is

$$\mathrm{Im}C_{\mathrm{h}0}(n)=-\left(\frac{2\pi m_0(z_1z_2e^2)^2\exp(-DK_h^2)}{M\hbar cv_ck_n(\Lambda^2+K_h^2)}\right)\left[\frac{m_0cK_h\cos\alpha}{2\hbar k_n}\ln\left(1+\frac{f_0^2}{\Lambda^2}\right)+\left(1+\frac{K_h\cos\alpha}{2k_n}\right)F_0(\Lambda,T)\right], \tag{39}$$

with

$$F_0(\Lambda,T)=f_0+2f_0(T/\Theta_D)[1-\exp(-\Theta_B/T)]-\Lambda\left\{\tan^{-1}\frac{f_0}{\Lambda}+\mathrm{ci}\left(\frac{\Lambda\hbar c}{k_BT}\right)\sin\left(\frac{\Lambda\hbar c}{k_BT}\right)-\mathrm{si}\left(\frac{\Lambda\hbar c}{k_BT}\right)\cos\left(\frac{\Lambda\hbar c}{k_BT}\right)\right\}, \tag{40}$$

where si and ci are well-known tabulated functions. We have extended the upper limit of the integral to ∞ in obtaining last two terms of Eq. (50), because the contribution from f greater than f_0 is small for the integral involved there at low temperatures.

Now from Eq. (39) we can write

$$\mathrm{Im}C_{h0}(n)=\mathrm{Im}C_{00}(n)\,\frac{\exp(-D_lK_h^2)}{1+K_h^2/\Lambda^2}\left[1+\frac{K_h\cos\alpha}{2k_n}+\frac{m_0cK_h\cos\alpha}{2\hbar k_nF_0(\Lambda,T)}\ln\left(1+\frac{f_0^2}{\Lambda^2}\right)\right], \tag{41}$$

so that the condition for anomalous transmission is

$$\frac{K_h\cos\alpha}{2k_n}\left[1+\frac{m_0c}{\hbar F_0(\Lambda,T)}\ln\left(1+\frac{f_0^2}{\Lambda^2}\right)\right]=\left[\left(1+\frac{K_h^2}{\Lambda^2}\right)\exp(D_lK_h^2)-1\right]. \tag{42}$$

Also,

$$|\varphi_n^+|^2\simeq\exp\left[-\frac{\pi m_0(z_1z_2e^2)^2F_0(\Lambda,T)}{M\hbar cv_c\gamma_nE_p\Lambda^2}(1-\epsilon_p)\hat{n}\cdot\boldsymbol{\gamma}\right], \tag{43}$$

where

$$\epsilon_p=\frac{\exp(-D_lK_h^2)}{1+K_h^2/\Lambda^2}\left[1+\frac{K_h\cos\alpha}{2k_n}+\frac{m_0cK_h\cos\alpha}{2\hbar k_nF_0(\Lambda,T)}\ln\left(1+\frac{f_0^2}{\Lambda^2}\right)\right]. \tag{44}$$

The effect of Λ on attenuation can be examined using Eq. (38). Thus for Λ^2 large compared to D_l^{-1}, so that $\Lambda^2\gg K_h^2$ and $\Lambda^2\gg f_0^2$, one gets

$$\mathrm{Im}C_{h0}(n)-\mathrm{Im}C_{00}(n)=\mathrm{Im}C_{00}(n)\left[1-\exp(-D_lK_h^2)\left(1+\frac{K_h\cos\alpha}{2k_n}\right)\right], \tag{45}$$

so that

$$\epsilon_p=\exp(-DK_h^2)(1+K_h\cos\alpha/2k_n)=\exp(-DK_h^2)(1-K_h^2/4k_n^2),$$

which is independent of Λ. Thus, when the screening is very strong, implying thereby that the potential is highly localized, the condition for anomalous transmission is independent of the screening parameter. On the other hand, if Λ is small compared to D_l^{-1} and can be taken to be of the order of f_0, then

$$\mathrm{Im}C_{h0}(n)-\mathrm{Im}C_{00}(n)=\mathrm{Im}C_{00}(n)\left\{1-\frac{\exp(-D_lK_h^2)}{1+K_h^2/\Lambda^2}\left[\left(1+\frac{K_h\cos\alpha}{2k_n}\right)+\frac{m_0cK_h\cos\alpha\ln 2}{2\hbar k_nf_0(1-(\Lambda/f_0)\tan^{-1}(f_0/\Lambda))}\right]\right\}, \tag{46}$$

showing that weak screening cannot lead to an anomalous effect.

IV. CONCLUSIONS

The present calculations lead to many interesting conclusions regarding the quantum theory of anomalous transmission of particles through perfect crystals. The fact that the Debye-model calculation approximately reproduces many results of the Einstein-model calculation of DHL is in itself interesting and is a confirmation of these results. Thus the condition for no attenuation given by Eq. (30) shows clearly that since the left-hand side is very small, $\exp(D_l'K_h^2)$ should be as close to unity as possible. This in turn implies that $1/4\beta^2$ should be very small compared to D_l and that is the case when the potential is highly localized. A comparison with Eq. (21) of DHL shows the identity of the two conclusions. It also follows that in this limit, the attenuation is independent of β as shown in DHL. The other conclusion of DHL that the potential be weak compared to E_p is implicit in the present case in assuming the two-wave solution. In the case of screened Coulomb interaction, Eq. (45) shows that the condition for anomalous transmission is independent of the screening parameter when the screening is very strong. The same conclusion follows from Eq. (31) of DHL. It is also clear that Eq. (30) goes over to the condition obtained from Eq. (21) of DHL if $(K_h/k_n)^2$ is neglected compared to unity.

The results obtained here differ from those of DHL in some respects. As already pointed out, it is difficult to satisfy Eq. (30) for a long-range interaction potential (β^{-1} large). This does not agree with the conclusion of DHL regarding the crucial role played by the ratio

TABLE I. Variation of $(1-\epsilon)$ with width of the potential β^{-1} and temperature when K_h corresponds to {100} planes in Cu (fcc).

β^{-1} (in units of $D_l^{1/2}$)	$(1-\epsilon)$ in units of 10^{-2} $T=5°$K	$T=15°$K	$T=25°$K	$T=35°$K
0.0	0.8081	0.8145	0.8271	0.8461
0.1	0.8101	0.8165	0.8292	0.8482
1.0	1.0091	1.0170	1.0328	1.0564
2.0	1.6097	1.6223	1.6474	1.6850
3.0	2.6026	2.6228	2.6631	2.7236
4.0	3.9759	4.0065	4.0676	4.1593
5.0	5.7131	5.7566	5.8437	5.9741
6.0	7.7937	7.8525	7.9698	8.1456
7.0	10.1935	10.2693	10.4207	10.6474
8.0	12.8850	12.9793	13.1677	13.4494
9.0	15.8380	15.9519	16.1792	16.5191
10.0	19.0201	19.1541	19.4216	19.8212

of $1/\beta^2$ and D_l in determining the attenuation when β is small. A similar situation is obtained when the screening is weak in the case of charged particles. Thus from Eq. (46), it follows that for small Λ, the attenuation depends on Λ. Apart from these limiting cases, our results in the general case show the energy dependence of the condition for the anomalous transmission as seen from Eq. (30). Since

$$K_h \cos\alpha/2k_n = -K_h^2/4k_n^2 = -\hbar^2 K_h^2/8m_0 E_p,$$

condition (30) is energy dependent. However, this energy dependence is seen to be quite feeble. Similarly apart from the temperature dependence of the condition via the mean-square displacement D_l, some extra dependence appears through $(T/\Theta_D)^3$ term in Eq. (30), which is again very small. It is clear that here the temperature dependence is a consequence of the assumption regarding a low-lying initial state $|\, n\rangle$.

It is important to note the importance of E_p^{-1} which appears in the exponent on the right-hand side of Eq. (31). When $(1-\epsilon)$ is not exactly zero but a small quantity, the wave φ_n^+ will channel the particles but there will be some attenuation The attenuation up to a given distance traversed will be governed by E_p^{-1}. Thus the distance at which a given fraction of the initially channeled particles is present in the channel will be proportional to E_p. On the other hand, φ_n^- must have been completely attenuated at any considerable distance within the crystal. Such considerations lead to the experimentally concluded[6] fact that $X_{1/2}$, the thickness into the crystal at which one-half of the initially channeled particles have escaped, is proportional to E_p. The present calculations can be extended so that any realistic vibrational spectrum $\xi_j = \xi_j(f)$ corresponding to a given lattice can be incorporated in Eq. (20), but then the problem will yield only to numerical computations.

One should be careful when using these results based on a two-wave calculation. Recently, DeWames *et al.*[12] have shown that such two-wave calculations are valid only for sufficiently weak interaction potentials or sufficiently small mass of the incident particle, regardless of the incident energy. As either the strength of the interaction or the mass of the particle increases, progressively more waves contribute substantially to the intensity, until ultimately particle motion becomes describable by the classical limit. The first of the two potential models considered here corresponds to neutrons and satisfies conditions for validity of the two-wave picture. The validity for the second potential model requires the mass of the charged particle to be small and it has been shown[12] that the electrons in low z-number crystals can be treated with these two-wave calculations but the protons should be treated classically.

Note added in proof. It should be noted that in Eq. (18), summing over various phonon wave vectors $\mathbf{f}$ and dividing by N, the number of values of $\mathbf{f}$, gives an average over processes in which phonons of different frequencies are exchanged. To make this point more clear, we notice from Eq. (19b) that the periodicity of $G_1(\mathbf{f})$ and $G_2(\mathbf{f})$, with period equal to a reciprocal lattice vector, can be used to show that even before the summation over $\mathbf{f}$ is made, the expression (19b) is independent of $\mathbf{f}$. Therefore, summation over $\mathbf{f}$ in Eq. (18) and in consequent equations, is accompanied by a multiplication by $(1/N)$.

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