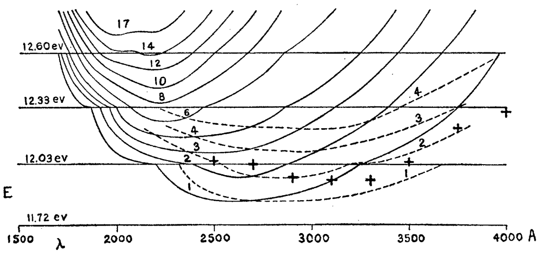

FIG. 7. Relations between I_λ, λ, and energy of exciting electrons E, for H_2. Lines of constant I_λ(——). Lines of constant illumination of plate in quartz spectrograph (- - - -). Data of Finkelnberg and Weizel (+ +). Intensities in arbitrary units.

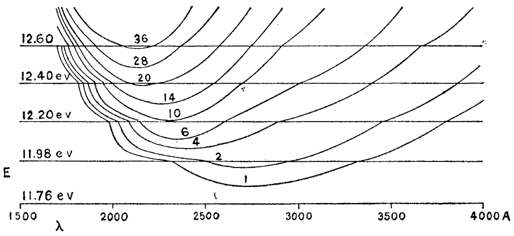

FIG. 8. Lines of constant I_λ for D_2. For explanation see Fig. 7.

plate, and this in turn corresponds to equal exposure, we may say that our calculations agree with their results to within the experimental error, estimated as 0.05 ev. Unfortunately there is no adequate reason to suppose that the assumed conditions are even approximately fulfilled. It seems more than ever desirable to obtain accurately controlled experimental results of this type also.

In conclusion, we wish to thank the Electrical Engineering Department of the Massachusetts Institute of Technology for the use of the differential analyzer. Also, one of us (H. M. J.) wishes to acknowledge gratefully a grant from the Society of Sigma Xi, which materially aided in the progress of this work.

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Capture of Neutrons by Atoms in a Crystal*

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The precise determination of the properties of nuclear resonance levels from the capture of slow neutrons is made difficult by the fact that most of the substances used for absorbers and detectors are in the solid state, so that the calculations of Bethe and Placzek for the influence of the Doppler effect are inapplicable, since these were based on the assumption of a perfect gas. In this paper, their calculations are generalized to include the effect of the lattice binding. Under the assumption that the crystal may be treated as a Debye continuum, it is shown that for sufficiently weak lattice binding, the absorption curve has the same form as it would in a gas, not at the temperature T of the crystal, however, but at a temperature which corresponds to the average energy per vibrational degree of freedom of the lattice (including zero-point energy). In cases of somewhat stronger lattice binding, the line form is found to be more complicated, and may even have a fine structure. Plots are given of the absorption line in several typical cases. An approximate formula for the cross section for self-indication is also derived.

ACCORDING to the theory of the compound nucleus proposed by Bohr and by Breit and Wigner,[1] the cross section for the capture of a slow neutron with an energy near to a resonance level of a nucleus at rest in free space is given by an equation of the form

$$\sigma=\frac{\Gamma^2}{4}\frac{\sigma_0}{(E-E_0-R)^2+\frac{1}{4}\Gamma^2},\tag{1}$$

where σ_0, the cross section at resonance, varies inversely with v, the velocity of the neutron in the rest system, E is the kinetic energy of the neutron, and E_0 is the energy that the neutron

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[1] N. Bohr, Nature **137**, 344 (1936); G. Breit and E. Wigner, Phys. Rev. **49**, 519 (1936).

would have at resonance if the atom were infinitely heavy so that the compound nucleus would take up no recoil energy. For atoms of finite mass, the recoil energy $R=(m/M)E$ must be included in the energy denominator.[2] (We assume that the mass M of the atom is much greater than the mass m of the neutron, and neglect terms of higher order in m/M.) Γ is the total half-value width of the resonance level, and is proportional to the rate of decay of the compound nucleus; in most cases this corresponds to the process of emission of a high energy gamma-ray.

Actually, of course, it never happens that one has to do with a free atom at rest. This somewhat complicates the determination of the properties of the resonance level from slow neutron data. The atoms in a gas may be treated as free, but at finite temperatures, there is a Maxwellian distribution of velocities, and Eq. (1) must be modified, as has been done by Bethe and Placzek[3, 4] for this case. It is here necessary to change the resonance energy denominator according to the relative velocity of the neutron and atom, and to average over the Maxwellian distribution of velocities of the gas atoms. The proportionality of the cross section to $1/v$ is thereby unaltered, as this factor arises just from the normalization of the incident neutron wave function to unit flux required by the definition of a cross section. The result of the averaging gives

$$\sigma=\sigma_0\psi(\xi, x), \tag{2}$$

where

$$x=(E-E_0-R)/\tfrac{1}{2}\Gamma, \quad \xi=\Gamma/\Delta \tag{3}$$

and

$$\Delta=2(RT)^{\frac{1}{2}} \tag{4}$$

is the "Doppler" width of the level.[5] The function

$$\psi(\xi, x)=\frac{\xi}{2\pi^{\frac{1}{2}}}\int_{-\infty}^{\infty} dy\frac{e^{-\frac{1}{4}\xi^2(x-y)^2}}{1+y^2} \tag{5}$$

becomes simple in the following limiting cases:

(a) $x\gg 1/\xi^2, \quad \psi\rightarrow 1/(1+x^2)$,

i.e., far enough from resonance, the line has its normal form.

(b) $\xi\gg 1, \quad \psi\rightarrow 1/(1+x^2)$,

i.e., when the natural breadth is much larger than the Doppler breadth, the line is again normal.

(c) $\xi\ll 1, \quad x\ll 1/\xi^2, \quad \psi\rightarrow\frac{1}{2}\pi^{\frac{1}{2}}\xi e^{-\frac{1}{4}\xi^2x^2}$,

i.e., when the natural width is small compared to the Doppler width, the absorption line has an effective width strongly dependent on the temperature.

The total activation induced in a thin detector by a beam of neutrons distributed smoothly in energy is proportional to the area under the absorption curve

$$\int dE\sigma_0\psi(\xi, x)=\tfrac{1}{2}\pi\Gamma\sigma_0, \tag{6}$$

independently of the temperature of the gas. Another quantity of experimental interest is σ_s, the cross section for self-indication[6]

$$\begin{aligned}\sigma_s=\int\sigma^2dE\Big/\int\sigma dE&=\tfrac{1}{2}\sigma_0\psi(\xi\sqrt{2}, 0)\\&=(\tfrac{1}{2}\pi)^{\frac{1}{2}}\xi e^{\frac{1}{2}\xi^2}[1-\Phi(\xi/\sqrt{2})],\end{aligned} \tag{7}$$

where Φ is the Gaussian error function.

The above results are valid, however, only for free atoms. Most of the experiments, of course, have been performed with solid absorbers and detectors in which the atoms are bound in a crystal lattice of some sort with a characteristic Debye temperature of the order of room temperature, and if the chemical binding is of importance, as we shall see is the case, it is clearly not permitted to apply the free atom theory of the Doppler broadening, as was done by Bethe,[4] to such cases as silver at ordinary temperatures.

We shall want, therefore, to calculate the shape of the absorption line for an atom which is bound in a crystal lattice. We do not expect that the chemical binding will cause any difference in

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[2] As it is usually written, the capture cross section refers to the coordinate system in which the compound nucleus is at rest, so that no energy of recoil appears in the denominator of Eq. (1).

[3] H. Bethe and G. Placzek, Phys. Rev. **51**, 462 (1937).

[4] H. Bethe, Rev. Mod. Phys. **9**, 140 (1937).

[5] We will measure temperatures in energy units, taking the Boltzmann constant to be unity. The results quoted here were derived on the assumption that the Doppler width of the level is much less than the energy E_0 at resonance of the neutron. This condition is satisfied in all cases of practical interest, and we shall have occasion to assume it in our calculations also.

[6] See reference 4, Eq. (520).

the $1/v$ variation of the capture cross section. This has been shown analytically for the case of capture by bound protons,[7] but the result is much more generally valid, following in every case just from the normalization of the neutron wave function. The calculation will be made without detailed assumptions about the crystal model, but in using the final result, for simplicity, we will treat the crystal as a Debye continuum, and hence the results will not admit of an exact application to experimental cases. Nevertheless, the general features of the dependence of the absorption line on the characteristics of the lattice and on the temperature may be expected to be fairly independent of the detailed model. For just as in the theory of specific heat, there are several limiting cases in which the results may not depend on the model of the lattice assumed, so that any fairly smooth interpolation should approximate the rigorous result fairly closely. For example, let us consider a crystal lattice at the temperature absolute zero. If the lattice binding is sufficiently strong (as defined below), the absorption line will be normal in form, but centered about $E=E_0$, while for very weak binding, as for instance might be the case with a different substance containing the atom in question, the absorption line will again be normal in form, but centered about an energy $E=E_0+R$. Since in practice, this shift R is often of the order of Γ, the half-width of the absorption line, this change in the curve can be experimentally important, even though the recoil energy is numerically quite small. It might thus be possible to detect the effect of the chemical binding, especially at low temperatures, by use of different crystals, containing in common an element with a slow neutron resonance capture level, but in which the remaining elements do not appreciably capture or scatter slow neutrons of the resonance energy.

In the intermediate cases, the shape of the absorption line is in general much more complicated. However, in the case of weak binding, as defined below, it will be possible to treat the bound atoms as if they were in a gas, not however with a temperature T, but at a larger temperature corresponding to the average energy per vibrational degree of freedom (including zero-point energy) of the crystal.

We must now ask for the probability $W(\{\beta_s\};\{\alpha_s\})$ for the capture of a neutron of momentum $\mathbf{p}$ by a definite lattice atom L of nuclear type A to form a nucleus B with emission of a gamma-ray of wave vector $\mathbf{k}$ when the crystal undergoes a transition from a state $\{\alpha_s\}$ to a state $\{\beta_s\}$. Here the set of numbers denoted by $\{\alpha_s\}$ gives the numbers α_s of quanta (phonons) in the various modes s of oscillation in the lattice. We must consider that the final state is reached through an intermediate state in which there is neither neutron nor gamma-ray, but a compound nucleus[8] C with the lattice in a state $\{n_s\}$. The usual dispersion theory gives, apart from a trivial constant factor,

$$W(\{\beta_s\};\{\alpha_s\}) = \left|\sum_{n_s} \frac{(B\beta_s\mathbf{k}|H'|Cn_s)(Cn_s|H'|A\alpha_s\mathbf{p})}{E_0-E+E(n_s)-E(\alpha_s)+(i/2)\Gamma(n_s)}\right|^2, \tag{8}$$

where $\Gamma(n_s)$ is the total half-value width of the intermediate state (C, n_s).[9] Because of the short range of nuclear forces and hence the independence of the motion in the crystal of the center of gravity and the internal degrees of freedom of the nucleus, the matrix elements of the perturbation H' which appear in the numerator of (8) can be factored into

$$\begin{aligned} (Cn_s|H'|A\alpha_s\mathbf{p}) &= (n_s|\exp(i\mathbf{p}\cdot\mathbf{x}_L/\hbar)|\alpha_s)M_{\text{comp}}, \\ (B\beta_s|H'|Cn_s) &= (\beta_s|\exp(-i\mathbf{k}\cdot\mathbf{x}_L/\hbar)|n_s)M_{\text{rad}}(\mathbf{k}), \end{aligned} \tag{9}$$

where $M_{\text{rad}}(k)$ and M_{comp} are the matrix elements for radiation and compound nucleus formation, respectively, for a free nucleus, and, for example,

$$(n_s|\exp(i\mathbf{p}\cdot\mathbf{x}_L/\hbar)|\alpha_s)$$

is the matrix element for transfer of a momentum

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[7] W. E. Lamb, Jr., Phys. Rev. **51**, 187 (1937).

[8] We will ignore throughout the circumstance that the compound nucleus C is heavier than the atom A. This neglect is certainly valid if $m \ll M$, as is the case in practice, and may be seen to subject our results to a limitation on the effective width of the level analogous to that met by Bethe and Placzek (reference 5) for free atoms. As there, this limitation is of no importance experimentally.

[9] The curly brackets denoting a set of numbers will be dropped when it will not cause confusion.

$\mathbf{p}$ to the crystal through the Lth atom with excitation of the lattice from a state $\{\alpha_s\}$ to a state $\{n_s\}$. In practice, the lattice is in thermal equilibrium, therefore not in a definite state $\{\alpha_s\}$, and further, because of the high energy of the gamma-ray, the experiments will give only the total probability of capture, i.e., not

$$W(\{\beta_s\};\ \{\alpha_s\})$$

but

$$W(E)=\sum_{\beta_s}\sum_{\alpha_s} g(\{\alpha_s\})W(\{\beta_s\};\{\alpha_s\}), \tag{10}$$

where the sum over the initial states of the lattice is weighted according to the Boltzmann factor $g(\{\alpha_s\})$ for each state when the temperature of the lattice is T. Because of over-all conservation of energy, the magnitude of the wave vector $\mathbf{k}$ in (8) is a function of the final state of the lattice $\{\beta_s\}$. In all cases of importance, however, one may neglect a variation of $\mathbf{k}$ of the order of the zero-point energy of oscillation in the lattice, and perform the sum over the final states of the lattice by use of the completeness relations, finding

$$W(E)=|M_{\mathrm{rad}}|^2|M_{\mathrm{comp}}|^2\sum_{\alpha_s} g(\alpha_s) \times\sum_{n_s}\frac{|(n_s|\exp(i\mathbf{p}\cdot\mathbf{x}_L/\hbar)|\alpha_s)|^2}{[E-E_0-\sum_s(n_s-\alpha_s)\hbar\omega_s]^2+\frac{1}{4}(\Gamma(n_s))^2}, \tag{11}$$

where the energy of the lattice has been expressed in terms of the frequencies ω_s of the lattice oscillations. Thus one sees that the probability of gamma-ray emission is proportional just to the probability of formation of a compound nucleus C irrespective of the state of the lattice, and this despite the fact that very often a gamma-ray may be emitted in a time short compared to the periods of oscillation of the lattice, giving the atom a recoil energy of the order of a hundred volts. Eq. (11) will be much less complicated if one may neglect the dependence of $\Gamma(n_s)$ on the state $\{n_s\}$ of the lattice. This will be so except in the case, unimportant for our purposes, that the main contribution to Γ comes from the emission of slow neutrons, i.e., in case of a large elastic scattering cross section instead of a large capture cross section. If one were also to neglect the energy given to the lattice, the expression (11), from which we will now drop the factor $|M_{\mathrm{comp}}M_{\mathrm{rad}}|^2$, by use once more of the completeness relation would reduce just to

$$1/[(E-E_0)^2+\tfrac{1}{4}\Gamma^2],$$

since

$$\sum_{\alpha_s} g(\{\alpha_s\})=1.$$

We now turn to an evaluation of the matrix elements in Eq. (11). In terms of the wave functions[9]

$$\psi_{n_s}(\mathbf{x}_1,\cdots,\mathbf{x}_N)$$

of the crystal, which is assumed to be periodic in a large volume containing N atoms whose positions are denoted by $\mathbf{x}_1,\cdots,\mathbf{x}_N$, this matrix element is

$$(\{n_s\}|\exp(i\mathbf{p}\cdot\mathbf{x}_L/\hbar)|\{\alpha_s\}) =\int\cdots\int d\mathbf{x}_1 d\mathbf{x}_2\cdots d\mathbf{x}_N\psi_{n_s}{}^*(\mathbf{x}_1\mathbf{x}_2\cdots\mathbf{x}_N) \times\exp(i\mathbf{p}\cdot\mathbf{x}_L/\hbar)\psi_{\alpha_s}(\mathbf{x}_1\cdots\mathbf{x}_N). \tag{12}$$

We introduce normal coordinates for the crystal in the usual form:[10]

$$\begin{aligned}\mathbf{x}_G&=\mathbf{x}_G{}^0+\mathbf{u}_G\\ \mathbf{u}_G&=\frac{1}{N^{\frac{1}{2}}}\sum_{\mathbf{q}}\sum_{j}\mathbf{e}_{\mathbf{q}j}(A_{\mathbf{q}j}\exp(i\mathbf{q}\cdot\mathbf{x}_G{}^0/\hbar)+\mathrm{conj.}),\end{aligned} \tag{13}$$

where $\mathbf{x}_G{}^0$ is the equilibrium position of the Gth atom, $\mathbf{u}_G$ its displacement from equilibrium, $\mathbf{e}_{\mathbf{q}j}$ is the unit polarization vector for the wave characterized by the propagation vector $\mathbf{q}$ and polarization j. The spectrum of eigenvibrations is determined by the periodic boundary conditions, and it is cut off at an upper frequency limit such that the number of degrees of freedom agrees with the number $3N$ belonging to the N atoms in the fundamental volume of the lattice. The single index s will often be used to denote the pair of indices $(\mathbf{q}, j)$. In terms of the quantities

$$\begin{aligned}Q_s&=A_s+A_s{}^*\\ P_s&=M\dot{Q}_s=iM\omega_s(A_s-A_s{}^*),\end{aligned} \tag{14}$$

where ω_s is the frequency belonging to the sth normal mode, the Hamiltonian of the crystal

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[10] See for instance, A. Sommerfeld and H. Bethe, *Handbuch der Physik*, vol. 24/2, second edition (1933), p. 500.

takes the form appropriate for a system of linear harmonic oscillators with coordinates Q_s and momenta P_s

$$H=\sum_s H_s,$$

$$H_s=\tfrac{1}{2}M\omega_s^2Q_s^2+P_s^2/2M. \tag{15}$$

The eigenvalues of this Hamiltonian are

$$E_s=(n_s+\tfrac{1}{2})\hbar\omega_s;\quad n_s=0,\,1,\,2,\,\cdots$$

and the wave functions normalized in terms of

$$\xi_s=Q_s(\hbar/2M\omega_s)^{-\frac{1}{2}}$$

are
$$\psi_{n_s}(Q_s)=(2\pi)^{-\frac{1}{4}}(n_s!)^{-\frac{1}{2}}e^{-\frac{1}{4}\xi_s^2}h_{n_s}(\xi_s),$$

where $h_{n_s}(\xi_s)$ is the n_sth Hermite polynomial. If, for convenience, we take the rest position of the capturing atom $\mathbf{x}_L{}^0=0$, as may be done without loss of generality, the matrix element (12) with the help of Eq. (13) takes the form

$$\prod_s\int_{-\infty}^{\infty}d\xi_s\psi_{n_s}(\xi_s)\exp\left(i\mathbf{p}\cdot\mathbf{e}\xi_s/(2M\hbar\omega_sN)^{\frac{1}{2}}\right)\psi_{\alpha_s}(\xi_s), \tag{16}$$

where the product is to be extended over all the normal modes. Integrals of the form

$$K(n_s,\,\alpha_s;\,q_s)=\int_{-\infty}^{\infty}d\xi\psi_{n_s}e^{iq_s\xi_s}\psi_{\alpha_s}(\xi_s)$$

are readily evaluated[11] by use of the generating formula for the Hermite polynomials. In our case,

$$q_s^2=\frac{(\mathbf{p}\cdot\mathbf{e}_s)^2}{2M\hbar\omega_sN}$$

and is arbitrarily small if we take the fundamental volume of the crystal large enough, so that only terms to the first order in q_s^2 need be kept in $K(n_s,\,\alpha_s;\,q_s)$, as will be seen more clearly below. Then there are three possibilities:

$$|K(\alpha_s,\,\alpha_s;\,q_s)|^2=(1-2\alpha_sq_s^2)e^{-q_s^2}, \tag{17a}$$

$$|K(\alpha_s+1,\,\alpha_s;\,q_s)|^2=(\alpha_s+1)q_s^2e^{-q_s^2}, \tag{17b}$$

$$|K(\alpha_s-1,\,\alpha_s;\,q_s)|^2=\alpha_sq_s^2e^{-q_s^2}, \tag{17c}$$

as all the other K's are of higher order. The q_s^2 will enter the final result only linearly in sums like

$$\sum_s q_s^2\backsimeq R/\theta,$$

where θ is the Debye temperature of the substance. Any sums of the form $\sum_s q_s^4$, etc. would vanish as the transition to the continuum is made, which provides a justification for neglect of the higher powers of the q_s^2 in Eqs. (17).

Consider now the expression

$$W(\alpha_s)=\sum_{n_s}\frac{\Pi_s|K(n_s,\,\alpha_s;\,q_s)|^2}{[E-E_0-\sum_s(n_s-\alpha_s)\hbar\omega_s]^2+\frac{1}{4}\Gamma^2}. \tag{18}$$

This is made difficult to evaluate only by the presence in the denominator of the term $\sum_s(n_s-\alpha_s)\hbar\omega_s$. This suggests that it will be convenient to group together the terms in the expression for which this quantity has the same value. One may accomplish this most easily by the introduction of a delta-function, writing (18) as

$$\int_{-\infty}^{\infty}d\rho\delta(\rho-\sum_s(n_s-\alpha_s)\hbar\omega_s)$$
$$\times\sum_{n_s}\frac{\Pi_s|K(\;)|^2}{(E-E_0-\rho)^2+\frac{1}{4}\Gamma^2}, \tag{19}$$

where for the delta-function, use is made of the usual representation

$$\delta(x)=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\mu e^{i\mu x}. \tag{20}$$

Thus one finds

$$W(\alpha_s)=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\rho\int_{-\infty}^{\infty}d\mu\frac{e^{i\mu\rho}}{(E-E_0-\rho)^2+\frac{1}{4}\Gamma^2}$$
$$\times\sum_{n_s}\prod_s\{|K(n_s,\,\alpha_s;\,q_s)|^2$$
$$\times\exp\left(-i\mu(n_s-\alpha_s)\hbar\omega_s\right)\}. \tag{21}$$

From Eqs. (17), one finds

$$I_s=\sum_{n_s}|K(n_s,\,\alpha_s;\,q_s)|^2\exp -i\mu(n_s-\alpha_s)\hbar\omega_s$$
$$=e^{-q_s^2}\{1+q_s^2[-2\alpha_s+(\alpha_s+1)e^{-i\mu\hbar\omega_s}$$
$$+\alpha_se^{i\mu\hbar\omega_s}]\}. \tag{22}$$

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[11] F. Bloch and A. Nordsieck, Phys. Rev. **52**, 54 (1937).

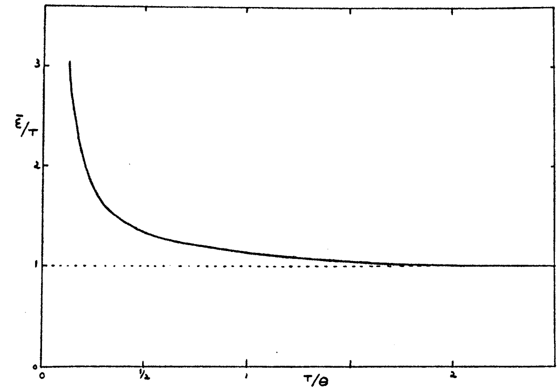

FIG. 1. Plot of the ratio of "effective temperature" and real temperature of a crystal as a function of the real temperature measured in units of the Debye temperature of the substance.

At this point it is most convenient to carry out the average over the values of the initial quantum numbers α_s, since now each α_s appears at most linearly. The result of the averaging is that each α_s above is replaced by its average value $\bar{\alpha}_s$ at thermal equilibrium, where

$$\bar{\alpha}_s = \frac{1}{e^{\hbar\omega_s/kT}-1}. \tag{23}$$

The product over the various oscillators s is then of the form

$$\prod_s (1+\lambda_s q_s^2) = 1 + \sum_s \lambda_s q_s^2 + \sum_{s<r}\sum \lambda_s \lambda_r q_s^2 q_r^2 + \cdots \tag{24}$$

and if one remembers the smallness of the q_s^2, the series may be summed to give $\exp(\sum_s \lambda_s q_s^2)$, so that

$$I = \prod_s I_s = \exp \sum_s q_s^2 \{(\bar{\alpha}_s+1)e^{-i\mu\hbar\omega_s} + \bar{\alpha}_s e^{i\mu\hbar\omega_s} - 2\bar{\alpha}_s\}. \tag{25}$$

Thus one has

$$W(E) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\rho \int_{-\infty}^{\infty} d\mu \frac{e^{i\mu\rho+g(\mu)}}{(E-E_0-\rho)^2+\frac{1}{4}\Gamma^2}. \tag{26}$$

where the function $g(\mu)$ is given by

$$g(\mu) = \sum_s q_s^2 \{(\bar{\alpha}_s+1)e^{-i\mu\hbar\omega_s} + \bar{\alpha}_s e^{i\mu\hbar\omega_s} - 1 - 2\bar{\alpha}_s\}. \tag{27}$$

The integral over ρ in (26) may be done at once by residue formation, and one has the generally valid final result

$$W(E) = 2/\Gamma \text{ Real} \int_0^{\infty} d\mu \times \exp[i\mu(E-E_0+i\Gamma/2)+g(\mu)]. \tag{28}$$

Naturally, it would be most difficult to evaluate $W(E)$ exactly. One may however easily obtain simple expressions which are valid in the various limiting cases. The function $g(\mu)$ is the cause of the complication, and it is possible to evaluate the integral (28) analytically only in cases where the values of μ given by $\mu\theta \sim 1$ do not play a dominant role. For $\mu\theta \ll 1$, one may expand in powers of μ and obtain

$$g(\mu) = -i\mu \sum_s q_s^2 \hbar\omega_s - \mu^2 \sum_s q_s^2 (\bar{\alpha}_s + \tfrac{1}{2})(\hbar\omega_s)^2 + \cdots. \tag{29}$$

The sums may be evaluated under the assumption of an isotropic crystal, i.e., the velocity of a wave is assumed to be independent of its direction of propagation, although not necessarily of its polarization; and one finds

$$g(\mu) = -i\mu R - \mu^2 R\bar{\epsilon}, \tag{30}$$

where R is again the recoil energy and $\bar{\epsilon}$ the average energy per vibrational degree of freedom of the crystal (including zero point energy). If the condition

$$\tfrac{1}{2}\Gamma + (R\bar{\epsilon})^{\frac{1}{2}} \gg \theta \tag{31}$$

("weak binding")

is met, only small values of μ in $g(\mu)$ in the integral (28) need be considered, and one finds

$$\begin{aligned} W(E) &= \frac{2}{\Gamma}\int_0^{\infty} d\mu \cos\mu(E-E_0-R) \times \exp(-\tfrac{1}{2}\Gamma\mu - \mu^2 R\bar{\epsilon}) \\ &= \frac{4}{\Gamma^2}\int_0^{\infty} dy \cos yx \exp(-y-y^2/\xi^2) \\ &\equiv (4/\Gamma^2)\psi(\xi, x), \end{aligned} \tag{32}$$

where $\psi(\xi, x)$,[12] x, and ξ are as defined by Eqs.

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[12] Equation (32) gives Reiche's form of the ψ-function. See Born, *Optik* (1933), p. 482.

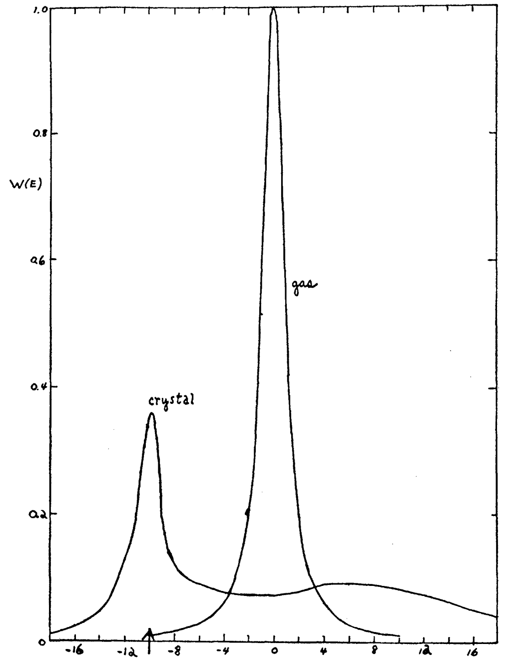

FIG. 2. Plot of the neutron resonance absorption curve in cold solid silver for an assumed value of Γ equal to $\theta/4$. The curve one would obtain with free atoms is shown for comparison. The abscissa measures the distance from resonance in units of $\frac{1}{2}\Gamma$. If the lattice binding were very strong, the curve for the crystal would have the same form for the gas, except that it would be centered about the point shown by the arrow.

(5) and (3), but now with an effective Doppler width

$$\Delta = 2(R\bar{\epsilon})^{\frac{1}{2}}, \tag{33}$$

which involves $\bar{\epsilon}$ instead of T. Thus we see that provided only the condition $\Delta + \Gamma \gg 2\theta$ is met, the atoms in a crystal at a temperature T give the same absorption line as they would in a gas at a temperature $\bar{\epsilon}$ equal to the average energy per vibrational degree of freedom of the crystal. This quantity is well known from the theory of specific heats

$$\bar{\epsilon} = \tfrac{1}{3}(\bar{\epsilon}_l + 2\bar{\epsilon}_t), \tag{34}$$

where

$$\bar{\epsilon}_j(T) = 3\left(\frac{T}{\theta}\right)^3 T \int_0^{\theta_j/T} dt\, t^3 \left(\frac{1}{e^t - 1} + \tfrac{1}{2}\right), \tag{34j}$$

where the indices l and t refer to the longitudinal and transverse waves. One has the limiting values

$$\bar{\epsilon} = T + \theta \cdot O(\theta/T) \qquad T \gg \theta \tag{34a}$$

$$\bar{\epsilon} = \tfrac{1}{8}(\theta_l + 2\theta_t) + T \cdot O(T^3/\theta^3). \tag{34b}$$

In Fig. 1, a plot is given of $\bar{\epsilon}(T)/T$ as a function of T/θ for the case that the various characteristic temperatures are equal.

The other limiting case is $\mu\theta \gg 1$. Here one finds

$$g(\infty) = -2\sum_s q_s^2(\bar{\alpha}_s + \tfrac{1}{2}) = -\tfrac{1}{3}[G(T/\theta_l) + 2G(T/\theta_t)], \tag{35}$$

where

$$G(x) = \frac{2R}{T} x^3 \int_0^{1/x} dt\, t\left(\frac{1}{e^t - 1} + \tfrac{1}{2}\right) \tag{36}$$

with

$$G(x) = xR/T \quad x \ll 1, \tag{36a}$$

$$G(x) = \frac{2R}{T} x^2 \quad x \gg 1. \tag{36b}$$

For special ranges of values of $E - E_0$, one may obtain a good approximation to $W(E)$ by splitting the range of integration in Eq. (28) at $\mu\theta = 1$, and in each range, using the appropriate expansion for $g(\mu)$. One finds in this way that for very strong binding of the atoms in the crystal ($\theta \to \infty$),

$$W(E) = \frac{1}{(E - E_0)^2 + \frac{1}{4}\Gamma^2}, \tag{37}$$

i.e., the normal absorption line centered about $E = E_0$.

In general, however, a certain amount of numerical integration is required to find the shape of the line. To illustrate the possibility of using the general Eqs. (28) and (27) except in the two limiting cases of Eqs. (31) and (37), we give plots of a $2\frac{1}{2}$-volt resonance energy absorption line in a substance at a temperature much lower than the Debye temperature of $\theta = 210°\text{K}$ (Case of cold silver if one abstracts from the difference between θ_l and θ_t), for several assumed values of Γ. In each case, the curve for free atoms at the same temperature is also shown. One sees that for these cases of intermediate binding, there is a rudimentary fine structure in the probability of capture which is suggestive of the neutron absorption *lines* that one would obtain from an atom harmonically bound, say in a molecule with energy levels separated by θ. (See Figs. 2 and 3.)

The area under the general absorption curve (28) may be evaluated immediately, again under the assumption of footnote (4), and one finds

$$\int_0^\infty dEW(E)=\frac{2}{\Gamma} \tag{38}$$

which, of course, agrees with the result for free atoms. The expression for the cross section for self-indication, which involves the integral of the square of $W(E)$ is more complicated, but may be reduced to

$$\sigma_s=\Gamma\int_0^\infty d\mu \exp\left[-\Gamma\mu+g(\mu)+g(-\mu)\right]. \tag{39}$$

In the case $\Gamma+\Delta\gg\theta$, this integral may again be evaluated by expanding $g(\mu)$ for small μ, and the cross section for self-indication has the value corresponding to that for a gas at an effective temperature $\bar{\bar{\epsilon}}$ instead of T. In the general case of arbitrary Γ, Δ and θ, however, one may derive an approximate formula by splitting the range of integration at $\mu\theta=1$,

$$\sigma_s=(\tfrac{1}{2}\pi)^{\frac{1}{2}}\xi e^{\frac{1}{2}\xi^2}\left[\Phi\left(\frac{\xi}{\sqrt{2}}+\frac{\Delta}{\sqrt{2}\theta}\right)-\Phi\left(\frac{\xi}{\sqrt{2}}\right)\right] +\exp\left[2g(\infty)-\Gamma/\theta\right], \tag{40}$$

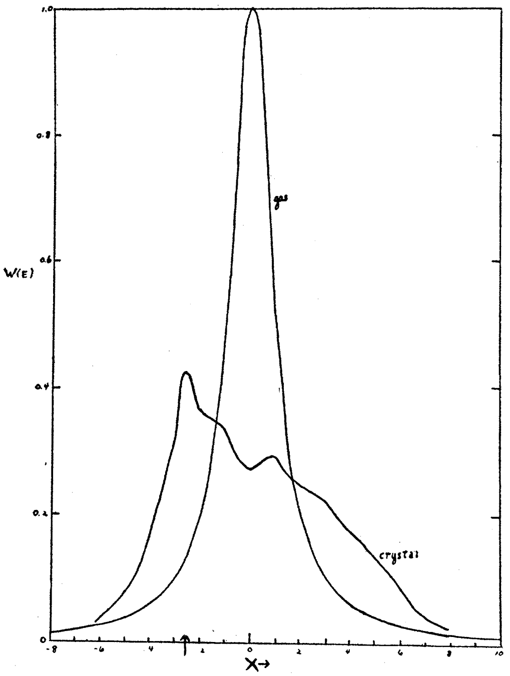

FIG. 3. Same as Fig. 2 except that the assumed value of Γ is now equal to θ. For values of $\Gamma\gtrsim 4\theta$, one is already in the domain of applicability of Eq. (32). The precise value of Γ for silver is not well known experimentally.

which may be used provided the result does not depend too much on the precise value of θ.

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