Note on the Interaction of an Electron and a Lattice Oscillator*

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The interaction of an electron and a lattice oscillator is studied for an interaction energy of a special type linear in the oscillator coordinates and momenta. The energy values and eigenfunctions for arbitrary coupling strength are found by solving a three-term recurrence relation. A plot of energy *vs* total momentum of electron plus oscillator reveals the role of degeneracies of states involving different numbers of quanta in the oscillator. As the frequency of the oscillator tends to zero, one finds the bandlike spectrum characteristic of an electron moving in a periodic potential. With increasing total momentum the electron makes Bragg reflections, transferring quanta of energy and momentum to the oscillator, and remaining bounded in velocity. For strong coupling the state of minimum energy is one of nonzero total momentum. For sufficiently strong coupling, regions of small effective electron mass cease to exist.

I. INTRODUCTION

In recent months increased attention has been directed to the interaction of electrons with the lattice vibrations of crystals.[1–4] In many cases as, for example, the motion of electrons in polar lattices the electron lattice interaction is so strong that ordinary perturbation methods are inadequate. The present note is concerned with the exact treatment of a very simple system: An electron interacting with a single lattice oscillator for a special form of interaction. The lattice oscillator is characterized by an angular frequency ω and a propagation vector $\mathbf{k}$, i.e., is a traveling wave. As the first of several main points we shall find the energy values and eigenfunctions of the system of electron plus oscillator and study the lowest state in detail. The energy is a function of three parameters: the total momentum of the system, the strength of interaction, and the ratio $(\hbar k)^2/m\hbar\omega$. By studying the energy values and eigenfunctions as a function of total momentum and interaction strength one can see the role of states in which many quanta are present in the oscillator and the effect on the effective mass of the electron. Second, the exact probability of scattering can be computed and compared with the results given by time-dependent perturbation theory. Third, we shall study the limit of zero frequency when the phase velocity (ω/k) of the wave tends to zero. The traveling wave then becomes stationary and, provided one can neglect the recoil motion of the oscillator, one has exactly the problem of an electron in a periodic potential with its characteristic band-energy spectrum. If a small electric field acts, continually imparting momentum to the electron, Bragg reflections occur in which momentum is transferred to the system providing the periodic potential, and the electron remains bounded in velocity and energy. For the case treated here it is interesting to understand in detail the momentum transfer process.

We adopt the notation used by Fröhlich[5] in the discussion of the motion of electrons in a polar lattice. A system consisting of one electron interacting with a set of oscillators in a polar crystal is governed by the approximate hamiltonian

$$\mathcal{H}=\frac{p^2}{2m}+\sum_k g_k\left(X_k \sin\mathbf{k}\cdot\mathbf{q}+\frac{Y_k}{M\omega}\cos\mathbf{k}\cdot\mathbf{q}\right)+\sum_k\left(\frac{M\omega^2}{2}X_k^2+\frac{Y_k^2}{2M}\right).$$

Here p_x, p_y, p_z are the canonical momenta and q_x, q_y, q_z the canonical coordinates of the electron, X_k and Y_k are canonical coordinates and momenta of a lattice oscillator with propagation vector $\mathbf{k}$ and frequency $\omega(\mathbf{k})$. M depends on the mass of the ions giving rise to the lattice vibration. The sum over k goes over all lattice vibrations and has a natural cutoff for wavelengths of the order of the lattice spacing. The coupling constant for the case of a polar crystal is approximately $g_k=4\pi e/k$. The form of interaction used here differs from that occurring in metals, being characteristic of the long-range coulomb forces due to the ionic nature of the constituents of a polar lattice, but is general in that it is linear in the oscillator coordinates and momenta. We are not concerned with the accuracy with which the above hamiltonian describes the actual situation in a polar crystal, but merely take advantage of the fact that the type of interaction term allows one to make an exact treatment of the interaction of an electron with one oscillator.

II. MOMENTUM INTEGRAL AND WAVE FUNCTION COEFFICIENTS

We now study the interaction of an electron with a radiation oscillator the direction of propagation of which coincides with that of the electron and with a hamiltonian

$$\mathcal{H}=p^2/2m+g_k(X_k \sin kq+(Y_k/m\omega)\cos kq)+\tfrac{1}{2}(M\omega^2X_k^2+Y_k^2/M). \quad (1)$$

* Sponsored by the ONR, the Army Signal Corps, and the Air Force under ONR contract.

[1] H. Fröhlich, Phys. Rev. **79**, 845 (1950).
[2] J. Bardeen, Phys. Rev. **79**, 167 (1950); **80**, 567 (1950).
[3] Fröhlich, Pelzer, and Zienau, Phil. Mag. **41**, 221 (1950).
[4] T. Muto and S. Ôyama, Prog. Theor. Phys. **5**, 833 (1950).
[5] H. Fröhlich, Proc. Roy. Soc. (London) **A160**, 230 (1937).

Since this is a system of two degrees of freedom, one additional integral of motion will suffice to determine the motion. Let us consider the operator

$$\Lambda = p + \tfrac{1}{2}(k/\omega)(M\omega^2 X_k^2 + Y_k^2/M),$$

which is the total momentum of the system. We form the Poisson bracket $[\Lambda, \mathcal{H}]$ and with the help of the relations $[p, f(q)] = -i\hbar\partial f/\partial q$, $[q, f(p)] = +i\hbar\partial f/\partial p$, which hold for any pair of canonical variables, we verify that $[\Lambda, \mathcal{H}] = 0$, so that the total momentum Λ is an integral of motion. As a result the eigenfunctions of $\mathcal{H}$ must simultaneously be eigenfunctions of Λ. Let the eigenvalues of Λ be λ, and the eigenfunctions be $\psi_\lambda(X_k, q)$. Now Λ is highly degenerate in the sense that a given value λ of total momentum has an eigenfunction which is an arbitrary linear combination of states corresponding to distribution of the given momentum in different ways on the electron and phonons. The coefficients in the Λ eigenfunctions must be so chosen that the ψ_λ's are simultaneously eigenfunctions of $\mathcal{H}$.

The eigenfunctions of Λ are determined from

$$\Lambda\psi_\lambda = \left\{ p + \frac{1}{2}\frac{k}{\omega}\left(M\omega^2 X_k^2 + \frac{Y_k^2}{M} \right) \right\} \psi_\lambda = \lambda\psi_\lambda(X_k, q). \quad (2)$$

Since Λ is the sum of operators for each of the degrees of freedom we may look for separable solutions, and it may be verified that the most general eigenfunction of Λ belonging to a total momentum λ is

$$\psi_\lambda = \exp\left[\frac{i}{\hbar}\left(\lambda - \frac{\hbar k}{2} \right) q \right] \sum_{n=0}^{\infty} a_n{}^\lambda e^{-ink q} \phi_n{}^\lambda(X_k). \quad (3)$$

The $a_n{}^\lambda$ are arbitrary complex numbers and the $\phi_n{}^\lambda$ are oscillator wave functions

$$\phi_n{}^\lambda = \left(\frac{(M\omega/\pi\hbar)^{\frac{1}{2}}}{2^n n!} \right)^{\frac{1}{2}} H_n\left[\left(\frac{M\omega}{\hbar} \right)^{\frac{1}{2}} X_k \right] \times \exp[-(M\omega/2\hbar)X_k^2] i^n. \quad (4)$$

We adopt periodic boundary conditions and normalize the wave function over a box of unit length so that

$$\sum_{n=0}^{\infty} a_n{}^{*\lambda} a_n{}^\lambda = 1.$$

For a given λ there are states where the electron has a negative momentum and many quanta are excited. Our treatment places no restrictions on λ so that it may range quasi-continuously from $-\infty$ to $+\infty$. The $a_n{}^\lambda$ are found by satisfying the Schrödinger equation $\mathcal{H}\psi_\lambda = E\psi_\lambda$. Operating on ψ_λ with the interaction part of the hamiltonian we find

$$g_k\left(X_k \sin kq + \frac{Y_k}{M\omega}\cos kq \right)\psi_\lambda = g_k\left(\frac{\hbar}{2M\omega} \right)^{\frac{1}{2}} \exp\left[\frac{i}{\hbar}\left(\lambda - \frac{\hbar k}{2} \right) q \right] \times \sum_{n=0}^{\infty} [a_{n+1}{}^\lambda (n+1)^{\frac{1}{2}} + a_{n-1}{}^\lambda n^{\frac{1}{2}}] e^{-ink q} \phi_n{}^\lambda, \quad (5)$$

where the coefficient $a_{-1}{}^\lambda = 0$. The result of satisfying the Schrödinger equation $\mathcal{H}\psi_\lambda = E\psi_\lambda$ is, therefore,

$$\sum_{n=0}^{\infty} \left[\left\{ (n+\tfrac{1}{2})\hbar\omega - E + \frac{(\lambda - \frac{1}{2}\hbar k - n\hbar k)^2}{2m} \right\} a_n{}^\lambda + g_k\left(\frac{\hbar}{2M\omega} \right)^{\frac{1}{2}} \{ a_{n+1}{}^\lambda (n+1)^{\frac{1}{2}} + a_{n-1}{}^\lambda n^{\frac{1}{2}} \} \right] e^{-ink q} \phi_n(X_k) = 0.$$

Multiplying both sides by $e^{ink q}\phi_n$ and integrating over q and X_k one obtains the recurrence relation

$$\left\{ (n+\tfrac{1}{2})\hbar\omega - E + \frac{(\lambda - \frac{1}{2}\hbar k - n\hbar k)^2}{2m} \right\} a_n{}^\lambda + g_k\left(\frac{\hbar}{2M\omega} \right)^{\frac{1}{2}} [a_{n+1}{}^\lambda (n+1)^{\frac{1}{2}} + a_{n-1}{}^\lambda n^{\frac{1}{2}}] = 0, \quad (6)$$

where $n = 0, 1, 2, \cdots$, and $a_{-1}{}^\lambda = 0$.

For the case of zero interaction we set $g_k = 0$, and find

$$E_{n\lambda}{}^0 = (n+\tfrac{1}{2})\hbar\omega + (\lambda - \tfrac{1}{2}\hbar k - n\hbar k)^2/2m, \text{ or } a_n{}^\lambda = 0. \quad (7)$$

The energy levels are specified by two quantum numbers: n which is discrete and λ which is continuous. The spectrum consists of continua which overlap over a portion of their ranges. When $n=0$ we have $E = \frac{1}{2}\hbar\omega + (\lambda - \frac{1}{2}\hbar k)^2/2m$ and $\psi_\lambda{}^0 = a_0{}^\lambda \exp[i/\hbar(\lambda - \hbar k/2)q]\phi_0(X_k)$ while for $n=1$ we have $E = 3\hbar\omega/2 + (\lambda - 3\hbar k/2)^2/2m$

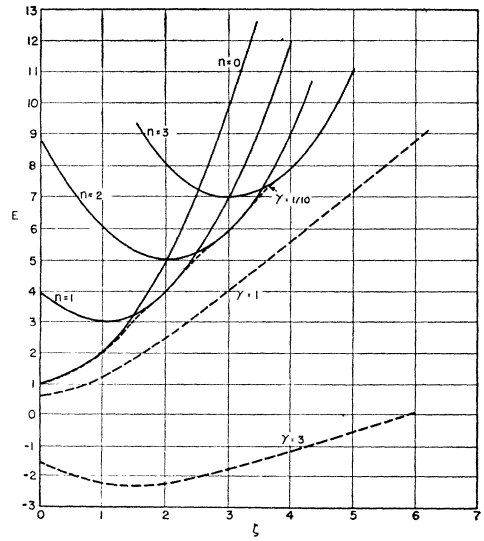

FIG. 1. Energy *vs* momentum for $\alpha = 1$. The quantities α and γ are defined by the equations $\frac{1}{2}\hbar\omega\alpha^2 = (\hbar k)^2/2m$ and $\frac{1}{2}\hbar\omega\gamma = g_k(\hbar/2M\omega)^{\frac{1}{2}}$.

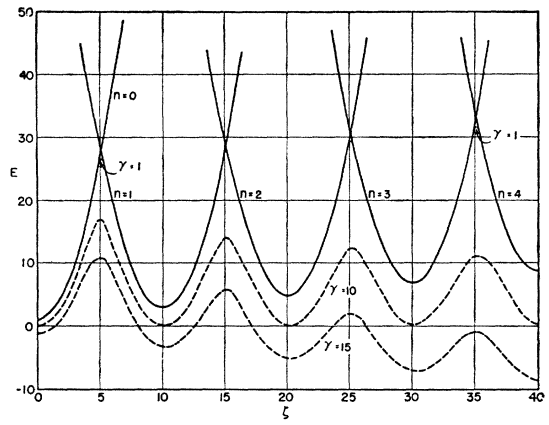

FIG. 2. Energy *vs* momentum for $\alpha=10$.

and $\psi_\lambda{}^1=\exp[i(\lambda-3\hbar k/2)q]a_1{}^\lambda\phi_1(X_k)$. The chief features of the energy spectrum for zero interaction may be illustrated by plotting E *vs* $\lambda-\hbar k/2$, one curve for each n value. This is done in Figs. 1 and 2 for different values of the ratio $(\hbar k)^2/m\hbar\omega$, using reduced units [see Eq. (8)]. Each curve is a parabola symmetric about the value $n\hbar k$ and has its minimum at that value. Two curves intersect at some value of ζ, so that for larger values of ζ the curve for the lower n value lies higher while for smaller ζ values it lies lower. It will be seen that the introduction of interaction removes the intersection of the curves in a way analogous to the removal of intersections of potential curves in the theory of molecules. The lowest curve to the right of the intersection point has a wave function similar to that of the higher curve before interaction was introduced. For sufficiently strong interaction even portions of the lowest curve near the minimum have several quantum terms in their wave functions. (Near the intersection points the effective mass of the electron is altered.)

III. ENERGY SPECTRUM AND SCATTERING PROBABILITY

We note that to deal with the case of finite interaction in the present method one must study the three-term recurrence relation Eq. (6). The energy values are the roots of an infinite determinant. After these have been determined one may find the corresponding ratios of the coefficients $a_n{}^\lambda$. The use of continued-fraction methods will permit us to find numerically the spectrum and the wave functions to any desired accuracy.

To study the recurrence relations we will put

$$(\hbar k)^2/2m=\tfrac{1}{2}\alpha^2\hbar\omega, \quad g_k(\hbar/2M\omega)^{\frac{1}{2}}=\tfrac{1}{2}\gamma\hbar\omega \tag{8}$$

and express all energies in units of $\hbar\omega/2$. Then with $\eta^2=\lambda^2/(2m\hbar\omega/2)$ and $\zeta=\eta-\alpha/2$

$$\{(2n+1)-E+(\zeta-n\alpha)^2\}a_n{}^\lambda +\gamma[a_{n+1}{}^\lambda(n+1)^{\frac{1}{2}}+a_{n-1}{}^\lambda n^{\frac{1}{2}}]=0. \tag{9}$$

Let us put $v_0=a_1/a_0$, $v_1=a_2/a_1\cdots v_r=a_{r+1}/a_r$. Noting that $v_0v_1=a_2/a_0$, we have for the $n=1$ equation

$$v_0{}^\lambda=-\gamma/[\{3-E+(\zeta-\alpha)^2\}+\gamma v_1\sqrt{2}]. \tag{10}$$

We find for the general term

$$v_{r-1}{}^\lambda=-\gamma r^{\frac{1}{2}}/[(2r+1)-E+(\zeta-r\alpha)^2+\gamma v_r{}^\lambda(r+1)^{\frac{1}{2}}]. \tag{11}$$

This last equation can be used to find $v_0{}^\lambda$ in terms of some v_r with r very large as a continued fraction. Inspection of Eq. (11) shows that there is a solution of the recurrence relation for which $v_r\to 0$ as $r\to\infty$. An expression for the energy spectrum is found by obtaining an independent equation for $v_0{}^\lambda$ and comparing with Eq. (10). One finds, using the $r=0$ equation of the recurrence relation,

$$v_0{}^\lambda=-(1-E+\zeta^2)/\gamma. \tag{12}$$

Hence the energy spectrum can be computed from

$$1-E+\zeta^2=\frac{\gamma^2}{3-E+(\zeta-\alpha)^2}\div\frac{\gamma^2\cdot 2}{5-E+(\zeta-2\alpha)^2} \div\frac{\gamma^2\cdot 3}{7-E+(\zeta-3\alpha)^2}\div\frac{\gamma^2\cdot 4}{9-E+(\zeta-4\alpha)^2}\div\cdots, \tag{13}$$

where we use the notation

$$\frac{1}{a}\div\frac{1}{b}\div\frac{1}{c}\equiv\cfrac{1}{a-\cfrac{1}{b-\cfrac{1}{c}}}.$$

Equation (13) has infinitely many roots representing the eigenvalues of ground and excited states for a given value of λ. We thus see that we should actually write $E_{\lambda\mu}$ and $\psi_{\lambda\mu}$ for the eigenvalues and eigenfunctions. To find the root which goes continuously to the zero interaction solution for a given quantum number n as $\gamma\to 0$, it may be convenient to invert the continued fraction n times. In Sec. IV we discuss the results of the numerical study of Eqs. (13) and (11) for several cases and compare them with the results of perturbation theory and other methods of dealing with the hamiltonian, Eq. (1).

The eigenfunctions Eq. (3) form a complete, orthonormal set if one takes all the functions with $-\infty<\lambda<+\infty$, $\mu=0, 1, 2, \cdots\infty$ and may be used to study the following type of scattering problem: If at $t=0$ the electron has a momentum p_0 and there are n quanta excited, we are to find the probability that at a later time t there are m quanta and an electron of momentum p_1. The problem may be solved by finding a linear combination of eigenfunctions satisfying the initial condition that at $t=0$ the wave function is $\exp[i(p_0/\hbar)q]\phi_n(X_k)$. A simple calculation shows that

$$P_{mp_1{}^{np_0}}=|\textstyle\sum_\mu a_n{}^{*\lambda\mu}a_m{}^{\lambda\mu}\exp[-(1/\hbar)E_{\lambda\mu}t]|^2, \tag{14}$$

where λ is fixed by specifying the initial state and p_0 and p_1 are linked by the law of conservation of momen-

tum $\lambda=p_0+n\hbar k=p_1+m\hbar k$. In Figs. 1 and 2 this means that only vertical transitions are permitted.

IV. DISCUSSION OF CASES

(1) Case of Infinite Wavelength, $\alpha=0$

As a first example, let us treat the limiting case $\alpha=0$, where it is possible to find exact expressions for the energy levels and wave functions for arbitrary strength of interaction. The main result is that all the energy levels are shifted by the same amount, which depends on the strength of interaction, while the wave functions are multiplied by a phase factor. Since the shapes of the energy-*vs*-momentum curves are unaltered, the effective mass and average velocity[6] remain that of a free electron. These results occur because one is dealing with the case $\hbar k=0$, or zero phonon recoil momentum. With the help of the exact wave functions the probabilities of occurrence of scattering processes are evaluated and compared with the time-dependent perturbation theory. For small values of the coupling constant the latter gives accurate results, but for stronger coupling it overestimates the scattering probability.

a. Exact Energy Values and Eigenfunctions

Let us take the limit $k\rightarrow 0$, assuming that g_k remains finite. The hamiltonian becomes

$$\mathcal{H}=p^2/2m+g_k(Y_k/M\omega)+\tfrac{1}{2}(M\omega^2X_k^2+Y_k^2/M). \quad (15)$$

The eigenfunctions and energy values of the system are

$$\psi_{n\lambda}=\exp\left(-\frac{i}{\hbar}\lambda q-i\frac{g_k}{\hbar\omega}X_k\right)H_n\left[\left(\frac{M\omega}{\hbar}\right)^{\frac{1}{2}}X_k\right]\times\exp\left(-\frac{M\omega}{2\hbar}X_k^2\right)\left[\frac{(M\omega/2\hbar)^{\frac{1}{2}}}{2^n n!}\right]^{\frac{1}{2}}(i)^n, \quad (16)$$

$$E_{n\lambda}=\hbar^2\lambda^2/2m+(n+\tfrac{1}{2})\hbar\omega-g_k^2/2M\omega^2. \quad (17)$$

In units of $\hbar\omega/2$ the expression is $E_{n\lambda}=E_{n\lambda}{}^0-\gamma^2/2$, the interaction causing a constant depression of energy.

In order to interpret these wave functions, we expand in terms of the complete set of wave functions without interaction

$$\psi_{n\lambda}=\sum_{n'\lambda'}(n\lambda|a|n'\lambda')\phi_{n'}\exp[-i(\lambda'/\hbar)q].$$

We find

$$(n\lambda|a|n'\lambda')=\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\phi_{n'}{}^*\exp(i\lambda' q/\hbar)\psi_{n\lambda}dqdX_k.$$

Inserting $\psi_{n\lambda}$ from Eq. (16) there results

$$(n\lambda|a|n'\lambda')=\delta_{\lambda\lambda'}\int_{-\infty}^{+\infty}\exp\left[-i\frac{g_k}{\hbar\omega}X_k-\frac{M\omega}{\hbar}X_k^2\right]\times H_nH_{n'}dX_k\frac{(M\omega/\pi\hbar)^{\frac{1}{2}}}{(2^n n!2^{n'}n'')^{\frac{1}{2}}}=\delta_{\lambda\lambda'}a_{nn'}, \quad (18)$$

where $\delta_{\lambda\lambda'}$ is the Kronecker delta. The $a_{nn'}$ may be evaluated by using the generating function for the Hermite polynomials. One finds for the lowest coefficients

$$\begin{aligned}
&a_{00}=\exp(-\gamma^2/8), \quad a_{01}=-\tfrac{1}{2}i\gamma\exp(-\gamma^2/8),\\
&a_{02}=-(\gamma^2/4\sqrt{2})\exp(-\gamma^2/8);\\
&a_{11}=(4-\gamma^2)/4\exp(-\gamma^2/8),\\
&a_{03}=(i\gamma^2/8\sqrt{3})\exp(-\gamma^2/8),\\
&a_{12}=[i(\gamma^3-8\gamma)/8\sqrt{2}]\exp(-\gamma^2/8),\\
&a_{00}=(\gamma^4/32\sqrt{6})\exp(-\gamma^2/8),\\
&a_{13}+[(\gamma^4-12\gamma^2)/16\sqrt{6}]\exp(-\gamma^2/8). \quad (19)
\end{aligned}$$

It is to be noted, in addition, that the relation $a_{mn}=a_{nm}$ is valid.

b. Time-Dependent Processes

The preceding formulas for the energy values and eigenfunctions may be also derived from stationary-state perturbation theory, if the perturbation theory is carried out to arbitrarily high accuracy. The factor $\exp(-\gamma^2/8)$ will enter if one takes care to normalize the perturbed wave functions. However, the time-dependent perturbation theory becomes very unwieldy in the higher approximations.

Using Eqs. (14) and (17) we compute

$$P_{0\lambda}{}^{0\lambda}=|\textstyle\sum_\mu|a_0{}^{\lambda\mu}|^2e^{-i\mu\omega t}|^2. \quad (20)$$

Inserting the values of $a_0{}^{\lambda\mu}$ given in Eq. (19), we find

$$P_{0\lambda}{}^{0\lambda}=\left|1+\frac{\gamma^2}{4}e^{-i\omega t}+\frac{\gamma^4}{32}e^{-2i\omega t}+\frac{\gamma^6e^{-3i\omega t}}{48\cdot 8}+\frac{\gamma^8e^{-4i\omega t}}{6\cdot 64\cdot 16}\right|^2\times\exp(-\gamma^2/2). \quad (21)$$

If $\gamma\ll 2$ we can keep only terms up to γ^2. Then

$$P_{0\lambda}{}^{0\lambda}\simeq 1-\tfrac{1}{2}\gamma^2(1-\cos\omega t). \quad (22)$$

Now $P_{0\lambda}{}^{0\lambda}$ is the probability that a system which has been observed to have zero quanta at time $t=0$ will have zero quanta at time t. This probability is less than unity and oscillates about the average value $1-\gamma^2/2$. If γ becomes of the order unity, the probability becomes small. The first approximation in time-dependent perturbation theory gives the same result as the exact probability expanded to order γ^2.

With the help of Eq. (21) we may find the probability $P_{0\lambda}{}^{0\lambda}$ to order γ^4. The result is

$$P_{0\lambda}{}^{0\lambda}=\left(1-\frac{\gamma^2}{2}+\frac{3}{16}\gamma^4\right)+\left(\frac{\gamma^2}{2}-\frac{\gamma^4}{4}\right)\cos\omega t+\frac{\gamma^4}{16}\cos 2\omega t. \quad (23)$$

We thus see that the nonfluctuating part of $P_{0\lambda}{}^{0\lambda}$ has

[6] With the help of methods used in the theory of electron motion in a periodic potential one may show that the mean electron velocity is given by $\bar{V}=\partial E/\partial\lambda$.

been increased to $(1-\frac{1}{2}\gamma^2+\frac{3}{16}\gamma^4)$. In general, the nonfluctuating part is

$$\exp(-\gamma^2/2)\left\{1+\left(\frac{\gamma^2}{4}\right)^2+\left(\frac{\gamma^4}{32}\right)^2+\left(\frac{\gamma^6}{8\cdot 48}\right)^2+\left(\frac{\gamma^8}{6\cdot 16\cdot 64}\right)^2+\cdots\right\}.$$

For $\gamma^2=4$ we find $e^{-2}\{1+1+(\frac{1}{2})^2+(\frac{1}{6})^2+\cdots\}\simeq 0.28$.

(2) Case of Intermediate α, $\alpha=1$

In Fig. 1 we have plotted, for several strengths of interaction, the energy curves obtained by solving Eq. (13). For weak interaction ($\gamma=\frac{1}{10}$) it is seen that the energy remains very close to the zero-quantum curve, giving an effective mass close to the free electron mass. Near the first intersection point, anomalies in average velocity and effective mass occur. The electron velocity decreases rapidly, and the electron has a negative and very small effective mass in this region. Beyond this region, as the total momentum increases, the velocity increases again since the electron must follow the one-quantum curve. The coefficients in the wave function are plotted in Figs. 3 and 4, where one sees the gradual increase of coefficients representing the many-quanta terms.

The moderate interaction curve ($\gamma=1$) starts at $\zeta=0$ with a small curvature, i.e., a large effective mass. As λ increases the curvature approaches zero and the electron velocity remains constant indicating practically infinite electron mass. We note that the region of small effective mass is no longer present. The momentum delivered to the electron is continuously transferred to the oscillators as shown by the increasing values of the higher coefficients, so that the electron velocity cannot increase. One sees from the wave-function curves that at $\zeta=0$ there is a greater contribution from a_1 coefficient than for the weak interaction case. The curves rise slowly showing that at any given value of ζ many of the coefficients are appreciable. As the interaction becomes stronger ($\gamma=3$) another feature comes into play. The absolute minimum, i.e., the most stable state of the system occurs at a nonzero value of λ. On either side the effective mass is very large.

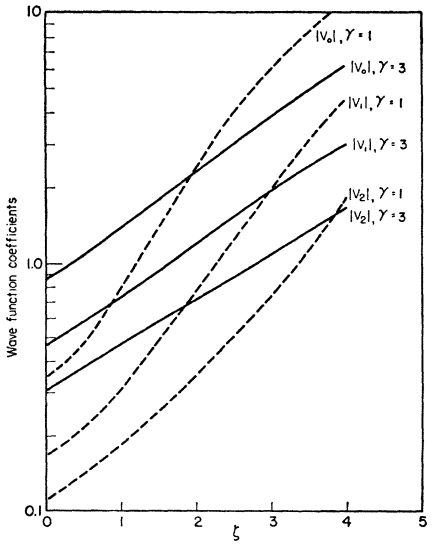

FIG. 3. Wave functions for $\alpha=1$.

The foregoing discussion is concerned with the stationary states. If, however, a sizable electric field is applied so that λ increases steadily and rapidly, there is an appreciable probability that an electron will jump to an excited-state curve.[7] If a transition takes place, the velocity does not experience anomalies and the electron continues to behave as a free particle. For weak interaction the probability of a transition is high.

Let us now compare the foregoing results with those obtained by applying second-order perturbation theory. If one is far from an intersection point, one expects to obtain accurate results for weak interaction. Consider the region between $\zeta=0$ and the first intersection point where the lowest energy curve is close to the zero-quantum curve. Second-order perturbation theory gives for the energy

$$E_0=1+\zeta^2-\gamma^2/(2-2\zeta\alpha+\alpha^2). \tag{24}$$

We find for $\zeta=0$, $\alpha=1$

$\gamma=1$, $|\delta E|=\frac{1}{3}$, as compared to $\frac{1}{3}$ for the exact theory;

$\gamma=3$, $|\delta E|=3$, as compared to 2.6;

$\gamma=5$, $|\delta E|=8.3$, as compared to 6.2.

We thus see that, for increasing interaction, perturbation theory predicts a shift proportional to γ^2, whereas, in reality, a saturation sets in. The accuracy depends, however, on the values of ζ and α. The perturbation expression is valid for strong interactions if $\alpha\gg 1$.

As ζ increases we come near the intersection point, the perturbation treatment breaks down, and one must first remove the degeneracy of the zero and one-quantum curves. Beyond the intersection point perturbation theory applied to the one-quantum curve gives sensible results for weak interactions.

Fröhlich, Pelzer, and Zienau,[3] in their discussion of the lowest levels of an electron interacting with the optical modes of a polar lattice, use a variational method to obtain results considerably more accurate than the perturbation theory. They take a trial wave-function involving the first two terms of our series Eq. (3) and choose the ratio a_1/a_0 so as to obtain the lowest value possible. It is clear from our results that this choice is adequate to handle the anomalies occurring near the intersection point. This method is, in fact, just the procedure which would be employed to remove the degeneracy. From Fig. 3 we see, however, for strong

[7] This probability can be computed using methods developed by W. V. Houston, Phys. Rev. 57, 184 (1940).

interaction ($\gamma=3$), the coefficient a_2 is large even at $\zeta=0$, so that this method will then give inaccurate results. A technique similar to that employed by Fröhlich, Pelzer, and Zienau could be used to handle the degeneracies at higher values of ζ.

(3) Case of the Transition to Periodic Potential, $\alpha\rightarrow\infty$

Let us now pass to the limit $\hbar\omega\rightarrow 0$, keeping $\hbar k$ finite. We also let the mass of the particles giving rise to the oscillation tend to infinity in such a way that $g_k(\hbar/2M\omega)^{\frac{1}{2}}$ remains finite. The recurrence relation Eq. (6) becomes

$$\left\{\frac{[\lambda-(n+\tfrac{1}{2})\hbar k]^2}{2m}-E\right\}a_n^{\lambda}+g_k\left(\frac{\hbar}{2M\omega}\right)^{\frac{1}{2}}[a_{n+1}^{\lambda}(n+1)^{\frac{1}{2}}+a_{n-1}^{\lambda}(n)^{\frac{1}{2}}]=0. \quad (25)$$

This three-term recurrence form is similar to that arising in the solution of Mathieu's equation and gives the same band-type spectrum. The quantity k takes the place of $2\pi/a$ where a is the lattice spacing in the periodic potential problem. The difference is that here values of λ differing by $\hbar k$ do have physical significance, corresponding to different values for the total momentum of the system. For the case where $\hbar\omega$ is small but not zero, the energy oscillates but slowly rises as the total momentum increases. If a weak electric field is applied, imparting momentum to the electron, one can say that a Bragg reflection occurs each time the total momentum passes a maximum. The electron transfers momentum and energy to the oscillators. These relations may be seen from Fig. 2. For small $\hbar\omega$ the curves for zero interaction representing different numbers of quanta in the oscillators have very nearly the same minimum values of energy. Interaction removes the crossing of curves and we find our bandlike spectrum.

As noted in case (2) perturbation theory is valid here unless one goes to extremely strong interactions (measured in units of $\hbar\omega/2$). That is, if one considers two oscillators of the same ω, the one of short wavelength satisfies perturbation theory for stronger interactions.

V. RESUMÉ

The lattice oscillator is characterized by an angular frequency ω and a propagation vector k. In the limit of zero frequency and finite k the phase velocity ω/k tends to zero and one obtains the solution of the problem of an electron moving in a periodic potential. For zero interaction between electron and oscillator the total energy is $E=(n+\frac{1}{2})\hbar\omega+p^2/2m$. Here n is the number of quanta in the oscillator and p in the momentum of the electron. Introducing the total momentum λ of the system, we have $p=\lambda-(n+\frac{1}{2})\hbar k$ and

$$E=(n+\tfrac{1}{2})\hbar\omega+\{\lambda-(n+\tfrac{1}{2})\hbar k\}^2/2m.$$

The energy thus depends on two quantum numbers, λ which is continuous, and n which is discrete. One plots E *vs* λ with one curve for each value of n. (See Figs. 1 and 2.) Although the plots differ, depending on the values of k and ω, a general feature is the intersection of curves. For values of λ less than that at the point of intersection, the curve representing n quanta lies lower than the curve for $n+1$, while beyond the intersection point the reverse is true. Thus the lowest energy state becomes that in which successively more quanta occupy the oscillator. Introduction of interaction removes the degeneracy and results in continuous curves but the same qualitative features remain. For moderate interactions the lowest energy curve has the shape of the asymptote of the zero energy curves. This means that the energy does not rise as rapidly as the zero quantum curve and results in a high effective electron mass.

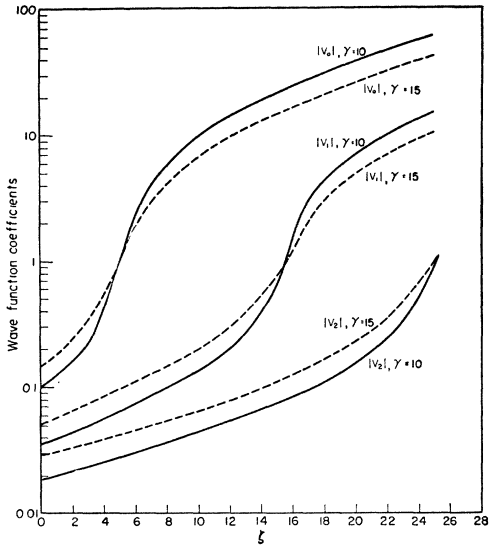

FIG. 4. Wave functions for $\alpha=10$.

If one examines the curves of Fig. 3, which are for the low frequency case, one sees that removal of degeneracy leads to a bandlike spectrum with energy slowly rising as the total momentum increases. The physical interpretation is that the electron makes Bragg reflections giving up a quantum of energy and momentum to the oscillator so that, as the total momentum increases, the electron velocity remains bounded, but more and more momentum and energy are present in the oscillator.

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