Anomalous Particle Penetration in Perfect Crystals

R. E. De Wames, W. F. Hall, and G. W. Lehman
North American Aviation Science Center, Thousand Oaks, California
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A quantum-mechanical calculation of the potential dependence of anomalous transmission of particles through crystals is made, showing that the anomalous effect can always be obtained at sufficiently high particle energy. Both the normal and the anomalous attenuation are found to depart markedly from that calculated from the free-particle cross section when the potential is broad compared to the atomic mean-square displacement. Two experiments to observe the predicted potential dependence are suggested.

I. INTRODUCTION

IN this paper the transmission of particles through crystals is examined theoretically in order to establish the conditions under which anomalous transmission, i.e., transmission with negligible attenuation, occurs. The possibility of anomalous neutron transmission was realized shortly after this effect had been identified and understood for the case of x rays.[1] However, no theoretical investigation was made at that time, and the only experiment directed toward seeing anomalous neutron transmission yielded a negative result,[2] apparently due to crystal imperfections. More recently, theorists interested in electron microscopy have made calculations along these lines for the transmission of electrons through crystals.[3,4] On the other hand, in the theory of radiation damage such effects have not yet been taken into account.

The existence of anomalous effects is a consequence of the crystal periodicity, which forces the particle wave function inside the crystal also to be periodic, and hence to be describable as a Bloch wave. It is precisely this departure of the particle wave function from a plane wave which has until recently[5] been ignored in the investigations of neutron scattering from crystals. There the crystal scattering cross section is calculated from the Golden rule, taking plane-wave matrix elements between different states of this crystal.[6] This approximation leads directly to the familiar quantization of scattered momentum expressed by the Bragg condition for elastic scattering, and to an intensity for Bragg scattering governed by the Debye-Waller factor e^{-2W}, W being given by

$$W=\mathbf{k}_h^2\langle x^2\rangle/2,$$

where $\mathbf{k}_h$ is the reciprocal lattice vector for the scattering plane and $\langle x^2\rangle$ is the mean-square displacement for a crystal atom.

The approach taken in this work has been to utilize the standard Born approximation, solving the coupled particle-crystal equations for the amplitude of the transmitted wave. In Sec. II we set forth these equations and outline the procedure for their solution for arbitrary interaction potentials. In Sec. III the conditions necessary to obtain anomalous behavior are derived. Section IV contains an evaluation of the attenuation as a function of the interaction potential for neutrons and high-energy electrons and protons. In Sec. V we suggest two types of experiments which could be used to test the predicted potential dependence of the attenuation.

II. PARTICLE DIFFRACTION IN CRYSTALS—BORN APPROXIMATION

For the scattering of particles of mass m in crystals with interaction potential V one may write the equations coupling particle and crystal wave functions in the form[3]

$$\left\{\nabla^2+\frac{2m}{\hbar^2}(E-E_\mathrm{n})-\frac{2m}{\hbar^2}\langle\mathbf{n}|V|\mathbf{n}\rangle\right\}\varphi_\mathrm{n}(\mathbf{r})=\frac{2m}{\hbar^2}\sum_{\mathrm{m}\neq\mathrm{n}}\langle\mathbf{n}|V|\mathbf{m}\rangle\varphi_\mathrm{m}(\mathbf{r}),\quad(1)$$

where one has expanded the total wave function Ψ in terms of the crystal eigenfunctions $|\mathbf{n}\rangle$ corresponding to energy E_n:

$$\Psi(\mathbf{r},\{\mathbf{R}_i\})=\sum_\mathbf{n}|\mathbf{n}\rangle\varphi_\mathrm{n}(\mathbf{r}),\quad(2)$$

$\mathbf{r}$ being the particle position and $\mathbf{R}_i$ being the position of the ith crystal nucleus. In order to study the effect of crystal structure on the attenuation of an incident particle beam, it is convenient to take the crystal as initially in its ground state $|\mathbf{0}\rangle$ and to set up an equation for the coefficient $\varphi_0(\mathbf{r})$ of this ground state. Assuming that φ_0 is the major driving term in the equations for the other φ_n, one obtains the result

$$\varphi_\mathrm{n}(\mathbf{r})=-\frac{2m}{\hbar^2}\int d\mathbf{r}'\frac{e^{ik_\mathrm{n}|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|}V_{\mathrm{n}0}(\mathbf{r}')\varphi_0(\mathbf{r}'),\quad(3)$$

with $k_\mathrm{n}^2=(2m/\hbar^2)(E-E_\mathrm{n})$ and $V_{\mathrm{n}0}=\langle\mathbf{n}|V|\mathbf{0}\rangle$, where one has neglected $\sum_{\mathrm{m}\neq0}\langle\mathbf{n}|V|\mathbf{m}\rangle\varphi_\mathrm{m}$ with respect to $\langle\mathbf{n}|V|\mathbf{0}\rangle\varphi_0$. This is equivalent to treating the deviation of the interaction potential from periodicity (due to

[1] For a review see B. W. Batterman, Rev. Mod. Phys. **36**, 681 (1964).
[2] J. W. Knowles, Acta Cryst. **9**, 61 (1956).
[3] H. Yoshioka, J. Phys. Soc. (Japan) **12**, 618 (1957).
[4] For a review see J. Phys. Soc. (Japan) **17**, Suppl. B-II (1962).
[5] Yu. Kagan and A. Afamasiev, Zh. Eksperim i Teor. Fiz. **49**, 1504 (1965) [English transl.: Soviet Phys.—JETP (to be published].
[6] R. J. Finkelstein, Phys. Rev. **72**, 907 (1947).

motion of the lattice ions) in the Born approximation. Substitution of this approximation to φ_n in the equation for φ_0 leads to the form

$$\left\{\nabla^2+k_0^2-\frac{2m}{\hbar^2}\langle 0|V|0\rangle\right\}\varphi_0=-\left(\frac{2m}{\hbar^2}\right)^2\int d\mathbf{r}'\varphi_0(\mathbf{r}')\times\sum_{n\neq 0}V_{0n}(\mathbf{r})V_{n0}(\mathbf{r}')\frac{e^{ik_n|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|}. \quad (4)$$

This is the general first-order perturbation equation for the particle beam including the renormalization of the ground-state wave function represented by the right-hand side above. In an infinite periodic crystal φ_0 must have the form $e^{i\mathbf{k}_M\cdot\mathbf{r}}u(\mathbf{r})$, where u is a periodic function, and $\mathbf{k}_M$ is to be determined; this follows from the periodicity of V_{00} and of the integral kernel on the right-hand side of Eq. (4). One therefore looks for periodic wave solutions, matching these to the appropriate boundary conditions at the crystal surfaces. Expanding V_{00} and u as reciprocal lattice sums transforms Eq. (4) into

$$(\hbar^2/2m)[(\mathbf{k}_h+\mathbf{k}_M)^2-k_0^2]u_h+\sum_g V_{h-g}u_g+\sum_g C_{hg}u_g=0 \quad (5)$$

where we have written

$$V_{00}=\sum_h V_h e^{i\mathbf{k}_h\cdot\mathbf{r}},\quad u=\sum_h u_h e^{i\mathbf{k}_h\cdot\mathbf{r}}, \quad (6)$$

and

$$C_{hg}=-\frac{1}{V'}\frac{2m}{\hbar^2}\int d\mathbf{r}\int d\mathbf{r}' e^{-i(\mathbf{k}_h+\mathbf{k}_0)\cdot\mathbf{r}+i(\mathbf{k}_g+\mathbf{k}_0)\cdot\mathbf{r}'}\times\sum_{n\neq 0}V_{0n}(\mathbf{r})V_{n0}(\mathbf{r}')\frac{e^{ik_n|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|}$$

$\mathbf{k}_h$ and $\mathbf{k}_g$ being reciprocal lattice vectors, and V' being the crystal volume. Since the imaginary part of $\mathbf{k}_M\cdot\mathbf{r}$ is small over many unit cells of the crystal, we have set $\mathbf{k}_M=\mathbf{k}_0$ in calculating C_{hg}. The physical significance of the quantities C_{hg} can be seen most easily by specializing the interaction potential to delta-function form

$$V=\frac{2\pi\hbar^2}{\mu}\sum_{j=1}^{N}a_j\delta(\mathbf{r}-\mathbf{R}_j), \quad (7)$$

with a_j being the scattering length at $\mathbf{R}_j$ and μ the reduced mass. The imaginary part of C_{hg} is then found to be

$$\mathrm{Im}C_{hg}=-\frac{\hbar^2 m}{V'\mu^2}\sum_{n\neq 0}\int d\mathbf{k}\langle 0|\sum_{i=1}^{N}a_i e^{i(\mathbf{k}-\mathbf{k}_0-\mathbf{k}_h)\cdot\mathbf{R}_i}|\mathbf{n}\rangle\times\langle\mathbf{n}|\sum_{j=1}^{N}a_j e^{-i(\mathbf{k}-\mathbf{k}_0-\mathbf{k}_g)\cdot\mathbf{R}_j}|0\rangle\times\delta(k^2-k_0^2+(2m/\hbar^2)(E_n-E_0)), \quad (8)$$

while the real part of C_{hg} is related by dispersion in E to the imaginary part. In Eq. (8) we have used the momentum representation of the free-space Green's function

$$\frac{e^{ik_n|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|}=\frac{1}{(2\pi)^3}\int d\mathbf{k}\frac{e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}{k^2-k_n^2}.$$

For $\mathbf{k}_h=\mathbf{k}_g=0$, Eq. (8) can be written in terms of the inelastic crystal scattering cross section $\sigma^{(i)}$ as given by the standard Born approximation, using the Golden rule[7]:

$$\mathrm{Im}C_{00}\sim-\frac{\hbar^2 k_0}{V'2m}\sigma^{(i)}. \quad (9)$$

This measures the rate of loss of particles from the incident beam when only the leading term in the expansion of φ_0 is important. For $\mathbf{k}_h$ and $\mathbf{k}_g$ different from zero, one is thus calculating one term in the absorption rate for a Bloch wave φ_0.

It thus becomes a matter of primary importance to determine the coefficients of those waves in the expansion of φ_0 which have appreciable magnitude in order to calculate the actual rate of loss for the Bloch wave. Once this has been done, we can proceed to investigate the dependence of the attenuation on the physical parameters of interest, namely the strength of the interaction relative to the particle energy, the range of interaction relative to the atomic mean square displacement, and the wavelength of the incident particle.

III. VALIDITY AND CHARACTERISTICS OF ONE- AND TWO-WAVE SOLUTIONS

Let us now examine closely the conditions under which only a few waves are needed in the periodic expansion of φ_0. From Eq. (5) if only u_0 is to be large then one must require that the solution for u_h obtained with u_0 as the source term be small:

$$u_h=-\frac{V_h+C_{h0}}{(\hbar^2/2m)[(\mathbf{k}_h+\mathbf{k}_M)^2-k_0^2]+V_0+C_{hh}}\ll 1. \quad (10)$$

Clearly, except at a Bragg condition, one is dividing a Fourier coefficient of the potential ($C_{hg}\ll V_h$) by an energy of the order of

$$E_h\simeq(\hbar^2/2m)[\mathbf{k}_h^2+2\mathbf{k}_h\cdot\mathbf{k}_0].$$

For reciprocal lattice vectors perpendicular to $\mathbf{k}_0$ this is about 50 eV for electrons and about 0.025 eV for protons and neutrons. Away from the perpendicular, but still not fulfilling a Bragg condition, for $k_0\gg k_h$, the second term dominates, tending toward $E_p(k_h/k_0)$. Therefore at sufficiently large energy only the planes parallel to $\mathbf{k}_0$ contribute appreciably to φ_0. To justify the one-wave picture when such planes exist, it is

[7] G. Placzek, Phys. Rev. 86, 377 (1952).

necessary that the Fourier coefficients of the potential V_h be small compared to $V_0+\hbar^2k_h^2/2m$. For sufficiently high order reflections V_h will in any case be small compared to V_0, limiting thereby the number of waves which must be taken into account.

The two-wave solution will be a valid approximation when the inequality (10) is violated for a single reflection—e.g., when a Bragg condition is fulfilled. In this case, as is well known, there will exist two solutions for φ_0 having $\mathbf{k}_M$ essentially parallel to $\mathbf{k}_0$:

$$\begin{aligned}&\varphi_0=\varphi_0{}^0+\varphi_0{}^1,\\&\varphi_0{}^0\simeq\{\exp i[\mathbf{k}_0+\eta_+\hat{n}]\cdot\mathbf{r}\}[1-e^{i\mathbf{k}_h\cdot\mathbf{r}}],\\&\varphi_0{}^1\simeq\{\exp i[\mathbf{k}_0+\eta_-\hat{n}]\cdot\mathbf{r}\}[1+e^{i\mathbf{k}_h\cdot\mathbf{r}}],\end{aligned}\tag{11}$$

where $\hat{n}$ is a unit normal to the entrance surface of the crystal, pointing inward, and $\eta_\pm$ is given by

$$\eta_\pm=(k_0/2\gamma_0E_p)[\pm(V_h+C_{h0})-(V_0+C_{00})],\tag{12}$$

γ_0 being $\hat{k}_0\cdot\hat{n}$. The decay of these two solutions with penetration distance is determined solely by the imaginary part of $\eta_\pm$:

$$\mathrm{Im}\eta_\pm=[\pm\mathrm{Im}C_{h0}-\mathrm{Im}C_{00}](k_0/2\gamma_0E_p),\tag{13}$$

and one notices that for $\mathrm{Im}C_{h0}\simeq\mathrm{Im}C_{00}$ the solution corresponding to η_+ will propagate almost without attenuation while the other is attenuated at twice the rate of the off-Bragg (one-wave) solution. This is physically reasonable, since $|\varphi_0{}^0|^2$ has nodes at the atomic sites, where scattering out of the beam occurs, while $|\varphi_0{}^1|^2$ has its maxima there. One thus obtains the familiar phenomenon of anomalous transmission, when the crystal is sufficiently thick to exclude transmission off Bragg. Even when several orders of reflection from the same plane contribute appreciably to φ_0, these two solutions dominate and one still gets anomalous transmission (see, e.g., Ref. 8 for the many-beam solution in electron microscopy).

IV. POTENTIAL DEPENDENCE OF ANOMALOUS PENETRATION

Summarizing the results of the previous section, one may say that the validity of the one- and two-wave pictures is determined by the requirement that the ratio V_h/E_h be small for all but one plane, while the characteristic anomalous attenuation is proportional to $\mathrm{Im}C_{00}-\mathrm{Im}C_{0h}$. Our investigation of the potential dependence of the attenuation will thus proceed in two steps: first, establishment of the range of energy where the few-wave picture holds and second, calculation of $\mathrm{Im}C_{h0}$ from the interaction potential.

For neutrons the two-particle interaction potential is very local, being on the order of nuclear dimensions. For wavelengths larger than the nuclear scattering length a one can replace the actual interaction by a potential whose width is intermediate between the scattering length and the wavelength. We shall choose a form which passes directly over to the Fermi pseudopotential[9] as the width β^{-1} vanishes:

$$v(r)=\frac{-2\pi a\hbar^2}{\mu}\frac{\beta^3}{(\pi)^{3/2}}e^{-\beta^2r^2},\tag{14}$$

where μ is the reduced mass for the neutron-nucleus interaction. The crystal itself we shall approximate by a cubic lattice of local, independent harmonic oscillators of mass M and frequency ω (Einstein crystal). With these assumptions we obtain

$$V_h=-(2\pi a\hbar^2/\mu)\rho e^{-k_h^2/4\alpha^2},\tag{15}$$

where ρ is the number density of atoms in the crystal and $1/2\alpha^2$ is the mean square displacement $\langle x^2\rangle$ of the crystal atoms. Because the scattering length is so small ($\sim10^{-12}$ cm), even V_0 is only 10^{-7} eV, so that V_h/E_h off Bragg is never larger than 10^{-5}, independent of the neutron energy. The attenuation is therefore accurately given by that for the one- or two-wave solution, in terms of $\mathrm{Im}C_{h0}$. This latter quantity can be written, assuming a Gaussian potential and an Einstein crystal, in the form

$$\begin{aligned}\mathrm{Im}C_{h0}=-\pi\rho\left(\frac{2\pi a\hbar^2}{\mu}\right)^2\int\frac{d\mathbf{k}}{(2\pi)^3}e^{-(k_1^2+k_2^2)/4\beta^2}\\\times\sum_{n=1}^{\infty}\delta\left(\frac{\hbar^2k^2}{2m}-E_p+n\hbar\omega\right)\\\times e^{-(k_1^2+k_2^2)/4\alpha^2}\left[\frac{\mathbf{k}_1\cdot\mathbf{k}_2}{2\alpha^2}\right]^n\frac{1}{n!},\end{aligned}\tag{16}$$

where $\mathbf{k}_1=\mathbf{k}-\mathbf{k}_h-\mathbf{k}_0$ and $\mathbf{k}_2=\mathbf{k}-\mathbf{k}_0$. Note that the sum above runs over the excited states of a single oscillator.

Let us restrict our attention to neutron wavelengths small compared to the atomic mean-square displacement. There, because the width of the interaction β^{-1} is smaller still, one obtains the approximate result [to lowest order in $(\hbar\omega/E)$]

$$\begin{aligned}\mathrm{Im}C_{h0}=-\left(\frac{2\pi a\hbar^2}{\mu}\right)^2\frac{\rho mk_0}{2\pi\hbar^2}\\\times e^{-k_h^2/4\alpha^2}\left\{\frac{\beta^2}{2k_0{}^2}(1-e^{-2k_0^2/\beta^2})\right.\\\left.+\left[\left(1+\frac{m}{M}\right)^{-2}-1\right]e^{-2k_0^2/\beta^2}\right\}\end{aligned}\tag{17}$$

[8] P. B. Hirsch *et al.*, *Electron Microscopy of Thin Crystals* (Butterworths Scientific Publications Ltd., London, 1965), Chap. 12, p. 276 ff.

[9] J. Blatt and V. Weisskopf, *Theoretical Nuclear Physics*, (John Wiley & Sons, Inc. New York, 1952), p. 74 ff.

which through dispersion gives for the real part

$$\mathrm{Re}C_{h0}=-\left(\frac{2\pi a\hbar^2}{\mu}\right)^2\frac{\rho m}{4\pi\hbar^2}\beta \times e^{-k_h^2/4\alpha^2}\left(\frac{2}{\pi}\right)^{1/2}\left[\left(1+\frac{m}{M}\right)^{-2}+1\right]. \quad (18)$$

We see that $\mathrm{Re}C_{h0}$ grows with β, so that the width of the interaction cannot be allowed to pass to zero to regain the Fermi pseudopotential. However, $\mathrm{Re}C_{h0}$ acts only as a small correction to V_h, since

$$|\mathrm{Re}C_{h0}/V_h|\simeq a\beta\ll 1.$$

At the same time, since the width of the Gaussian must be chosen small compared to the neutron wavelength, $\mathrm{Im}C_{h0}$ becomes approximately

$$\mathrm{Im}C_{h0}\simeq-\sigma_{\mathrm{free}}\rho(\hbar^2k_0/2m)e^{-k_h^2/4\alpha^2}=e^{-k_h^2/4\alpha^2}\,\mathrm{Im}C_{00}, \quad (19)$$

where $\sigma_{\mathrm{free}}=4\pi a^2$ is the total neutron cross section of a free atom. Therefore the one-wave solution at short neutron wavelength is attenuated by the free atomic cross section[7]:

$$|\varphi_0{}^0|^2\sim\exp(-\rho\sigma_{\mathrm{free}}\hat{n}\cdot\mathbf{r}) \quad (20)$$

while the anomalously transmitted solution has attenuation given by

$$|\varphi_0{}^0|^2\sim\exp(-\rho\sigma_{\mathrm{free}}(1-\epsilon)\hat{n}\cdot\mathbf{r}), \quad (21)$$

where $1-\epsilon=1-e^{-k_h^2/4\alpha^2}\simeq 10^{-2}$. We thus see that for an interaction potential narrow compared to the mean square displacement, the attenuation at short wavelength is independent of the width of the potential.

For electrons or protons three types of transitions in the crystal become important: excitation of nonlocalized electrons, excitation of the electron cloud surrounding the lattice ion, and vibrational transition of the lattice ion. The first effect contributes a large directionally independent background to the total attenuation, while the latter two, because of their localization, will show anomalous behavior at Bragg angles. We shall illustrate the effect of the localization by consideration of the purely vibrational transitions, taking for simplicity a screened Coulomb interaction of appropriate range as the potential of interaction between incident charged particles and lattice atoms:

$$v(r)=(Z_1Z_2e^2/r)\exp(-\Lambda r), \quad (22)$$

where Λ^{-1} is the screening length, Z_1 is the charge (in units of e) on the incident particle, and Z_2 is the atomic number for the lattice atom. One obtains immediately

$$V_h=+\rho[4\pi Z_1Z_2e^2/(k_h^2+\Lambda^2)\exp(-k_h^2/4\alpha^2), \quad (23)$$

which is a number typically of the order of a few electron volts. Thus, to ensure that only the plane parallel to $\mathbf{k}_0$ contributes in the expansion of φ_0, we must take $\hbar^2k_hk_0/2m$ for the incident particle to be at least 100 eV. For electrons this requires an incident energy of about 400 eV and for protons, an energy of 1 MeV.

Because the one-wave attenuation as given by $\mathrm{Im}C_{00}$ has interesting structure as a function of $x_0\equiv\Lambda^2/2\alpha^2$, we shall consider this case separately. For the screened Coulomb the expression for $\mathrm{Im}C_{h0}$ becomes

$$\mathrm{Im}C_{h0}=-\pi\rho(4\pi Z_1Z_2e^2)^2 \times\int\frac{d\mathbf{k}}{(2\pi)^3}\frac{e^{-(k_1^2+k_2^2)/4\alpha^2}}{[k_1^2+\Lambda^2][k_2^2+\Lambda^2]} \times\sum_{n=1}^{\infty}\delta\left(\frac{\hbar^2k^2}{2m}-E_p+n\hbar\omega\right)\left(\frac{\mathbf{k}_1\cdot\mathbf{k}_2}{2\alpha^2}\right)^n\frac{1}{n!}. \quad (24)$$

At high energy one may write to lowest order in $(\hbar\omega/E)$

$$\mathrm{Im}C_{00}=\frac{-\hbar^2k_0}{2m}\rho\sigma_{\mathrm{free}}\int_{x_0}^{\infty}dx\,e^{-(x-x_0)}(x_0/x), \quad (25)$$

where σ_{free} is the screened-Coulomb free-particle elastic-scattering cross section in the Born approximation:

$$\sigma_{\mathrm{free}}=2\pi(Z_1Z_2e^2)^2m/\hbar^2E_p\Lambda^2. \quad (26)$$

The asymptotic behavior of the so-called exponential integral in Eq. (25) is well known. For large $x_0(\Lambda^2/2\alpha^2\gg 1)$ it tends to unity, while for small x_0 one has

$$\int_{x_0}^{\infty}dx\,e^{-(x-x_0)}(x_0/x)\sim x_0[-\gamma-\ln x_0], \quad (27)$$

where $\gamma=0.57721\cdots$ is Euler's constant. Thus, when the screening length is small compared to the atomic mean-square displacement the one-wave solution is attenuated by the full free cross section, just as in the case of neutrons. But when the interaction potential becomes broad compared to the mean square displacement, the attenuation of the one-wave solution falls far below the free cross-section value, going approximately as $\Lambda^2\langle x^2\rangle\ln(\Lambda^2\langle x^2\rangle)$. This result can also be obtained by considering only the one-phonon transition in the original expression [Eq. (2)] for $\mathrm{Im}C_{00}$ (dipole approximation). For $\Lambda=0$ (pure Coulomb) one must retain first-order terms in $\hbar\omega/E$ in the expression for $\mathrm{Im}C_{00}$, giving

$$\mathrm{Im}C_{00}\simeq\frac{\hbar^2k_0}{2m}\rho\frac{\pi(Z_1Z_2e^2)^2}{E_p\hbar\omega}\frac{m}{M}\ln\left(\frac{4\hbar\omega}{E_p}\frac{m}{M}\right). \quad (28)$$

The character of the screened-Coulomb attenuation is essentially undisturbed by consideration of more than one wave. For k_h small compared to Λ one obtains (for $|\mathbf{k}_0+\mathbf{k}_h|=k_0$)

$$\mathrm{Im}C_{h0}=-\frac{\hbar^2k_0}{2m}\sigma_{\mathrm{free}} \times e^{-k_h^2/4\alpha^2}\left[\left(1+\frac{k_h^2}{8\alpha^2}\right)\int_{x_0}^{\infty}e^{-(x-x_0)}(x_0/x)dx-\frac{k_h^2}{6\alpha^2}\right] \quad (29)$$

which for $\Lambda^2\langle x^2\rangle$ small tends to

$$\mathrm{Im}C_{h0}\sim(\hbar^2k_0/2m)\sigma_{\mathrm{free}}[x_0\ln x_0+k_h^2/6\alpha^2] \quad (30)$$

while for $\Lambda^2\langle x^2\rangle$ large one, has

$$\mathrm{Im}C_{h0}\sim e^{-k_h^2/4\alpha^2}(1-k_h^2/24\alpha^2)\,\mathrm{Im}C_{00} \quad (31)$$

which differs only by the factor in parentheses from the relation obtained in the neutron case, Eq. (19). The attenuation for the anomalously transmitted solution for $\Lambda^2\langle x^2\rangle$ small is, from Eqs. (13) and (30),

$$\mathrm{Im}\eta_+=(\rho\sigma_{\mathrm{free}}/\gamma_0)(k_h^2/12\alpha^2) \quad (32)$$

which is typically a factor of 100 smaller than the attenuation one would calculate from the free cross section.

V. CONCLUSIONS

From the foregoing calculations several characteristics of anomalous particle penetration emerge. First, the existence of an anomalous effect has nothing directly to do with the wavelength of the incident particle, but rather is determined by two criteria, namely that the interaction potential be sufficiently weak compared to the particle energy [Eq. (10)] and that the interaction is localized in the vicinity of the lattice sites. This last condition ensures that the anomalous solution will be negligibly attenuated compared to the one-wave solution. At high particle energy the effect of the atomic mean-square displacement has been shown to be negligible when the range of the potential is small compared to it; however, when the reverse is true, the attenuation depends strongly on the ratio of these two lengths, falling markedly below the attenuation which one would calculate using the total free-particle cross section. This suggests that one could observe experimentally variations in the intensity of the transmitted elastic wave with atomic mean-square displacement. Such an experiment might be carried out with high-energy electrons, providing that the large inelastic background could be sufficiently reduced by energy selection on the transmitted beam.

For MeV protons there exists the possibility of detecting anomalous behavior by observation of nuclear reactions such as neutron production, even in the presence of large nonlocal electronic attenuation. If the crystal is thick enough to absorb the incident proton beam, a dip in the number of neutrons produced will be observed at the Bragg angle, the intensity ratio being given by

$$\frac{I_N(\mathrm{Bragg})}{I_N(\mathrm{Normal})}\simeq 1-\epsilon_p\left(\frac{\sigma_p}{\sigma_f+\sigma_p}\right), \quad (33)$$

where σ_p and σ_f are the charged-particle scattering cross sections from the lattice atoms and the free electrons, respectively, and ϵ_p for a broad screened-Coulomb potential is, from Eqs. (25) and (30)

$$\epsilon_p=[1-k_h^2/3\Lambda^2\ln(2\alpha^2/\Lambda^2)]. \quad (34)$$

These formulas apply so long as the neutron production cross section is small compared to either σ_p or σ_f. Thompson[10] has performed an experiment of this type with 2.8-MeV protons incident on copper in the $\langle 110\rangle$ direction, where a 5% decrease in neutron production was observed at the Bragg angle. This is consistent with a value of ϵ_p near unity, since σ_p/σ_f is generally considered to be about 5% at these energies. One sees from Eq. (33) that even when the atomic interaction potential is poorly localized, so that ϵ_p departs significantly from unity, the anomalous effect persists, providing a means of probing the distribution of charged particles inside the crystal.

[10] M. W. Thompson, Phys. Rev. Letters **13**, 756 (1964).