APPENDIX 3. SPECTRUM OF THE CHARGE DISTRIBUTION IN POLYCRYSTALS

From Eqs. (19) and (42) for the one-dimensional case

$$|q^k|^2/e^2=1+\sum_{m=1}^{L}(1-m/L)\{\exp[i(\kappa-\pi)m]+\text{c.c.}\}\,, \quad \text{(A7)}$$

where $\kappa=kd$. Using the relations

$$\sum_{m=1}^{L}\exp(imx) =\exp[\tfrac{1}{2}ix(L+1)]\sin(\tfrac{1}{2}xL)/\sin(\tfrac{1}{2}x)\,, \quad \text{(A8)}$$

$$\sum_{m=1}^{L} m\exp(imx) =\frac{\exp[\tfrac{1}{2}ix(L+1)]}{2\sin^2(\tfrac{1}{2}x)}\{(L+1)\sin(\tfrac{1}{2}xL)\sin(\tfrac{1}{2}x) -i[L\cos(\tfrac{1}{2}xL)\sin(\tfrac{1}{2}x)-\sin(\tfrac{1}{2}xL)\cos(\tfrac{1}{2}x)]\}\,, \quad \text{(A9)}$$

one finds after trivial calculations

$$|q^k|^2/e^2=\sin^2\tfrac{1}{2}L(\kappa-\pi)/L\cos^2\tfrac{1}{2}\kappa\,, \quad \text{(A10)}$$

which is equivalent to Eq. (43).

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Energy Levels of Polarons in a Magnetic Field

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A variational method closely related to the intermediate coupling method of Lee, Low, and Pines is used to calculate the ground-state energy and low-lying excited states of the Fröhlich Hamiltonian with a uniform time-independent magnetic field. The energy is calculated in a power series in ω_c/ω to order $(\omega_c/\omega)^2$, where ω_c is the cyclotron resonance frequency of the electron in the absence of electron-phonon interaction and ω is the frequency of the longitudinal optical phonons. It is shown that in the presence of electron-phonon interaction the energy of the nth magnetic level is no longer proportional to n and that the effective mass for motion along the direction of the magnetic field is a function of n. The calculated variational energies approach the weak field result expected from the calculation of Lee, Low, and Pines (LLP) when $\omega_c/\omega\to 0$, and in the weak coupling limit the ground-state energy becomes exact to order $(\omega_c/\omega)^2$.

INTRODUCTION

IT is well known that if one wishes to compute the energy spectrum of a spinless electron of mass m in a magnetic field, $\mathbf{H}$, with associated vector potential $\mathbf{A}$, one replaces the energy operator $p^2/2m$ for the free electron by $(\mathbf{p}-e\mathbf{A}/c)^2/2m$ and solves the resulting Schrödinger equation. The energy spectrum so obtained can be written

$$(p_z^2/2m)+(n+\tfrac{1}{2})\hbar\omega_0\,, \quad (1)$$

where $\omega_0=eH/mc$, p_z is the component of electron momentum along $\mathbf{H}$, e is the magnitude of the electron charge, and n takes on values $(0,1,2,\cdots)$.

In this paper we shall discuss what happens to the energy of an electron (more precisely, a polaron) in a polarizable but magnetically inert crystal when a relatively weak magnetic field is turned on. Polaron theory[1–3] predicts that in the absence of external fields the polaron energy spectrum has the form

$$p^2/2m^*+(\bar{K}p^4/4m^2\hbar\omega)+O(p^6/m^3(\hbar\omega)^2)\,, \quad (2)$$

if $(p^2/2m)\ll\hbar\omega$, where ω is the frequency of the longitudinal optical phonons and m is now and henceforth the band mass of the electron. In (2) m^* is the "effective mass" of the polaron and $\bar{K}$ is a dimensionless constant.

If we could proceed in analogy to the free electron we would regard (2) as the energy operator for the polaron, replace $p^2/2m$ in (2) by $(\mathbf{p}-e\mathbf{A}/c)^2/2m$ and solve the resulting Schrödinger equation. The energy levels of the polaron in the magnetic field would then take the form

$$\mu[(n+\tfrac{1}{2})\hbar\omega_c+p_z^2] +(\bar{K}/\hbar\omega)[(n+\tfrac{1}{2})\hbar\omega_c+(p_z^2/2m)]^2 +O[((n+\tfrac{1}{2})\hbar\omega_c+p_z^2/2m)^3/(\hbar\omega)^2]\,, \quad (3)$$

where

$$\mu=m/m^* \quad (4)$$

and

$$\omega_c=eH/mc\,.$$

At this point (3) is only suggestive; it motivates the more careful study of low-lying polaron energy levels to be undertaken in the present paper. We shall show, to the accuracy of our calculation, that in fact (3) becomes

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[1] H. Fröhlich, *Advances in Physics* (Taylor & Francis, Ltd., London, 1954), Vol. 3, p. 325. We use the notation of Fröhlich unless otherwise specified.

[2] T. D. Lee, F. E. Low, and D. Pines, Phys. Rev. **90**, 297 (1953). This paper will henceforth be referred to as LLP.

[3] Particularly useful as a survey of the entire subject of polarons is the book *Polarons and Excitons*, edited by C. G. Kuper and G. D. Whitfield (Oliver & Boyd, Ltd., Edinburgh, 1963).

exact in the limit

$$\omega_c \to 0 \quad \text{with} \quad n\omega_c \text{ constant}. \tag{5}$$

The Fröhlich Hamiltonian will be used to describe the electron-phonon system, which means that we treat the lattice as a continuous polarizable medium and assume that, aside from the polarization energy, the electron-lattice interaction can be taken into account by merely replacing the electron mass by an effective band mass (which may be field-dependent).[4]

VARIATIONAL CALCULATION

We can omit the electron spin energy without loss of generality so that the Fröhlich Hamiltonian with magnetic field can be written[1,5,6]

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_1, \tag{6}$$

$$\mathcal{H}_0=\sum b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}+(\hat{p}_x+\tfrac{1}{2}\lambda^2 y)^2+\hat{p}_y^2+\hat{p}_z^2, \tag{7}$$

$$\mathcal{H}_1=\left(\frac{4\pi\alpha}{S}\right)^{1/2}\sum\frac{1}{k}(e^{-i\mathbf{k}\cdot\mathbf{r}}b_{\mathbf{k}}^{\dagger}+\text{h.c.}), \tag{8}$$

where $(\hat{p}_x,\hat{p}_y,\hat{p}_z)$ is the electron momentum operator, $\lambda=(\omega_c/\omega)^{1/2}$, $\mathbf{r}=(x,y,z)$ is the electron displacement, and we have used the vector potential $\mathbf{A}$ defined by

$$e\mathbf{A}/(2m\hbar\omega)^{1/2}c=(-\tfrac{1}{2}\lambda^2 y,\,0,\,0)$$

to describe the external, uniform, time-independent magnetic field in the z direction.

We shall build up our variational wave function step by step by a succession of unitary transformations on the normalized wave function

$$e^{i(p_x x+p_z z)}|\Phi(n)\rangle|0\rangle\equiv|p_z,n,0\rangle, \tag{9}$$

where $|0\rangle$ is the phonon vacuum and $|\Phi(n)\rangle$ is the one-dimensional harmonic-oscillator eigenfunction defined by

$$(\hat{p}_y^2+\tfrac{1}{4}\lambda^4 y^2)|\Phi(n)\rangle=(n+\tfrac{1}{2})\lambda^2|\Phi(n)\rangle.$$

However, since we are interested only in the energy spectrum of $\mathcal{H}$ it will not be necessary to deal explicitly with wave functions; thus if our variational wave function is $\mathfrak{U}^{-1}|p_z,n,0\rangle$, where $\mathfrak{U}$ is a unitary operator, the corresponding variational energy is

$$\langle 0,n,p_z|\mathfrak{U}\mathcal{H}\mathfrak{U}^{-1}|p_z,n,0\rangle.$$

If $\mathfrak{U}$ is a product of unitary operators:

$$\mathfrak{U}=\mathfrak{U}_4\mathfrak{U}_3\mathfrak{U}_2\mathfrak{U}_1 \tag{10}$$

and if we define $\mathfrak{U}_i\mathcal{H}^{(i-1)}\mathfrak{U}_i^{-1}=\mathcal{H}^{(i)}$ with $\mathcal{H}^{(0)}=\mathcal{H}$ then the variational energy we seek is the diagonal part of $\mathcal{H}^{(4)}$ in the states $|p_z,n,0\rangle$. The purpose of the rest of this section is to build up a set of operators $\mathfrak{U}_1\cdots\mathfrak{U}_4$ which yield a variational energy, E_T, for low-lying states which has the properties: (a) E_T goes over to the form expected from the LLP variational energy[2] in the limit (5), (b) E_T is exact to order λ^4 in the weak coupling limit ($\alpha\to 0$). By "low-lying states" we shall mean states with excitation energy well below $\hbar\omega$.

All our transformations $\mathfrak{U}_i$ will be represented in the form $\mathfrak{U}_i=e^{S_i}$ where $S_i^{\dagger}=-S_i$, and we shall define the various $\mathfrak{U}_i$ by specifying the corresponding S_i. $\mathcal{H}^{(i)}$ is then computed from S_i and $\mathcal{H}^{(i-1)}$ by applying the well known identity:

$$\mathcal{H}^{(i)}=e^{S_i}\mathcal{H}^{(i-1)}e^{-S_i}\equiv\mathcal{H}^{(i-1)}+[S_i,\mathcal{H}^{(i-1)}]+(1/2!)[S_i,[S_i,\mathcal{H}^{(i-1)}]]+\cdots. \tag{11}$$

We begin with the first canonical transformation of LLP, defined by

$$S_1=i\mathbf{r}\cdot\sum\mathbf{k}b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}. \tag{12}$$

The effect of $\mathfrak{U}_1$ on $\mathcal{H}^{(0)}$ can be readily calculated by computing the effect of $\mathfrak{U}_1$ on the different operators in $\mathcal{H}^{(0)}$ using (13), below.

$$\begin{aligned}&\mathfrak{U}_1\hat{p}\mathfrak{U}_1^{-1}=\hat{p}-\sum\mathbf{k}b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}},\\ &\mathfrak{U}_1 b_{\mathbf{k}}^{\dagger}\mathfrak{U}_1^{-1}=e^{i\mathbf{k}\cdot\mathbf{r}}b_{\mathbf{k}}^{\dagger},\\ &\mathfrak{U}_1\mathbf{r}\mathfrak{U}_1^{-1}=\mathbf{r}.\end{aligned} \tag{13}$$

The purpose of this transformation is to locate the origin of the coordinate system describing the phonon field, at the position of the electron.

Transforming operators in (6)–(8) according to (13) we obtain

$$\mathcal{H}^{(1)}=\sum n_{\mathbf{k}}+(\hat{p}_x-\sum k_x n_k+\tfrac{1}{2}\lambda^2 y)^2+(\hat{p}_y-\sum k_y n_{\mathbf{k}})^2+(p_z-\sum k_z n_{\mathbf{k}})^2+(4\pi\alpha/S)^{1/2}\sum(1/k)(b_{\mathbf{k}}^{\dagger}+b_{\mathbf{k}}). \tag{14}$$

As in the case of a free electron in a magnetic field in our gauge, the energy of the system will not depend upon $\hat{p}_x$. To show this we eliminate $\hat{p}_x$ from (14) by introducing

$$\mathfrak{U}_2=\exp-(2i\hat{p}_x\hat{p}_y/\lambda^2),$$

which shifts the y coordinate of the electron. In our units $[p_y,y]=-i$ so that

$$\mathfrak{U}_2 y\mathfrak{U}_2^{-1}=y-(2\hat{p}_x/\lambda^2).$$

Thus

$$\mathcal{H}^{(2)}=\sum n_{\mathbf{k}}+\sum\mathbf{k}\cdot\mathbf{l}n_{\mathbf{k}}n_1+\mathbf{\Pi}^2-2\mathbf{\Pi}\cdot\sum\mathbf{k}n_{\mathbf{k}}+(4\pi\alpha/S)^{1/2}\sum(1/k)(b_{\mathbf{k}}^{\dagger}+b_{\mathbf{k}}), \tag{15}$$

where

$$\mathbf{\Pi}=(\tfrac{1}{2}\lambda^2 y,\hat{p}_y,\hat{p}_z)$$

and, as in (14),

$$n_{\mathbf{k}}=b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}.$$

Since we will ultimately have to take expectation values in the state (9), which contains the state $|\Phi(n)\rangle$ as a factor, it is convenient to rewrite (15) in terms of the

[4] In this way we sidestep the important but difficult problem of the energy levels of an electron interacting simultaneously with a rigid periodic lattice and an external magnetic field.

[5] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Addison-Wesley Publishing Company Inc., Reading, Massachusetts, 1958).

[6] From this point on all lengths are taken in units of $r_0=(\hbar/2m\omega)^{1/2}$, all momenta and wave numbers are in units of $\hbar/r_0$ and $1/r_0$, respectively, and all energies are in units of $\hbar\omega$.

harmonic oscillator raising and lowering operators defined by:

$$a^\dagger=\lambda^{-1}(\hat{p}_y+(i/2)\lambda^2 y),\quad a=\lambda^{-1}(\hat{p}_y-(i/2)\lambda^2 y). \quad (16)$$

In terms of these operators we write (15) in the form

$$\begin{aligned}\mathcal{H}^{(2)}=&\sum n_{\mathbf{k}}+\sum \mathbf{k}\cdot\mathbf{l}n_{\mathbf{k}}n_1+\hat{p}_z^2+\lambda^2(a^\dagger a+\tfrac{1}{2})-2\hat{p}_z\sum k_z n_{\mathbf{k}}\\&-\lambda[(a^\dagger+a)\sum k_y n_{\mathbf{k}}-i(a^\dagger-a)\sum k_x n_{\mathbf{k}}]\\&+(4\pi\alpha/\mathcal{S})^{1/2}\sum(1/k)(b_{\mathbf{k}}^\dagger+b_{\mathbf{k}}). \quad (17)\end{aligned}$$

In order to motivate our final two transformations we note that (15) is the same as the corresponding LLP Hamiltonian [see LLP Eq. (9)] with the c number P in LLP replaced by the operator $\mathbf{\Pi}$. This suggests that we replace $\tilde{f}_k(\mathbf{P})$ in the LLP transformation $\exp[\sum_{\mathbf{k}}\tilde{f}_{\mathbf{k}}(\mathbf{P})(b_{\mathbf{k}}^\dagger-b_{\mathbf{k}})]$ by $\tilde{f}_k(\mathbf{\Pi})$. We do this in our next two transformations, which amount to using an $\tilde{f}_{\mathbf{k}}(\mathbf{\Pi})$ expanded to second order in powers of $\mathbf{k}\cdot\mathbf{\Pi}$.

From another point of view we can regard our final two transformations as eliminating operators linear in phonon operators which contribute to the ground-state energy in order λ^4 and lower. This is done in analogy to the procedure in LLP, the effect of which is to remove *all* terms linear in the phonon operators from the Hamiltonian. In the field-free case, considered by LLP, this can be done in a simple way because the only operators in the LLP Hamiltonian corresponding to (17) are phonon operators.

To eliminate the dominant terms linear in the phonon operators we introduce

$$S_3=\sum_{\mathbf{k}}[f_{\mathbf{k}}+(a^\dagger+a)s_{\mathbf{k}}+i(a^\dagger-a)u_{\mathbf{k}}](b_{\mathbf{k}}^\dagger-b_{\mathbf{k}}), \quad (18)$$

where $f_{\mathbf{k}}$, $s_{\mathbf{k}}$, and $u_{\mathbf{k}}$ serve as variational parameters and are assumed to be real functions of $\mathbf{k}$.

$$\begin{aligned}\mathfrak{U}_3 b_{\mathbf{k}}^\dagger\mathfrak{U}_3^{-1}=&b_{\mathbf{k}}^\dagger-f_{\mathbf{k}}-(a^\dagger+a)s_{\mathbf{k}}-i(a^\dagger-a)u_{\mathbf{k}}\\&+i\sum_{\mathbf{m}}(u_{\mathbf{m}}s_{\mathbf{k}}-s_{\mathbf{m}}u_{\mathbf{k}})(b_{\mathbf{m}}^\dagger-b_{\mathbf{m}}),\\ \mathfrak{U}_3 a^\dagger\mathfrak{U}_3^{-1}=&a^\dagger+\sum_{\mathbf{m}}(s_{\mathbf{m}}-iu_{\mathbf{m}})(b_{\mathbf{m}}^\dagger-b_{\mathbf{m}}).\end{aligned} \quad (19)$$

At this point we remark that $\hat{p}_z$ in (17), can be replaced by a c number since it commutes with $\mathfrak{U}_3$ specified by (18) above, with $\mathfrak{U}_4$ to be given below, and with $\mathcal{H}^{(2)}$. Thus, although in the ground state of $\mathcal{H}^{(2)}$, $p_z=0$, we will be able to obtain an upper bound to the energy of the lowest lying state of $\mathcal{H}^{(2)}$ for given p_z by minimizing the expectation value of $\mathcal{H}^{(4)}$ in the states (9) for each value of p_z.

Examination of $\mathcal{H}^{(3)}$ shows that the largest terms which are linear in phonon operators are terms with coefficients of order λ^2 and are quadratic in "a" operators. To eliminate such terms to lowest order in λ we specify $\mathfrak{U}_4$ by

$$S_4=\sum_{\mathbf{k}}\sigma_{\mathbf{k}}(b_{\mathbf{k}}^\dagger-b_{\mathbf{k}}), \quad (20)$$

where $\sigma_{\mathbf{k}}=(a^\dagger+a)^2r_{\mathbf{k}}+(a^\dagger-a)^2t_{\mathbf{k}}+i(a^\dagger a^\dagger-aa)q_{\mathbf{k}}$, and $r_{\mathbf{k}}$, $t_{\mathbf{k}}$, and $q_{\mathbf{k}}$ are variational parameters assumed to be real functions of $\mathbf{k}$.

If the reader has explicitly constructed $\mathcal{H}^{(3)}$ from (19) and (17), he will have verified that it is a very bulky and ungainly expression. Worse yet, the commutator expansion for $\mathcal{H}^{(4)}$ obtained by inserting S_4 and $\mathcal{H}^{(3)}$ into (11) does not even terminate. In order to proceed further we must make certain assumptions about the size and structure of our six variational parameters. These assumptions, listed below, will be shown to be self-consistent at the end of the calculation. Thus we assume

$$\begin{aligned}f_{\mathbf{k}}&=f(k,k_z,p_z)=O(\lambda^0),\\ s_{\mathbf{k}}&=k_y s(k,k_z,p_z)=O(\lambda),\\ u_{\mathbf{k}}&=k_x\lambda u(k,k_z,p_z)=O(\lambda),\end{aligned} \quad (21)$$

and

$$r_{\mathbf{k}}=O(\lambda^2),\quad t_{\mathbf{k}}=O(\lambda^2),\quad q_{\mathbf{k}}=O(\lambda^2). \quad (22)$$

The assumed order in λ of the various variational parameters in (21) and (22) is just equal to the order of the terms which they are designed to eliminate. For example, the term $\sum_{\mathbf{k}}s_{\mathbf{k}}(b_{\mathbf{k}}^\dagger-b_{\mathbf{k}})(a^\dagger+a)$ in S_3 of (18) is designed to eliminate the term $\lambda(a^\dagger+a)\sum_k k_y f_{\mathbf{k}}(b_{\mathbf{k}}^\dagger+b_{\mathbf{k}})$ which would have been present in $\mathcal{H}^{(3)}$ had we set $s_k=0$ in (18). Thus $s_{\mathbf{k}}$ is assumed to be of order λ.

From (21) it follows that the largest terms in $\mathcal{H}^{(3)}$ are of order λ^0; therefore, the expectation value of $\mathcal{H}^{(4)}$ in states (9) is correctly given to order λ^4 by the expectation value of the operator

$$\mathcal{H}^{(3)}+[S_4,\mathcal{H}^{(3)}]+\tfrac{1}{2}[S_4,[S_4,\mathcal{H}^{(3)}]]. \quad (23)$$

Furthermore, we can extract the part of $\mathcal{H}^{(3)}$ which contributes to the expectation value of (23) to order λ^4 in the states (9) and replace $\mathcal{H}^{(3)}$ in (23) by this extracted part, $\mathcal{H}_E^{(3)}$. Picking out the terms of $\mathcal{H}^{(3)}$ which contribute to $\mathcal{H}_E^{(3)}$ is simpler than one might expect because a large majority of operators in $\mathcal{H}^{(3)}$ have coefficients of order λ or higher. Such operators can contribute to E_T to order λ^4 only if they are diagonal or if their commutator with S_4 is diagonal. Using (20)–(23), we can write down $\mathcal{H}_E^{(3)}$ almost by inspection from $\mathcal{H}^{(3)}$. The result is

$$\begin{aligned}\mathcal{H}_E^{(3)}=&\sum(1-2k_z(1-\eta)p_z)n_{\mathbf{k}}+\sum\mathbf{k}\cdot\mathbf{l}n_{\mathbf{k}}n_1+\tfrac{1}{2}\lambda^2+\lambda^2a^\dagger a+E_3-\sum[(1-2k_z(1-\eta)p_z+k^2)f_{\mathbf{k}}-(4\pi\alpha/\mathcal{S})^{1/2}(1/k)]\\&\times(b_{\mathbf{k}}^\dagger+b_{\mathbf{k}})-\lambda\sum[(a^\dagger+a)^2k_y s_{\mathbf{k}}+(a^\dagger-a)^2k_x u_{\mathbf{k}}+i(a^\dagger a^\dagger-aa)(k_y u_{\mathbf{k}}-k_x s_{\mathbf{k}})](b_{\mathbf{k}}^\dagger+b_{\mathbf{k}})\\&+\sum_{\mathbf{k}\neq 1}\mathbf{k}\cdot\mathbf{l}f_{\mathbf{k}}f_1(b_{\mathbf{k}}^\dagger+b_{\mathbf{k}})(b_1^\dagger+b_1)-2\sum\mathbf{k}\cdot\mathbf{l}[(a^\dagger+a)^2s_{\mathbf{k}}^2-(a^\dagger-a)^2u_{\mathbf{k}}^2]f_1(b_1^\dagger+b_1)\\&-4\sum\mathbf{k}\cdot\mathbf{l}f_{\mathbf{k}}[(a^\dagger+a)^2s_{\mathbf{k}}s_1-(a^\dagger-a)^2u_{\mathbf{k}}u_1+i(a^\dagger a^\dagger-aa)(s_{\mathbf{k}}u_1+u_{\mathbf{k}}s_1)](b_1^\dagger+b_1)\end{aligned} \quad (24)$$

and

$$E_3=\sum(1-2k_zp_z+k^2)f_k^2-2(4\pi\alpha/\mathcal{S})^{1/2}\sum(1/k)f_k+(\sum k_zf_k^2)^2+\sum(1-2k_z(1-\eta)p_z+k^2)(s_k^2+u_k^2)(1+2a^\dagger a)$$
$$+4(I_s^2+I_u^2)(1+2a^\dagger a)+2\lambda(I_s-I_u)(1+2a^\dagger a)+\mathcal{G}_u[\sum(1+k^2)s_k^2+4I_s^2]$$
$$+\mathcal{G}_s[\sum(1+k^2)u_k^2+4I_u^2]+\lambda^2(\mathcal{G}_s+\mathcal{G}_u)+4\lambda(\mathcal{G}_uI_s-\mathcal{G}_sI_u), \quad (25)$$

where

$$I_s=\sum k_ys_kf_k, \quad I_u=\sum k_xu_kf_k,$$
$$\mathcal{G}_s=\sum s_k^2, \quad \mathcal{G}_u=\sum u_k^2,$$
$$\eta p_z=\sum k_zf_k^2.$$

In (25) and in the following we consider p_z^2 to be a quantity of order λ^2, and we therefore neglect terms which contribute only to order p_z^6, $\lambda^2p_z^4$, $\lambda^4p_z^2$ or higher. While it would have been possible to calculate E_3 to higher order in p_z^2 we feel that there is not much point in doing so (thereby adding further complication to an already complicated expression) when we are only able to calculate the energy associated with motion in the x–y plane to order λ^4. The variational result in any case is expected to be most accurate when $\lambda^2\ll1$ and $p_z^2\ll1$.

In (23) we replace $\mathcal{H}^{(3)}$ by $\mathcal{H}_E^{(3)}$, insert S_4 from (20), and evaluate the commutators using the orthogonality properties among f_k, u_k, and s_k implied by (21).

Omitting only, but not all, terms which have no diagonal part to order λ^4 or $\lambda^2p_z^2$ in the states (9), we obtain for our effective Hamiltonian, $\mathcal{H}_E^{(4)}$:

$$\mathcal{H}_E^{(4)}=p_z^2+\tfrac{1}{2}\lambda^2+\lambda^2a^\dagger a+E_3+\sum(1-2k_z(1-\eta)p_z+k^2)\sigma_k^2+2\sum[(1-2k_z(1-\eta)p_z+k^2)f_k-(4\pi\alpha/\mathcal{S})^{1/2}(1/k)]\sigma_k$$
$$+2\lambda\sum[(a^\dagger+a)^2k_ys_k+(a^\dagger-a)^2k_xu_k+i(a^\dagger a^\dagger-aa)(k_yu_k-k_xs_k)]\sigma_k$$
$$+8\sum[(a^\dagger+a)^2k_ys_kI_s-(a^\dagger-a)^2k_xu_kI_u+i(a^\dagger a^\dagger-aa)(k_yu_kI_s-k_xs_kI_u)]\sigma_k-2\sum\mathbf{k}\cdot\mathbf{l}f_kf_l\sigma_k\sigma_l. \quad (26)$$

If we let E_4 be the diagonal part of $\mathcal{H}_E^{(4)}-(\frac{1}{2}\lambda^2+\lambda^2a^\dagger a+E_3+p_z^2)$ we get

$$E_4=\{\sum[(1-2k_z(1-\eta)p_z+k^2)(r_k^2+t_k^2)+2(\lambda+4I_s)k_ys_kr_k+2(\lambda-4I_u)k_xu_kt_k]$$
$$-2(\sum\mathbf{k}f_kt_k)^2-2(\sum\mathbf{k}f_kr_k)^2\}[3+6a^\dagger a+6(a^\dagger a)^2]$$
$$+2\{\sum[(1-2k_z(1-\eta)p_z+k^2)r_kt_k+(\lambda+4I_s)k_ys_kt_k$$
$$+(\lambda-4I_u)k_xu_kr_k]-2(\sum\mathbf{k}f_kr_k)\cdot(\sum\mathbf{l}f_lt_l)\}[1-2a^\dagger a-2(a^\dagger a)^2]$$
$$+2\{\sum[(1-2k_z(1-\eta)p_z+k^2)q_k^2+2(\lambda+4I_s)k_yu_kq_k-2(\lambda-4I_u)k_xs_kq_k]\}[1+a^\dagger a+(a^\dagger a)^2]$$
$$+2\{\sum[[(1-2k_z(1-\eta)p_z+k^2)f_k-(4\pi\alpha/\mathcal{S})^{1/2}(1/k)](r_k-t_k)]\}(1+2a^\dagger a). \quad (27)$$

In (27) we have used the following relations for the diagonal parts of operators

$$(a^\dagger+a)^4|_D=(a^\dagger-a)^4|_D=3+6a^\dagger a+6(a^\dagger a)^2,$$
$$(a^\dagger-a)^2(a^\dagger+a)^2|_D=(a^\dagger+a)^2(a^\dagger-a)^2|_D$$
$$=1-2a^\dagger a-2(a^\dagger a)^2,$$
$$(a^\dagger a^\dagger-aa)^2|_D=-2(1+a^\dagger a+(a^\dagger a)^2),$$

where if B is an operator, $B|_D$ is the diagonal part of B in the states (9).

To complete the variational calculation we must minimize the ground-state energy from (26) and (27) with respect to f_k, s_k, u_k, r_k, t_k, and q_k. At first sight this seems formidable. However our initial postulate that f_k is of order λ^0, s_k and u_k of order λ and r_k, t_k, and q_k of order λ^2 suggests that to obtain a first approximation for f_k we should consider only terms in $\langle0,0,p_z|(E_3+E_4)\times|p_z,0,0\rangle$ of order λ^0 and minimize them with respect to f_k. These terms appear in E_3; they give exactly the polaron energy of LLP, E_{LLP}, when the polaron momentum is in the z direction, namely,

$$\sum(1-2k_zp_z+k^2)f_k^2+(\sum\mathbf{k}f_k^2)^2$$
$$-(8\pi\alpha/\mathcal{S})\sum(1/k)f_k. \quad (28)$$

Minimizing with respect to f_k gives, as in LLP,

$$f_k=\left(\frac{4\pi\alpha}{\mathcal{S}}\right)^{1/2}\frac{1}{k(1-2k_z(1-\eta)p_z+k^2)}. \quad (29)$$

Next we find a first approximation to s_k and u_k by minimizing all terms in the ground-state energy for fixed p_z which depend upon s_k and u_k and are of no higher order than λ^2. These terms also appear only in E_3 and are

$$\sum(1-2k_z(1-\eta)p_z+k^2)s_k^2+2I_s(\lambda+2I_s)$$
$$+\sum(1-2k_z(1-\eta)p_z+k^2)u_k^2+2I_u(-\lambda+2I_u). \quad (30)$$

Minimizing the expression (30) we find

$$s_k=-\frac{(\lambda+4I_s)k_yf_k}{1-2k_z(1-\eta)p_z+k^2},$$
$$u_k=-(k_x/k_y)s_k,$$
$$I_s=-[\lambda+4I_s]\sum\frac{k_y^2f_k^2}{1-2k_z(1-\eta)p_z+k^2} \quad (31)$$
$$=-\lambda I/(1+4I),$$
$$I_u=-I_s,$$

where

$$I=\sum \frac{k_y^2 f_k^2}{1-2k_z(1-\eta)p_z+k^2}.$$

Using the solutions (31) we calculate r_k, t_k, and q_k from (27). Since we are neglecting terms of order $\lambda^4 p_z^2$ we can set $p_z=0$ in our expressions (29) and (31) for f_k, s_k, and u_k before substituting them into (27). The result upon minimizing the ground-state energy of E_4 (at fixed p_z) with respect to r_k, t_k, and q_k is

$$\begin{aligned} r_k&=-\frac{(\lambda+4I_s)k_y s_k}{1-2k_z(1-\eta)p_z+k^2},\\ t_k&=-\frac{(\lambda-4I_u)k_x u_k}{1-2k_z(1-\eta)p_z+k^2},\\ q_k&=\frac{(\lambda-4I_u)k_x s_k-(\lambda+4I_s)k_y u_k}{1-2k_z(1-\eta)p_z+k^2}. \end{aligned} \tag{32}$$

Note that (29), (31), and (32) are consistent with (21) and (22).

If we now go back and recalculate f_k using values of the other parameters given by (31) and (32) we find no correction to order λ^2 to the expression for f_k given by (29). Thus for purposes of calculating E_3+E_4 to order λ^4, (29) is exact. By inspection there are no corrections to s_k and u_k in (31) of order lower than λ^3. Corrections to s_k and u_k of order λ^3 contribute to the energy in order λ^6. We therefore conclude that (29), (31), and (32) are exact to the order of our calculation.

Evaluating the energy expectation value in the limit of infinite volume using (25), (27), (29), (31), and (32) we obtain finally

$$\begin{aligned} E_T=&-\alpha+\mu\left(\frac{\omega_c}{\omega}(n+\tfrac{1}{2})+p_z^2\right)\\ &-\frac{3}{40}\mu^4\alpha\left(p_z^4+2\left(n\frac{\omega_c}{\omega}\right)p_z^2+\left(n\frac{\omega_c}{\omega}\right)^2\right)\\ &-\frac{3}{40}\mu^4\frac{\omega_c}{\omega}\alpha\left((n+\tfrac{1}{2})\frac{\omega_c}{\omega}+p_z^2\right)\\ &+\frac{1}{96}(\mu+3)\mu^2\left(\frac{\omega_c}{\omega}\right)^2\alpha, \end{aligned} \tag{33}$$

where

$$\mu=6/(6+\alpha).$$

In obtaining (33) we have used the variational result of LLP that the energy of a polaron with momentum p is given by

$$-\alpha+\mu p^2-(3/40)\mu^4 p^4\alpha+O(p^6). \tag{34}$$

We have neglected terms of order $\lambda^4 p_z^2$ and $\lambda^2 p_z^4$ in (33), assuming, as before, that p_z^2 and λ^2 are of the same order of smallness. It should be emphasized again that (33) is expected to be most accurate for low-lying states, $p_z^2\ll 1$, $n\lambda^2\ll 1$.

Comparing (33) and (34) we find that in the limit (5) if we formally replace $n\omega_c/\omega$ in (33) by $p_\perp^2$, (33) becomes equal to (34). Thus our calculation, within its limits of accuracy, verifies (3).

We now inspect terms of (33) which vanish in the limit (5). The term $\frac{1}{2}\mu(\omega_c/\omega)$ is easily identified as the zero-point energy of the polaron with the LLP effective mass, in the magnetic field. To understand the term

$$-\frac{3}{40}\mu^4\frac{\omega_c}{\omega}\alpha\left((n+\tfrac{1}{2})\frac{\omega_c}{\omega}+p_z^2\right), \tag{35}$$

we must recognize the possibility that the presence of an external field can alter the internal structure of the polaron so that the effective mass becomes explicitly field dependent.[7] We therefore regard the factor $-3\mu^4\omega_c\alpha/40\omega$ as the lowest order field-dependent correction to μ (where μ is the ratio of the band mass to the LLP effective mass).

Finally, we identify the remaining term

$$(\mu+3)\mu^2\omega_c^2\alpha/96\omega^2$$

as the lowest order residual magnetic correction to the field-free polaron ground-state energy, since we cannot regard this term as arising from an effective mass correction associated with the zero-point motion of the polaron.

In order to compare (33) with the weak coupling solution to be derived in the next section, we evaluate E_T to order α in the ground state and first excited magnetic state ($n=1$). The weak coupling limit for the ground-state energy of (33) is

$$-\alpha+\frac{1}{2}\left(1-\frac{\alpha}{6}\right)\frac{\omega_c}{\omega}+\frac{1}{240}\left(\frac{\omega_c}{\omega}\right)^2\alpha, \tag{36}$$

while the energy difference between the ground state and first excited magnetic state is

$$\left(1-\frac{\alpha}{6}\right)\frac{\omega_c}{\omega}-\frac{3}{20}\left(\frac{\omega_c}{\omega}\right)^2\alpha. \tag{37}$$

PERTURBATION THEORY

In this section we calculate the ground-state energy and the energy of the $n=1$, $p_z=0$ state by treating $\mathcal{H}_1$ in (8) as a perturbation on the eigenfunctions of $\mathcal{H}_0$ given by (7). We do this in order to show that to order λ^4 the corresponding variational energies of (33) are exact in the weak coupling limit. Also, it turns out to be relatively easy to calculate the energy to higher order than λ^4 in the weak coupling case by the method given.

[7] This has been demonstrated for a polaron in an electric field in the weak coupling case. D. M. Larsen, Phys. Rev. **133**, A860 (1964).

The unperturbed states may be written

$$|\psi(n,p_x,p_z)\rangle|\{n_k\}\rangle,$$

where $|\psi\rangle$ and $|\{n_k\}\rangle$ are assumed normalized,

$$[(\hat{p}_x+\tfrac{1}{2}\lambda^2 y)^2+\hat{p}_y^2+\hat{p}_z^2]|\psi(n,p_x,p_z)\rangle = [(n+\tfrac{1}{2})\lambda^2+p_z^2]|\psi(n,p_x,p_z)\rangle \quad (38)$$

and

$$b_1^\dagger b_1|\{n_k\}\rangle=N_1|\{n_k\}\rangle, \quad (39)$$

where N_1 is the number of phonons of wave vector $\mathbf{l}$ in the state $|\{n_k\}\rangle$. We shall denote the phonon vacuum state by $|0\rangle$ with $|\mathbf{k}\rangle$ defined by $b_k^\dagger|0\rangle=|\mathbf{k}\rangle$.

We take as unperturbed ground-state wave function the state

$$|\psi(0,0,0)\rangle|0\rangle. \quad (40)$$

From (8) we observe that $\mathcal{H}_1$ connects (40) only to unperturbed states of the form

$$|\psi(n,k_x,k_z)\rangle|\mathbf{k}\rangle,$$

with energy $1+(n+\frac{1}{2})\lambda^2+k_z^2$. The matrix element

$$\langle\mathbf{k}|\langle\psi(n,k_x,k_z)|e^{-i\mathbf{k}\cdot\mathbf{r}}b_k^\dagger|\psi(0,0,0)\rangle|0\rangle$$

contains, besides trivial factors, a factor of the form I_n

$$I_n=\int_{-\infty}^{\infty}dyH_n\left(\frac{\lambda(y-y_0)}{\sqrt{2}}\right)e^{-\lambda^2[(y-y_0)^2+y^2]/4}e^{-ik_y y}, \quad (41)$$

where $H_n(x)$ is the Hermite polynomial in x of nth order. To evaluate (41) we evaluate $\sum t^n I_n/n!$ by replacing $\sum t^n H_n(x)/n!$ by e^{-t^2+2tx} and performing the resulting integral. We then extract I_n from its generating function by differentiation. The result is that the perturbation expression giving the energy correction in order α is

$$-\frac{4\pi\alpha}{\mathcal{S}}\sum_k\frac{\exp-(k_\perp/\lambda)^2}{k^2}\sum_n\frac{1}{n!}\left(\frac{k_\perp}{\lambda}\right)^{2n}\frac{1}{1+n\lambda^2+k_z^2}. \quad (42)$$

We propose to evaluate (42) in a power series in λ^2. To do this we observe that for fixed $k_\perp^2$ the summand in (42) is a sharply peaked function of n as $\lambda\to 0$ because of the factor $(1/n!)(k_\perp/\lambda)^{2n}$. The value of n which maximizes this factor is approximately

$$n_0=(k_\perp/\lambda)^2. \quad (43)$$

This motivates the expansion of the factor $(1+n\lambda^2+k_z^2)^{-1}$ in (42) as follows:

$$\begin{aligned}&(1+n\lambda^2+k_z^2)^{-1}\\ &=[(1+n_0\lambda^2+k_z^2)+(n-n_0)\lambda^2]^{-1}\\ &=\frac{1}{1+k^2}\left[1-\frac{(n-n_0)\lambda^2}{1+k^2}+\left(\frac{(n-n_0)\lambda^2}{1+k^2}\right)^2-\cdots\right].\end{aligned} \quad (44)$$

We insert expansion (44) into (42) and perform the summation on n on each term of the expansion. To do this in a systematic way consider sums of the form

$$S_l=e^{-\chi}\sum_{n=0}^{\infty}n^l(\chi^n/n!)\quad\text{for}\quad l\neq 0, \quad (45)$$
$$S_0=1.$$

From (45) it is easy to show

$$S_{l+1}=\chi[1+(d/d\chi)]S_l \quad (46)$$

so that $S_1=\chi$, $S_2=\chi^2+\chi$, $S_3=\chi^3+3\chi^2+\chi$, etc. If we make the identification

$$\chi=n_0=(k_\perp/\lambda)^2, \quad (47)$$

then (42) becomes

$$-\frac{4\pi\alpha}{\mathcal{S}}\sum_k\frac{1}{k^2(1+k^2)}\left[1-\frac{\lambda^2(S_1-\chi)}{1+k^2}+\frac{\lambda^4(S_2-2\chi S_1+\chi^2)}{(1+k^2)^2}-\frac{\lambda^6(S_3-3S_2\chi+3S_1\chi^2-\chi^3)}{(1+k^2)^3}+\cdots\right]. \quad (48)$$

First we note from (47) that χ is of order λ^{-2}. From (46) it follows that the highest power of χ in S_l occurs as χ^l. It is clear that if we keep only these highest powers in each S_l (which amounts to replacing S_l by χ^l), all terms in the bracket in (48) vanish except for the first. This means that to order λ^0 the only contribution from (42) is

$$-\frac{4\pi\alpha}{\mathcal{S}}\sum_k\frac{1}{k^2(1+k^2)}. \quad (49)$$

Next we look for contributions in order λ^2 in (48). These come only from terms in S_l of order χ^{l-1}. From the recursion relation of (46) it is easy to show that the coefficient of this term in S_l is $\frac{1}{2}l(l-1)$. Therefore we can replace S_l by $\frac{1}{2}l(l-1)\chi^{l-1}$ in (48) to obtain all contributions to order λ^2. The contribution of the $(m+1)$st term in the bracket in (48) is

$$\tfrac{1}{2}m(m-1)\sum_{r=0}^{m-2}\frac{(m-2)!}{(m-2-r)!r!}(-1)^{r+m}\chi^{m-1}\left(\frac{\lambda^2}{1+k^2}\right)^m = \lambda^2\frac{k_\perp^2}{(1+k^2)^2}\delta_{m,2},$$

where $\delta_{i,j}$ is the Kronecker delta. Thus the total contribution to order λ^2 in (48) comes solely from the third term $(m=2)$ in the bracket and is

$$-\frac{4\pi\alpha}{\mathcal{S}}\lambda^2\sum_k\frac{k_\perp^2}{k^2(1+k^2)^3}. \quad (50)$$

Finally, in order λ^4 we can replace S_l by $(1/24)\,l(l-1)\times(l-2)(3l-5)\chi^{l-2}$ and proceeding as above we find

that only the fourth and fifth terms in the bracket contribute, the sum of the contributions being

$$-4\pi\alpha\lambda^4\left[-\sum\frac{k_\perp^2}{k^2(1+k^2)^4}+3\sum\frac{k_\perp^4}{(1+k^2)^5}\right]. \quad (51)$$

Converting the summations on $\mathbf{k}$ to integrations in the limit of infinite volume and adding the contributions (49)–(51) to the zero-point energy, $\frac{1}{2}\lambda^2$, of the unperturbed state (40), we obtain the weak coupling results for the ground-state energy, $E_{\rm wc}$, to order λ^4:

$$E_{\rm wc}=-\alpha+\frac{1}{2}\frac{\omega_c}{\omega}\left(1-\frac{\alpha}{6}\right)+\left(\frac{\omega_c}{\omega}\right)^2\frac{\alpha}{240}. \quad (52)$$

The energy of the first excited magnetic state is obtained from perturbing

$$|\psi(1,0,0)\rangle|0\rangle,$$

which yields the expression (53) corresponding to (42)

$$\frac{4\pi\alpha}{S}\lambda^2\sum_{\mathbf{k}}\frac{\exp-(k_\perp/\lambda)^2}{k_\perp^2k^2}\sum_n\frac{1}{n!}\times\left(\frac{k_\perp}{\lambda}\right)^{2n}\frac{(n-\lambda^{-2}k_\perp^2)^2}{1+(n-1)\lambda^2+k_z^2}. \quad (53)$$

We expand the factor $(1+(n-1)\lambda^2+k_z^2)^{-1}$ in powers of $[(n-1)\lambda^2-k_\perp^2]/(1+k^2)$ and evaluate (53) by the same technique used to evaluate (42). We find that the weak coupling excitation energy of the first excited magnetic state is

$$\left(1-\frac{\alpha}{6}\right)\frac{\omega_c}{\omega}-\frac{3}{20}\left(\frac{\omega_c}{\omega}\right)^2\alpha+O\left(\left(\frac{\omega_c}{\omega}\right)^3\right). \quad (54)$$

Comparing (52) and (54) to (36) and (37), respectively, shows that the variational ground-state and first excited-state energy become exact in the weak-coupling limit.

DISCUSSION

It should be possible to observe the main features of the energy spectrum (33). Ascarelli and Brown[8] have observed a polaron cyclotron resonance line in AgBr at 70 kMc/sec in a field of 6600 Oe. The line was narrow enough so that its peak could be located within a few percent. In a field ten times stronger a much narrower resonance line would be expected, and for reasonable values of α one should in principle be able to resolve a magnetic fine structure and observe the nonlinear dependence of the resonance energy levels on the magnetic-field strength.

Of course we have simplified the theoretical calculation by assuming that to order λ^4 we can still describe the interaction of the electron with the rigid lattice by a band mass. It may be that the correct band mass depends upon ω_c, in which latter case additional nonlinear effects in the cyclotron resonance will be observed.

It is difficult to estimate the accuracy of our variational energy. We have proved that it is exact to order α in the weak coupling limit but we do not really know how rapidly the error increases with α. If we assume that the LLP effective mass for $\alpha=2$ is within 5% of the correct value in the field-free case, then we might expect that correction terms in (33) which go as μ^4 would be within perhaps 20% of their true value for $\alpha=2$. This error would decrease rapidly with decreasing α.

A calculation of the magnetic energy levels of the polaron has been made previously by Tulub.[9] He finds that the polaron effective mass for weak fields is given by the LLP effective mass plus a term proportional to $(\omega_c/\omega)^2$. This result is in disagreement with (33) of the present paper. Tulub does not calculate the ground-state energy of the system nor does he recognize that the polaron magnetic levels at fixed p_z are not equally spaced. Although derived for the intermediate coupling region, Tulub's effective mass does not approach the weak coupling result to order α. It is not completely clear that the mathematical method and approximations used by Tulub are appropriate for the problem of the polaron in a magnetic field.

Hellwarth and Platzman[10] (henceforth called HP) have calculated the free energy of polarons in a magnetic field by Feynman's method. This method is superior in accuracy to the LLP method (a modification of which is employed in the present paper) for calculating the ground-state energy and effective mass for free polarons. It would be interesting to compare the energy spectrum which produces the HP free energy to the spectrum obtained here. Unfortunately, HP do not calculate energy levels explicitly, and the comparison is difficult.

Because the LLP method normally produces a ground-state energy which goes over to the ground-state energy of perturbation theory for small α, it is of some interest to investigate the result of perturbation theory in the case $\lambda\gg1$ with arbitrarily small nonzero α. To this end we examine the order of the individual terms of the sum on n in (42) in the limit $\lambda\to\infty$. We find that for $n\neq0$ every term is of order $-\alpha/\lambda$ and that the sum on all $n\neq0$ is convergent; however, the $n=0$ term is of order $-\alpha\ln\lambda$. Thus for λ sufficiently large the energy correction in perturbation theory to order α is given by the $n=0$ term. The perturbed energy is therefore

$$\frac{1}{2}\lambda^2-\sum_{\mathbf{k}}\frac{|\langle\mathbf{k}|\langle\psi(0,k_x,k_z)|\mathcal{H}_1|\psi(0,0,0)\rangle|0\rangle|^2}{1+k_z^2}. \quad (55)$$

Assuming that a perturbation expansion in α for the

[8] G. Ascarelli and F. C. Brown, Phys. Rev. Letters **9**, 209 (1962).

[9] A. V. Tulub, Zh. Eksperim. i Teor. Fiz. **36**, 565 (1959) [English transl.: Soviet Phys.—JETP **9**, 392 (1959)].

[10] R. W. Hellwarth and P. M. Platzman, Phys. Rev. **128**, 1599 (1962).

ground state is possible when λ is very large and fixed, we conclude that a power-series expansion in λ^2 of the ground-state energy has a finite radius of convergence in the weak-coupling limit. This suggests strongly that the modified LLP variational method employed in this paper, even if carried out to all orders in λ, would fail for $\lambda \gg 1$. We should note, however, that in typical ionic crystals $\lambda = 1$ when the applied fields are in the hundreds of kilogauss. At such field strengths the validity of the Fröhlich Hamiltonian, given by (6)–(8), is doubtful.

The question of how the size of α affects the radius of convergence of an expansion of the ground-state energy in powers of λ^2 obtained from carrying out the modified LLP variational method to all orders in λ^2, remains unanswered.

In the limit of very weak field, namely, the limit (5), one can show, using a method due to Platzman[11] for performing the summation on n in (42), that the weak-coupling energy to order α is correctly given by the eigenvalues of the effective Hamiltonian obtained by replacing p^2 by $\boldsymbol{\Pi}^2$ in the field-free weak-coupling polaron energy, given by[1]

$$E_{\mathrm{wc}}(p^2)=\left[p^2-\alpha\frac{\sin^{-1}[(p^2)^{1/2}]}{(p^2)^{1/2}}\right].$$

The essential step in the proof of this result is to neglect the commutator $[p_y,y]$ wherever it appears. This neglect can be rigorously justified in the limit (5). The effective Hamiltonian $E_{\mathrm{wc}}(\boldsymbol{\Pi}^2)$ is applicable only when the condition

$$n\lambda^2+p_z^2<1$$

is satisfied.

The validity of replacing the field-free polaron energy spectrum $E(p^2)$ by $E(n\lambda^2+p_z^2)$ in the presence of a sufficiently weak magnetic field is undoubtedly not restricted to the weak coupling limit, but the author has not yet found a rigorous proof of this for the intermediate coupling case.

[11] P. M. Platzman, Phys. Rev. **125**, 1961 (1962).

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Volume Magnetostriction in Gadolinium Single Crystals*

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The magnetostriction of single-crystal gadolinium has been measured from 77 to 325°K in magnetic fields up to 20 kOe. A preliminary result of this work is the behavior of the forced volume magnetostriction. These results have been employed to obtain the partial differential coefficient of Curie temperature as a function of pressure over the above temperature range by means of the well-known thermodynamic expression due to Kornetzki. It is found that $\partial\theta/\partial P=-1.26\pm0.10$ °K/1000 atm at 290°K. These results are compared with the results obtained by direct measurement and discussed further.

THE forced volume magnetostriction above technical saturation in ferromagnetics is related to the pressure dependence of the magnetization through the thermodynamic relation

$$(\partial\omega/\partial H)_P=-(\partial I/\partial P)_H, \quad (1)$$

where $\omega=\Delta V/V$. Kornetzki,[1] assuming that a change in the spontaneous magnetization with a change in the volume at a definite temperature and at a definite magnetic field can occur only through a volume dependence of the Curie temperature or the exchange interaction energy and an arbitrary form for $M_{H,T}=f(T/\theta,H)$, where θ is the Curie temperature, finds that the forced volume magnetostriction and the pressure dependence of the Curie temperature are related through[2]

$$1/\theta(\partial\theta/\partial P) = 1/T(\partial\omega/\partial H)\Big/\left[\rho\frac{\partial\sigma}{\partial T}-\beta/K(\partial\omega/\partial H)\right], \quad (2)$$

where ρ is the density, σ the specific magnetization, β the volume thermal expansion coefficient, and K the volume compressibility.

The magnetostriction of single crystals of gadolinium has been measured from 77 to 325°K in magnetic fields up to 20 kOe. A preliminary result from this study

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[1] M. Kornetzki, Z. Physik **98**, 289 (1935).

[2] The right band of Eq. (2) should be multiplied by $(1+H/NI)$, where N is the Weiss molecular field factor. Calculating N from the susceptibility measurements in the paramagnetic region H/NI was found to be less than 0.03 and consequently was neglected.