remains a puzzle, since all of the splittings should be anisotropic. In many respects, however, the CdSe lines were similar to those of CdS and ZnO, as can be seen from the typical line complexes of Table II. Not unlike CdS, the CdSe complex lines also showed both linear and nonlinear magnetic splittings, as well as zero-field-split pairs and isotropic electron g values. Several of the linearly split lines undoubtedly arose from neutral complexes, but thermalization effects were not observed in the split components of these lines; consequently, it was not possible to determine, in the usual way, whether the neutral complex was of donor or acceptor origin. The excited states of a bound-exciton complex were rather dramatically demonstrated in the magnetic splittings of the line group, $I_{9a}-I_{9b}$. Since diamagnetic shifts are observed in intrinsic exciton spectra,[4] and since such shifts are to be expected from theory,[4,23] the observed negative diamagnetic shift in the spectral splitting of I_9 serves as further confirmation of excited states in this bound-exciton complex.

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Electron and Phonon Bound States and Scattering Resonances for Extended Defects in Crystals

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By making use of the translational symmetry associated with line and plane defects in crystals, we define certain subbands of the unperturbed electron and phonon bands. Certain Wannier functions and Green's functions associated with these subbands are defined and are used to study the existence of localized electron and phonon states and scattering resonances associated with extended defects. By firstly considering very simple examples of such perturbations, of arbitrary strength and secondly considering perturbations of quite general form but of small strength, we establish the general existence of electron and phonon bound states for line and plane defects, and the existence of electron and phonon scattering resonances for line defects. The effects of different characteristics of the unperturbed band structure are indicated. In contrast to the above results, bound states for point defects and scattering resonances for point and plane defects do not occur unless the perturbation exceeds a certain minimum strength. Our results underline the basic importance of including the band structure in scattering problems of this type and also the dangers of relying on perturbation approaches. Attempts which have been made to arrive at properties of crystal defects by the study of one dimensional models should also be reviewed in the light of our results. The above-mentioned bound levels form continuous bands which may lie partly between or within the allowed bands of the unperturbed crystal, and those electron levels that lie in the forbidden regions should have an important influence on the properties of semiconductors and insulators. Such effects have long been observed, and have been interpreted usually in terms of the "dangling bond" theory of Shockley and Read; our theory gives a much more general basis for their existence and, although the difficulties are considerable, seems to offer a means of quantitative investigation which previously did not exist. The electron and phonon scattering resonances seem to afford a natural explanation of the long-standing discrepancy between theory and experiment on the subject of dislocation contributions to electrical and thermal resistivities.

I. INTRODUCTION

THE problem of the scattering of conduction electrons in metals by localized point imperfections, using the Wannier-function–Green's-function technique of Koster and Slater[1] has been treated by several authors on the basis of simplified models, and has been discussed by Seeger[2] and Callaway,[3] who give further references. For our purposes, the important point to emerge from this work is that a localized point perturbation can give rise to neither bound states nor scattering resonances[4] in the electron spectrum unless its strength exceeds a certain value. Similar techniques have also been applied by several authors to the problem of phonon scattering by point defects, and Callaway[3] gives appropriate references. Again we find the perturbation must exceed a certain minimum strength in order to give rise to either bound states or scattering resonances in the phonon spectrum.

In this paper we adapt these methods to the study of electron and phonon scattering from line and surface defects which preserve the crystal periodicity in one and two dimensions, respectively. In Sec. II we make use of this periodicity to define certain subbands of the unperturbed electron and phonon energy bands, and we use these subbands to generate Green's func-

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[4] To avoid confusion we use the term *scattering resonance* rather than *virtual bound state*, so that *bound state* refers to a real localized state whose amplitude is significant only near the perturbed region.

tions analogous to those appearing in the point-defect problems, but differing from these in one important respect as shown in Sec. III. On the basis of simplified models it is shown in Sec. IV that for line perturbations of any strength both bound states and scattering resonances associated with these subbands occur for phonons and electrons. For surface defects the same results hold for bound states but the existence of scattering resonances depends on the strength of the perturbation. In Sec. V we consider more general perturbations and indicate in what way the existence of bound states and resonances may depend on the form of the perturbation and on the degeneracy of the sub-band edges. We deduce the existence of bands of resonances and bands of bound-state energies associated with each band of the original crystal. In Sec. VI we briefly discuss some implications of these results.

The existence of real phonon bound states associated with a line or plane of isotopes has been shown by Kobori[5] on the basis of a simple model and using a Green's-function method, but he does not extend his argument to other defects, to electrons, or to the existence of scattering resonances. Using more restricted techniques, other authors[6–10] have examined the existence of bound states for simple models of plane defects and dislocations. The "dangling bond" acceptor states of dislocations in semiconductors are well known; we give some discussion of semiconductors in Sec. VI.

Regarding the experimental observation of localized and resonant states, it seems possible[11,12] that localized phonon states, associated with *point* defects, could be observed by Mössbauer or neutron-scattering experiments. Resonances in the phonon scattering by point defects have been observed[13] by their effect on the thermal conductivity, while Friedel[14] has explained trends in the electronic properties of transition metal alloys in terms of resonance scattering associated with the d band of the impurity.

Direct observation of bound and resonant states associated with line or surface defects is obviously complicated by the fact that such states occur right through the unperturbed energy bands, as indicated in Sec. V; hence we do not expect any *sharp* resonance effects such as those observed[13,14] for point defects. However, the existence of localized states associated with dislocations in semiconductors is well established on the basis of photoconductivity and excess carrier lifetime measurements. Moreover, it seems that the resonance scattering of conduction electrons and phonons from dislocations affords a natural explanation of the high electrical and thermal resistivities which are experimentally attributed to dislocations and which perturbation treatments of the scattering severely underestimate. This point is taken up in detail in another paper[15] where it is shown that the resonance scattering can indeed lead to resistivities of the right order of magnitude.

II. GENERAL FORMULATION

In this section we will derive in some detail the equations necessary for the study of electron and phonon bound states and scattering resonances associated with a straight-line defect; the procedure for plane defects follows in an obvious manner and we shall merely quote appropriate results.

For simplicity we consider a crystal having one atom per unit cell which is defined by the primitive vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$, and containing a single line defect with period $\mathbf{a}_3$.[16] We impose periodic boundary conditions so that the electron and phonon states of the unperturbed crystal are characterized by, amongst other labels, a wave vector $\mathbf{k}=\mathbf{k}_*+\mathbf{k}_3$, where

$$\mathbf{k}_*=2\pi\sum_{i=1}^{2} n_i\mathbf{b}_i/N_i \quad \text{and} \quad \mathbf{k}_3=2\pi n_3\mathbf{b}_3/N_3. \quad (2.1)$$

Here $0\leqslant n_i\leqslant N_i-1$, the N_i arising from the boundary conditions in the usual way. The $\mathbf{b}_i$ are the primitive reciprocal lattice vectors derived from the $\mathbf{a}_i$. If the unit cell volume is Ω, then our crystal is of volume $N\Omega$, where $N=N_1N_2N_3$. As far as notation is concerned, we shall use throughout this paper the letters $\mathbf{k}$ and $\mathbf{l}$ with or without primes, and with appropriate subscripts as in (2.1), to denote wave vectors; likewise the letters $\mathbf{m}$ and $\mathbf{n}$ will be used to denote lattice vectors of the unperturbed crystal, so that, e.g., $\mathbf{m}=\mathbf{m}_*+\mathbf{m}_3$, where

$$\mathbf{m}_*=\sum_{i=1}^{2} n_i\mathbf{a}_i, \quad \mathbf{m}_3=n_3\mathbf{a}_3, \quad \text{and} \quad 0\leqslant n_i\leqslant N_i-1. \quad (2.2)$$

At this stage we need to consider the electron and phonon problems separately.

A. Electron States

We denote the one-electron Hamiltonians of the unperturbed and perturbed crystals by H_0 and $H=H_0+V$, respectively. Since H is invariant under transla-

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[16] If the perturbation has some other period, we can still regard this as a primitive translation of the unperturbed crystal which we must now regard as having more than one atom per unit cell. The results of the following sections are essentially unaltered by considering more than one atom per unit cell and it does not seem justified to deal with this added complication at this stage.

tions $\mathbf{a}_3$ we can, as discussed by Holland,[17] label the perturbed wave functions by the wave vectors $\mathbf{k}_3$, as well as other labels bearing one-to-one correspondence with the $N_*=N_1N_2$ vectors $\mathbf{k}_*$ and the band indices j. So with $b_j(\mathbf{k}_3+\mathbf{k}_*, \mathbf{r})$ denoting the Bloch function corresponding to the jth band and wave vector $\mathbf{k}_3+\mathbf{k}_*$ of the unperturbed crystal and normalized over the crystal volume $N\Omega$, we define the orthonormal Wannier functions

$$a_j(\mathbf{n}_*,\mathbf{r};\mathbf{k}_3)=N_*^{-1/2}\sum_{\mathbf{k}_*} b_j(\mathbf{k}_3+\mathbf{k}_*,\mathbf{r})e^{-i\mathbf{k}_*\cdot\mathbf{n}_*}, \quad (2.3)$$

the sum being over all N_* vectors $\mathbf{k}_*$.

These Wannier functions are localized[17] about lines parallel to the line defect and through the points $\mathbf{n}_*$. They also have the Bloch property of transforming irreducibly under the translations $n_3\mathbf{a}_3$. It follows from this and from their completeness property that any wave function of the perturbed crystal corresponding to the wave vector $\mathbf{k}_3$ can be expanded

$$\Psi_{\mathbf{k}_3}(\mathbf{r})=\sum_j\sum_{\mathbf{n}_*} C_j(\mathbf{n}_*,\mathbf{k}_3)a_j(\mathbf{n}_*,\mathbf{r};\mathbf{k}_3). \quad (2.4)$$

On substituting this expansion in the Schrödinger equation for Ψ and carrying through the procedure of Seeger,[2] we get for the coefficients

$$C_q(\mathbf{n}_*,\mathbf{k}_3)=\sum_{j,\mathbf{m}_*,\mathbf{m}_*'} C_j(\mathbf{m}_*',\mathbf{k}_3)V_{qj}(\mathbf{m}_*,\mathbf{m}_*') \times G_{E,q}(\mathbf{n}_*-\mathbf{m}_*). \quad (2.5)$$

Although not explicitly labelled, V and G in (2.5) depend on $\mathbf{k}_3$ and are given by

$$V_{qj}(\mathbf{m}_*,\mathbf{n}_*)=\int_{N\Omega} a_q^*(\mathbf{m}_*,\mathbf{r};\mathbf{k}_3)V(\mathbf{r})a_j(\mathbf{n}_*,\mathbf{r};\mathbf{k}_3)d^3r, \quad (2.6)$$

the integral being over the crystal of volume $N\Omega$, and

$$G_{E,q}(\mathbf{n}_*-\mathbf{m}_*)=-\frac{1}{N_*}\sum_{\mathbf{k}_*}\frac{e^{i\mathbf{k}_*\cdot(\mathbf{n}_*-\mathbf{m}_*)}}{E_{0,q}(\mathbf{k}_3;\mathbf{k}_*)-E}, \quad (2.7)$$

where $E_{0,q}(\mathbf{k}_3;\mathbf{k}_*)\equiv E_{0,q}(\mathbf{k}_3+\mathbf{k}_*)$ is the eigenvalue of H_0, corresponding to $b_q(\mathbf{k}_3+\mathbf{k}_*,\mathbf{r})$.

The eigenvalues E of the perturbed problem are obtained from (2.5) as the roots of

$$D(E)\equiv\det[\delta_{qj}\delta_{\mathbf{m}_*\mathbf{n}_*}-\sum_{\mathbf{m}_*'} V_{qj}(\mathbf{m}_*',\mathbf{n}_*) \times G_{E,q}(\mathbf{m}_*-\mathbf{m}_*')]=0, \quad (2.8)$$

and this equation is particularly suitable for the study of the real bound levels which lie[17] above or below the various $\mathbf{k}_3$ subbands,[18] separated from the subband edge by an amount independent of N_*.[19]

To study the scattering resonances, which lie within the $\mathbf{k}_3$ subbands, we find it convenient to treat the problem explicitly from a scattering viewpoint and, following Callaway,[3] verify that the $C_j(\mathbf{n}_*,\mathbf{k}_3)$ representing an outgoing scattered wave of energy E and corresponding to an incident Bloch wave of wave vector $\mathbf{k}_3+\mathbf{k}_*$ and band s such that $E_{0,s}(\mathbf{k}_3;\mathbf{k}_*)=E$, are given by

$$C_q^{(s)}(\mathbf{n}_*,\mathbf{k}_3)=C_{0,q}^{(s)}(\mathbf{n}_*,\mathbf{k}_3)+\sum_{j,\mathbf{m}_*,\mathbf{m}_*'} C_j^{(s)}(\mathbf{m}_*',\mathbf{k}_3) \times V_{qj}(\mathbf{m}_*,\mathbf{m}_*')\mathcal{G}_{E,q}(\mathbf{n}_*-\mathbf{m}_*), \quad (2.9)$$

where

$$C_{0,q}^{(s)}(\mathbf{n}_*,\mathbf{k}_3)=N_*^{-1/2}\delta_{qs}e^{i\mathbf{k}_*\cdot\mathbf{n}_*} \quad (2.10)$$

is an appropriately normalized solution of the unperturbed problem, and

$$\mathcal{G}_{E,q}(\mathbf{n}_*-\mathbf{m}_*)=\lim_{\epsilon\to+0} G_{E+i\epsilon,q}(\mathbf{n}_*-\mathbf{m}_*). \quad (2.11)$$

Following Callaway we associate our resonant state energies with the (complex) poles of the scattering amplitude so that from (2.9) we need the roots E of

$$\mathfrak{D}(E)\equiv\det[\delta_{qj}\delta_{\mathbf{m}_*\mathbf{n}_*}-\sum_{\mathbf{m}_*'} V_{qj}(\mathbf{m}_*',\mathbf{n}_*) \times\mathcal{G}_{E,q}(\mathbf{m}_*-\mathbf{m}_*')]=0. \quad (2.12)$$

The only physically important solutions of (2.12) are those close to a real E_0 satisfying

$$\mathcal{R}[\mathfrak{D}(E_0)]=0, \quad (2.13)$$

where $\mathcal{R}$ denotes real part. The scattering cross section near such an E_0 has a large value independent of the strength of the perturbation.[3]

B. Phonon States

We start from the classical equations of motion[3,20] in terms of the Cartesian components[21] $U_\alpha(\mathbf{m})$ of the displacement of the atom at the lattice site $\mathbf{m}$ from its equilibrium position. Thus, for atoms of mass M we find for a wave of angular frequency ω,

$$M\omega^2U_\alpha(\mathbf{m})-\sum_{\mathbf{n},\beta}\Phi_{\alpha\beta}{}^{\mathbf{mn}}U_\beta(\mathbf{n})=\sum_{\mathbf{n}\beta}\Delta_{\alpha\beta}{}^{\mathbf{mn}}U_\beta(\mathbf{n}). \quad (2.14)$$

Here the $\Phi_{\alpha\beta}{}^{\mathbf{mn}}=\Phi_{\alpha\beta}{}^{\mathbf{m}-\mathbf{n}}$ are the coupling constants for

[7] B. W. Holland, Phil. Mag. 8, 87 (1963).

[18] Following Holland, we refer to the set of levels formed from the $E_{0q}(\mathbf{k}_3;\mathbf{k}_*)$ as $\mathbf{k}_*$ runs over its N_* values, as a $q\mathbf{k}_3$ subband of the unperturbed crystal. Thus a bound state, which lies outside a given subband, may still lie within an allowed band of the original crystal.

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[21] Unless otherwise specified, Greek subscripts take the values 1, 2, 3.

the unperturbed crystal and the $\Delta_{\alpha\beta}{}^{\mathrm{mn}}$ represent the perturbation. For our line defect, Δ depends on $\mathbf{m}_3$ and $\mathbf{n}_3$ only through the difference $\mathbf{m}_3-\mathbf{n}_3$ so we write

$$\Delta_{\alpha\beta}{}^{\mathrm{mn}}=\Delta_{\alpha\beta}(\mathbf{m}_*,\ \mathbf{n}_*,\ \mathbf{m}_3-\mathbf{n}_3). \tag{2.15}$$

Because of this property it is readily verified that the solutions of (2.14) can be labeled by the wave vector $\mathbf{k}_3$ and can be written as a normal coordinate expansion[20] over the $\mathbf{k}_3$ subbands of all three polarizations as follows:

$$U_\alpha{}^{\mathrm{k}_3}(\mathbf{m})=(MN)^{-1/2}\sum_{\mathbf{k}_*,j} e_\alpha(\mathbf{k}_3+\mathbf{k}_*,\ j)Q(\mathbf{k}_3+\mathbf{k}_*,\ j) \times\exp[i(\mathbf{k}_3+\mathbf{k}_*)\cdot\mathbf{m}]. \tag{2.16}$$

Here the polarization index j takes the values 1, 2, 3 and the polarization vectors $e_\alpha(\mathbf{k},j)$, real for monatomic crystals, satisfy

$$\omega_j{}^2(\mathbf{k})e_\alpha(\mathbf{k},j)=\sum_\beta D_{\alpha\beta}(\mathbf{k})e_\beta(\mathbf{k},j), \tag{2.17}$$

and consequently the orthogonality and completeness relations

$$\sum_\alpha e_\alpha(\mathbf{k},j)e_\alpha(\mathbf{k},j')=\delta_{jj'}, \tag{2.18}$$

and

$$\sum_j e_\alpha(\mathbf{k},j)e_\beta(\mathbf{k},j)=\delta_{\alpha\beta}. \tag{2.19}$$

The $\omega_j{}^2(\mathbf{k})$, being the squares of the eigenfrequencies of the unperturbed lattice, are the eigenvalues of the 3×3 matrices

$$D_{\alpha\beta}(\mathbf{k})=M^{-1}\sum_{\mathbf{m}}\Phi_{\alpha\beta}{}^{\mathrm{m}}e^{-i\mathbf{k}\cdot\mathbf{m}}. \tag{2.20}$$

We substitute the expression (2.16) into the left side of (2.14), multiply both sides by $e^{-i\mathbf{m}\cdot\mathbf{k}'}$, and sum over $\mathbf{m}$. Then, simplifying by use of (2.20) and (2.17), we get

$$\sum_j e_\alpha(\mathbf{k},j)Q(\mathbf{k},j)[\omega^2-\omega_j{}^2(\mathbf{k})] =(MN)^{-1/2}\sum_{\mathbf{m},\mathrm{n},\beta}\Delta_{\alpha\beta}{}^{\mathrm{mn}}U_\beta{}^{\mathrm{k}_3}(\mathbf{n})e^{-i\mathbf{m}\cdot\mathbf{k}}.$$

Now multiply by $e_\alpha(\mathbf{k},j')$ and sum over α using (2.18) to solve for $Q(\mathbf{k},j)$, and then substitute this expression back in (2.16) to obtain finally

$$U_\alpha{}^{\mathrm{k}_3}(\mathbf{m})=\sum_{\mathrm{n},\mathrm{n}',\beta,\gamma}U_\gamma{}^{\mathrm{k}_3}(\mathbf{n}')\Delta_{\beta\gamma}{}^{\mathrm{nn}'} \times G_{\alpha\beta}(\mathbf{m}-\mathbf{n},\omega^2;\mathbf{k}_3), \tag{2.21}$$

where we have written

$$G_{\alpha\beta}(\mathbf{m}-\mathbf{n},\omega^2;\mathbf{k}_3) =\frac{1}{MN}\sum_{\mathbf{k}_*,j}\frac{e_\alpha(\mathbf{k}_3+\mathbf{k}_*,\ j)e_\beta(\mathbf{k}_3+\mathbf{k}_*,\ j)}{\omega^2-\omega_j{}^2(\mathbf{k}_3;\mathbf{k}_*)}e^{i\mathbf{k}\cdot(\mathbf{m}-\mathrm{n})}. \tag{2.22}$$

The set of equations (2.21) is of order $3N\times3N$, but we can reduce this by noticing, from (2.16), that the U's are of the form

$$U_\alpha{}^{\mathrm{k}_3}(\mathbf{m})=v_\alpha{}^{\mathrm{k}_3}(\mathbf{m}_*)e^{i\mathbf{k}_3\cdot\mathbf{m}_3}. \tag{2.23}$$

Using (2.23) in (2.21), we get $3N_*$ independent equations in the $3N_*$ variables $v_\alpha{}^{\mathrm{k}_3}(\mathbf{m}_*)$, viz.

$$\sum_{\mathbf{n}_*'\gamma}v_\gamma{}^{\mathrm{k}_3}(\mathbf{n}_*')\{\delta_{\alpha\gamma}\delta_{\mathbf{m}_*\mathbf{n}_*'}-\sum_{\mathbf{n}_*\beta}\Lambda_{\beta\gamma}(\mathbf{n}_*,\mathbf{n}_*') \times F_{\alpha\beta}(\mathbf{m}_*-\mathbf{n}_*,\omega^2;\mathbf{k}_3)\}=0, \tag{2.24}$$

where

$$\Lambda_{\beta\gamma}(\mathbf{n}_*,\mathbf{n}_*')=\sum_{\mathbf{n}_3}\Delta_{\beta\gamma}(\mathbf{n}_*,\mathbf{n}_*',\mathbf{n}_3)e^{-i\mathbf{k}_3\cdot\mathbf{n}_3}, \tag{2.25}$$

and

$$F_{\alpha\beta}(\mathbf{m}_*-\mathbf{n}_*,\omega^2;\mathbf{k}_3) =\frac{1}{MN_*}\sum_{\mathbf{k}_*,j}\frac{e_\alpha(\mathbf{k}_3+\mathbf{k}_*,\ j)e_\beta(\mathbf{k}_3+\mathbf{k}_*,\ j)}{\omega^2-\omega_j{}^2(\mathbf{k}_3;\mathbf{k}_*)} \times e^{i\mathbf{k}_*\cdot(\mathbf{m}_*-\mathbf{n}_*)}. \tag{2.26}$$

Thus the eigenvalues ω^2 of the perturbed problem are the roots of

$$M(\omega^2)\equiv\det[\delta_{\alpha\gamma}\delta_{\mathbf{m}_*\mathbf{n}_*}-\sum_{\mathbf{n}_*'\beta}\Lambda_{\beta\gamma}(\mathbf{n}_*',\mathbf{n}_*) \times F_{\alpha\beta}(\mathbf{m}_*-\mathbf{n}_*',\omega^2;\mathbf{k}_3)]=0, \tag{2.27}$$

and as with (2.8) we use this equation to study those states which lie outside the unperturbed subbands. The fact that such states are localized near the defect follows from Eq. (2.21) or (2.24) using the arguments of Holland[17]; the method of stationary phase shows the Green's functions (2.7) and (2.26) decrease exponentially for large $|\mathbf{m}_*-\mathbf{n}_*|$. One difference to be observed between the phonon and electron problems is that only solutions $\omega^2>0$ of (2.27) are acceptable in order to yield real frequencies of vibration.

As in Sec. IIA, we use a slightly different formalism to study the in-band scattered states, and using Eqs. (2.17)–(2.20) we verify that with $v_\alpha{}^{\mathrm{k}_3}(\mathbf{m}_*)$ given by (2.23), the solution of (2.14) representing an outgoing scattered wave of frequency ω, corresponding to an incident wave of polarization j and wave vector $\mathbf{k}_3+\mathbf{k}_*$ such that $\omega_j(\mathbf{k}_3+\mathbf{k}_*)=\omega$, is

$$v_\alpha{}^{\mathrm{k}_3}(\mathbf{m}_*)=v_{0,\alpha}{}^{\mathrm{k}_3}(\mathbf{m}_*)+\sum_{\mathbf{n}_*,\mathbf{n}_*',\beta,\gamma}\Lambda_{\beta\gamma}(\mathbf{n}_*,\mathbf{n}_*') \times\mathfrak{F}_{\alpha\beta}(\mathbf{m}_*-\mathbf{n}_*,\omega^2;\mathbf{k}_3)v_\gamma{}^{\mathrm{k}_3}(\mathbf{n}_*'), \tag{2.28}$$

where

$$\mathfrak{F}_{\alpha\beta}(\mathbf{m}_*-\mathbf{n}_*,\omega^2;\mathbf{k}_3) =\lim_{\epsilon\to+0}F_{\alpha\beta}(\mathbf{m}_*-\mathbf{n}_*,\omega^2+i\epsilon;\mathbf{k}_3). \tag{2.29}$$

Thus the poles of the scattering amplitude are at the

solutions ω^2 of

$$\mathfrak{M}(\omega^2)\equiv\det[\delta_{\alpha\gamma}\delta_{m_*n_*}-\sum_{n_*'\beta}\Lambda_{\beta\gamma}(\mathbf{n}_*',\mathbf{n}_*)\times\mathfrak{F}_{\alpha\beta}(\mathbf{m}_*-\mathbf{n}_*',\omega^2;\mathbf{k}_3)]=0. \quad (2.30)$$

Again we are interested in solutions $\omega^2\simeq\omega_0^2$, where

$$\mathfrak{R}[\mathfrak{M}(\omega_0^2)]=0. \quad (2.31)$$

C. Plane Defects

The equations of Secs. IIA and IIB can be made to apply to plane, rather than line, defects simply by interchanging * and 3 subscripts on the wave vectors and lattice vectors. The only significant effect of this is to change the behavior of the Green's functions (2.7), (2.11), (2.26), and (2.29) as the energy approaches a subband edge. This will be discussed in the next section.

III. BEHAVIOR OF THE GREEN'S FUNCTIONS

The proofs of the existence of bound and resonant states depend on the fact that the Green's functions mentioned above became infinite as the energy approaches a subband edge, as we now show.

First consider (2.7). We replace the sum over the two-dimensional space of $\mathbf{k}_*$ by an integral[22] over the subband,

$$\sum_{k_*}\rightarrow N_*\sigma_*\int d^2k_*, \quad (3.1)$$

where[23] there are $N_*\sigma_*d^2k_*$ points $\mathbf{k}_*$ in the area element d^2k_*.

Now since $E_{0,q}(\mathbf{k}_3;\mathbf{k}_*)$ is an analytic function of $\mathbf{k}_*$, we can expand it about the bottom of the subband in a power series in κ_1 and κ_2, the Cartesian components of $\mathbf{k}_*$ relative to an origin at the subband minimum, thus

$$E_0(\mathbf{k}_3;\mathbf{k}_*)=\mathcal{E}_B(\mathbf{k}_3)=\sum_{i,j=1}^{2}a_{ij}(\mathbf{k}_3)\kappa_i\kappa_j+\text{higher powers}, \quad (3.2)$$

where the quadratic form is positive definite. Here $\mathcal{E}_B(\mathbf{k}_3)$ is the bottom of the $\mathbf{k}_3$ subband and we have dropped the band index q. If the minimum occurs in the interior of that section of the Brillouin zone corresponding to the $\mathbf{k}_3$ subband the absence of linear terms in (3.2) requires no explanation; if the minimum occurs at a boundary of this section it is explained by the orthogonality of the energy surfaces to the Brillouin zone boundary. The terms corresponding to small κ_i dominate in the sum (2.7) as $E-\mathcal{E}_B\rightarrow-0$, so we do not need to consider the higher-order terms of (3.2).

[22] This is permissible for E outside the subband when the integral is a slowly varying function of $\mathbf{k}_*$. We have to be more careful when considering the in-band scattered states.

[23] σ_* depends on the crystal structure and the direction of the defect line, but is of order a^2 for a crystal of lattice constant a.

Using (3.2) and (3.1) in (2.7) we show in Appendix A that, as $E-\mathcal{E}_B(\mathbf{k}_3)\rightarrow-0$,

$$G_E(0)\rightarrow a(\mathbf{k}_3)\sigma_*\ln[\mathcal{E}_B(\mathbf{k}_3)-E], \quad (3.3)$$

where

$$a(\mathbf{k}_3)=\frac{1}{2}\int_0^{2\pi}[a_{11}\sin^2\theta+2a_{12}\sin\theta\cos\theta+a_{22}\cos^2\theta]^{-1}d\theta, \quad (3.4)$$

which exists unless $a_{12}^2=a_{11}a_{22}$, in which unlikely case further terms of (3.2) need to be considered. Since the quadratic form in (3.2) is positive definite, $a(\mathbf{k}_3)>0$; thus by (3.3)

$$G_E(0)\rightarrow-\infty \quad \text{as} \quad E-\mathcal{E}_B\rightarrow-0. \quad (3.5)$$

Precisely the same considerations apply as E approaches the top, $\mathcal{E}_T$, of a subband from above and we find

$$G_E(0)\rightarrow+\infty \quad \text{as} \quad E-\mathcal{E}_T\rightarrow+0. \quad (3.6)$$

Note that we have implicitly assumed in writing (3.2) that there is a unique state $\mathbf{k}$ corresponding to the subband minimum. If on the contrary this level is degenerate, we simply expand about each such minimum point and add their separate contributions to the integral. The conclusions (3.5) and (3.6) are unchanged.

It is clear from (2.7) that for a subband edge at a nondegenerate state $\mathbf{k}_3+\mathbf{k}_*^e$,

$$G_E(\mathbf{n}_*)\rightarrow e^{i\mathbf{k}_*^e\cdot\mathbf{n}_*}G_E(0), \quad (3.7)$$

as E approaches the edge from outside the subband. For a degenerate subband maximum or minimum $G_E(\mathbf{n}_*)$ approaches a sum of such terms, one for each degenerate state. In Sec. IV we are mostly concerned with the behavior of $G_E(0)$.

Moving on to the Green's function (2.11) we write it as, using (3.1),

$$\mathcal{G}_E(0)=\lim_{\epsilon\rightarrow+0}\sigma_*\int\frac{d^2k_*}{E+i\epsilon-E_0(\mathbf{k}_3;\mathbf{k}_*)},$$

i.e.,

$$\mathcal{G}_E(0)=[I(E)-i\pi\eta(E)], \quad (3.8)$$

where $N_*\eta(E)$ is the number of subband states per unit energy range in the unperturbed crystal, and

$$I(E)=P\int\eta(E')/(E-E')dE'. \quad (3.9)$$

Here P denotes principal part and the integral is over the $\mathbf{k}_3$ subband.

We can proceed using the general expansion (3.2), but nothing essential is lost if we adopt the simpler version

$$E_0(\mathbf{k}_3;\mathbf{k}_*)=\mathcal{E}_B(\mathbf{k}_3)+\frac{\hbar^2k_*^2}{2m^*(\mathbf{k}_3)}+O(k_*^4) \quad (3.10)$$

in which we write the constant explicitly as an effective mass. For the bands (3.10) we readily find

$$\eta(E) \to 2\pi\sigma_* \hbar^{-2} m^*(\mathbf{k}_3) \tag{3.11}$$

independent of E, as $E-\mathcal{E}_B \to +0$. Thus, from (3.9),

$$I(E) \to 2\pi\sigma_* \hbar^{-2} m^*(\mathbf{k}_3) \log[E-\mathcal{E}_B(\mathbf{k}_3)], \tag{3.12}$$

i.e.,

$$I(E) \to -\infty \quad \text{as} \quad E-\mathcal{E}_B \to +0, \tag{3.13}$$

and likewise we find

$$I(E) \to +\infty \quad \text{as} \quad E-\mathcal{E}_T \to -0. \tag{3.14}$$

Regarding $E_0(\mathbf{k}_3;\mathbf{k}_*)$ as a function of $\mathbf{k}_*$, its absolute maximum and minimum for the $\mathbf{k}_3$ subband are $\mathcal{E}_T$ and $\mathcal{E}_B$, respectively. If it also has local maxima $\mathcal{E}_{Mi}$ and minima $\mathcal{E}_{mj}$, we similarly find (see appendix A)

$$I(E) \to -\infty \quad \text{as} \quad E \to \mathcal{E}_{mj}, \quad \text{all} \quad j, \tag{3.15}$$

and

$$I(E) \to +\infty \quad \text{as} \quad E \to \mathcal{E}_{Mi}, \quad \text{all} \quad i. \tag{3.16}$$

The general existence of such local extrema is a consequence of the general existence[24,25] of saddle points of the function $E_0(\mathbf{k}_3+\mathbf{k}_*)$ when regarded as a function of $(\mathbf{k}_3+\mathbf{k}_*)$; the intersection of this generalized surface with the plane $\mathbf{k}_3=$ constant yields the surface $E_0(\mathbf{k}_3;\mathbf{k}_*)$ which will have either maxima, minima, or saddle points, depending on the relative dispositions of the plane and the generalized surface. We show in Appendix A that $I(E)$ *does not* become infinite near saddle points of the surface $E_0(\mathbf{k}_3;\mathbf{k}_*)$, so that resonances are not generally associated with these points.

In considering the phonon Green's function (2.26), much the same considerations apply. In general the sub-bands corresponding to different polarizations will have different maxima and minima, $\omega=\Omega_T(j;\mathbf{k}_3)$ or $\Omega_B(j;\mathbf{k}_3)$. Also[20] $\omega_j^2(\mathbf{k}_3+\mathbf{k}_*)$ is an even function of $\mathbf{k}$ so we expand, for instance, in the same spirit as (3.10),

$$\omega_j^2(\mathbf{k}_3+\mathbf{k}_*)=\Omega_B^2(j;\mathbf{k}_3)+v_j^2(\mathbf{k}_3)k_*^2+O(k_*^4), \tag{3.17}$$

where, in the Debye approximation, v_j is the velocity of sound at the minimum of the $j\mathbf{k}_3$ subband.

Using (3.17) and (3.1) in (2.26) we find, if the minimum of the $j\mathbf{k}_3$ subband occurs at $\mathbf{k}=\mathbf{k}_j$,

$$F_{\alpha\beta}(0,\omega^2;\mathbf{k}_3) \to \frac{\sigma_*}{M}\pi e_\alpha(\mathbf{k}_j,j)e_\beta(\mathbf{k}_j,j) \times\log[\Omega_B^2(j;\mathbf{k}_3)-\omega^2], \tag{3.18}$$

as $\Omega_B^2(j;\mathbf{k}_3)-\omega^2 \to +0$, $j=1, 2, 3$. In particular then

$$F_{\alpha\alpha}(0,\omega^2;\mathbf{k}_3) \to -\infty \text{ as } \Omega_B^2(j;\mathbf{k}_3)-\omega^2 \to +0, \tag{3.19}$$

and likewise we find

$$F_{\alpha\alpha}(0,\omega^2;\mathbf{k}_3) \to +\infty \text{ as } \Omega_T^2(j;\mathbf{k}_3)-\omega^2 \to -0. \tag{3.20}$$

[24] L. van Hove, Phys. Rev. **89**, 1189 (1953).
[25] Reference 20, Chap. III, Sec. 3.

Similarly we find

$$\mathfrak{F}_{\alpha\beta}(0,\omega^2;\mathbf{k}_3) \to M^{-1}e_\alpha(\mathbf{k}_j;j)e_\beta(\mathbf{k}_j,j) \times[J_j(\omega^2)-i\pi\xi_j(\omega^2)], \tag{3.21}$$

where

$$J_j(\omega^2)=P\int \frac{\xi_j(x)}{\omega^2-x}dx, \tag{3.22}$$

the integral being over the subband and $N_*\xi_j(\omega^2)d\omega^2$ being the number of j $\mathbf{k}_3$ subband states in the range $d\omega^2$. For the bands (3.17) we find

$$\xi_j(\omega^2) \to \pi\sigma_* v_j^{-2} \tag{3.23}$$

near the subband minimum, and so

$$J_j(\omega^2) \to \pi\sigma_* v_j^{-2} \log[\omega^2-\Omega_B^2(j;\mathbf{k}_3)]. \tag{3.24}$$

Thus

$$J_j(\omega^2) \to -\infty \quad \text{as} \quad \omega^2-\Omega_B^2(j;\mathbf{k}_3) \to +0. \tag{3.25}$$

Likewise

$$J_j(\omega^2) \to +\infty \quad \text{as} \quad \omega^2-\Omega_T^2(j;\mathbf{k}_3) \to -0, \tag{3.26}$$

and equations similar to (3.15) and (3.16) also follow.

Similarly it is a simple matter to verify that for a plane defect the Green's functions behave in the same way as the corresponding line-defect ones G and F when the energy approaches the subband edge from *outside*. On the contrary, those Green's functions corresponding to $\mathcal{G}$ and $\mathfrak{F}$ *remain finite* as the energy approaches the subband edge from *inside*, and also as the energy approaches subsidiary extrema.

As a point of comparison it is also readily shown that the corresponding Green's functions for the point-defect problem remain finite in all cases.

We shall show in the next section how these differences in behavior of the Green's functions lead to fundamental differences between the three classes of defects with regard to the existence of bound and resonant states.

IV. SIMPLE MODELS

The models employed in this section are the obvious analogs, for the line and plane defects, of the usual simple model used to represent a point defect.[1–3] We consider it best to use them here, as they facilitate direct comparison of the bound-state and resonant-state properties of the three types of defect, and in Sec. V we consider models which more closely represent dislocations and stacking faults, which are of obvious interest. The use of this one-band, highly localized, model has been criticized by Beeby.[26] His objections do not affect our arguments where, for the energy near a given subband edge, the divergence of the Green's function corresponding to that band swamps the contri-

[26] J. L. Beeby, Phys. Rev. **137**, A933 (1965).

bution from all other bands and so makes the one-band approximation redundant.

A. Electron States

We put

$$V_{qj}(\mathbf{m}_*,\mathbf{n}_*)=\delta_{qj}\delta_{\mathbf{m}_*,0}\delta_{\mathbf{n}_*,0}V_0 \tag{4.1}$$

in (2.8), which then reduces to

$$1-V_0G_E(0)=0. \tag{4.2}$$

Now from (2.7) it is obvious that $G_E(0)\to 0$ as E moves a long way from the subband, either above or below. Further, for E outside the subband, (2.7) is a finite sum of continuous functions, and so $G_E(0)$ is a continuous function of E. Then using (3.5) and (3.6) it is clear that (4.2) has a solution below the subband if $V_0<0$, and above the subband if $V_0>0$, so that at least one bound state always exists. On this model, owing to the monotonic nature of the function $G_E(0)$ for E outside the subband, there can be only one bound state; however, if the one-band model is not used, there may be more than one bound state between two given subbands.

The existence of bound states for the corresponding model of a plane defect is established in the same way.

To study the resonant states we use (4.1) to reduce (2.13) to

$$1-V_0I(E_0)=0. \tag{4.3}$$

Then from (3.13) and (3.14) there is obviously at least one resonance within the subband, whatever the value of V_0.

It is instructive to consider Fig. 1, drawn for a subband having no subsidiary extrema. The function $I(E)$ must have the general form shown there, although the behavior well inside the asymptotes $\mathcal{E}_B$ and $\mathcal{E}_T$ cannot be determined without detailed knowledge of $\eta(E)$. We see, however, that for any perturbation V_0, whatever its sign or magnitude, there is an even number of solutions of (4.3). One of these is the real bound state discussed above, so that there is always an odd number of scattering resonances in each subband. We show in the following paper[15] that the density of subband states is increased above $\eta(E)$ near points such as X_3 where $dI/dE<0$, and is decreased near X_2, X_4, and Y_1 where $dI/dE>0$. We further show that just one state is removed from (or introduced to) the vicinity of each of these resonances, so that in particular one considers the perturbation to have shifted a state from Y_1 inside the subband to the bound-state position Y_2, or, for an attractive potential, from X_2 to X_1.

If the subband has subsidiary extrema we may be able to establish the existence of more than one resonance state by using (3.13)–(3.16) and without needing the detailed knowledge necessary to consider the region between the asymptotes as in Fig. 1. The situation depends on the relative values of the $\mathcal{E}_{Mi}$ and the $\mathcal{E}_{mj}$; if all the $\mathcal{E}_{mj}$ are less than all the $\mathcal{E}_{Mi}$ we can only predict one resonance state from the asymptotic behavior of $I(E)$, but more than one if the $\mathcal{E}_{mj}$ and $\mathcal{E}_{Mi}$ are interspersed.

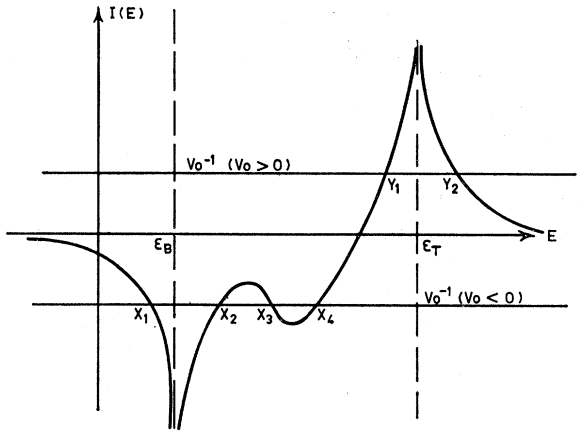

FIG. 1. The solutions of Eqs. (4.2) and (4.3).

We might expect the above discussion, based on (4.1), to give us some insight into the electronic states associated with a screw dislocation. Similarly we might expect analysis of the antisymmetric perturbation

$$V_{qj}(\mathbf{m}_*,\mathbf{n}_*)=\delta_{qj}\delta_{\mathbf{m}_*\mathbf{n}_*}(\delta_{\mathbf{m}_*,\mathbf{p}_*}-\delta_{\mathbf{m}_*,-\mathbf{p}_*})V_0 \tag{4.4}$$

to give us similar insight into edge-dislocation states. In (4.4) $\mathbf{p}_*$ is the shortest of the vectors $\mathbf{m}_*$ normal to the slip plane. In the same way as above we find that independent of the strength of the perturbation this simple model of an edge dislocation always gives rise to *two* real bound states, one below and one above each subband. Likewise there is always an *even* number of resonances, and again there is just one state excluded from or introduced to the vicinity of each resonance. The state excluded from each of the two resonances lying respectively nearest to the subband top or bottom is regarded as being shifted to the bound state outside the respective subband edge.

For plane defects, the finite behavior of the Green's functions near subband extrema enables no conclusions to be drawn regarding the existence of scattering resonances.

B. Phonon States

In the same spirit as (4.1) we choose for the coefficients (2.15)

$$\Delta_{\alpha\beta}(\mathbf{m}_*,\mathbf{n}_*,\mathbf{m}_3-\mathbf{n}_3)=-\omega^2\delta M\delta_{\mathbf{m}_*,0}\delta_{\mathbf{n}_*,0}\delta_{\mathbf{m}_3,\mathbf{n}_3}\delta_{\alpha\beta}, \tag{4.5}$$

for which (2.27) reduces to

$$\det[\delta_{\alpha\gamma}+\omega^2\delta MF_{\alpha\gamma}(0,\omega^2;\mathbf{k}_3)]=0. \tag{4.6}$$

For cubic crystals, when[20] the $e_\alpha(\mathbf{k},j)$ have the symmetry of the k_α we see from (2.26) that

$$F_{\alpha\gamma}(0,\omega^2;\mathbf{k}_3)=\delta_{\alpha\gamma}F_{\alpha\alpha}(0,\omega^2;\mathbf{k}_3),$$

so that (4.6) has the three solutions

$$1+\omega^2\delta M F_{\alpha\alpha}(0,\omega^2;\mathbf{k}_3)=0, \quad \alpha=1, 2, 3. \quad (4.7)$$

Using Eqs. (3.19) and (3.20), and proceeding as for the electronic case, we establish the existence of at least one bound state for each polarization j, whatever the perturbation δM. If for a given j and corresponding subband extremum $\mathbf{k}_j$ more than one $e_\alpha(\mathbf{k},j)$ is nonzero, then (3.18) shows that more than one of (4.7) may have solutions for different ω^2 outside the subband, and so we may get up to three bound states per subband of each polarization. It should be mentioned that, because of the appearance of ω^2 in the perturbation, bound states below *low-lying* $\mathbf{k}_3$ subbands will be very close to the subband edge.

Plane-defect bound states are established in the same way.

For resonances, (2.31) reduces to

$$1+\omega^2\delta M \Re[\mathfrak{F}_{\alpha\alpha}(0,\omega^2;\mathbf{k}_3)]=0, \quad \alpha=1, 2, 3, \quad (4.8)$$

and analysis using (3.21)–(3.26) gives results analogous to the above. Again we cannot establish the existence of scattering resonances for plane defects.

The antisymmetric perturbation

$$\Delta_{\alpha\beta}(\mathbf{m}_*, \mathbf{n}_*, \mathbf{m}_3-\mathbf{n}_3) = -\omega^2\delta M\delta_{\alpha\beta}\delta_{\mathbf{m}_3,\mathbf{n}_3}\delta_{\mathbf{m}_*,\mathbf{n}_*}(\delta_{\mathbf{m}_*,\mathbf{p}_*}-\delta_{\mathbf{m}_*,-\mathbf{p}_*}) \quad (4.9)$$

gives the same type of duplication effects discussed for the electronic case.

The models (4.5) and (4.9) suffer from the obvious drawback that they do not take into account any changes in the force constants between atoms, but simply consider changes in mass. The consideration of the force constants leads to considerably more complicated equations than (4.7) and (4.8) and we do not consider the extra effort justified at present. Equations (4.5) and (4.9) presumably give reasonable representations of dislocations provided the dilatation about these defects is their most important characteristic.

V. MORE GENERAL MODELS

Up to this stage we have done nothing more than make an obvious extension, to linear and plane defects, of a very simple model which has previously yielded results of interest concerning point defects. Although the results we have already obtained are clearly of considerable interest, we need to investigate as far as is practicable the extent to which these results apply to perturbations more closely representing defects actually occurring in crystals. The general situation is too complicated for any general trends to show through and in fact requires for its treatment a detailed knowledge, which we usually do not possess, of the Green's functions and the perturbation matrix elements. However, in Sec. VA, by considering a perturbation of general form but of very low strength, we are able to obtain some idea of how the form of the perturbation and the band structure of the unperturbed crystal effect the existence or otherwise of bound states and resonances. Unfortunately we are not able to carry these results over at all exactly to stronger perturbations and can only regard them as a guide to the situation existing in a real crystal, which we discuss in Sec. VB. The arguments for the electron and phonon problems are very similar, so we consider only the former.

A. Very Weak Perturbations

With the crystal undergoing the perturbation V we firstly treat the problem corresponding to a perturbation $v(\lambda)=\lambda V$ in the limit as $\lambda \to +0$. To avoid convergence difficulties and problems associated with determinants of infinite order we assume that the perturbation only extends over a finite number of sites $\mathbf{m}_*$, say p of them, such that $V_{ij}(\mathbf{m}_*,\mathbf{n}_*)$ is zero unless $\mathbf{m}_*$ and $\mathbf{n}_*$ both belong to this set of sites.

Now with $\lambda \to 0$ we look for solutions close to the edge of some sub-band; then the Green's functions of that subband[27] dominate all others and Eq. (2.8) reduces to the one-band equation

$$D(E)\equiv\det[\delta_{\mathbf{m}_*,\mathbf{n}_*}-\sum_{\mathbf{m}_*'}\lambda V(\mathbf{m}_*',\mathbf{n}_*) \times G_E(\mathbf{m}_*-\mathbf{m}_*')]=0, \quad (5.1)$$

where we have dropped the band index, and the labels $\mathbf{m}_*$ take the p values of the set defined above.

It is easy to show, as in (3.7) that when $E \to \mathcal{E}_B$ or $\mathcal{E}_T$ from outside the subband $G_E(\mathbf{m}_*)$ approaches the form

$$G_E(\mathbf{m}_*) \to \ln\Delta \sum_{r=1}^{\nu} a(\mathbf{k}_*^r)e^{i\mathbf{k}_*^r\cdot\mathbf{m}_*}+g(\mathbf{m}_*) +0(\Delta\ln\Delta), \quad (5.2)$$

where $\Delta=E-\mathcal{E}_B$ or $E-\mathcal{E}_T$ and $g(\mathbf{m}_*)$ is independent of Δ. The vectors $(\mathbf{k}_3+\mathbf{k}_*^r)$ correspond to the level $\mathcal{E}_B$ or $\mathcal{E}_T$ which is assumed ν-fold degenerate. The constants $a(\mathbf{k}_*^r)$ are positive for E near $\mathcal{E}_B$, negative for E near $\mathcal{E}_T$. The term of order $\Delta\ln\Delta$ in (5.2) can only lead to terms of type $\Delta^s(\ln\Delta)^t$ in (5.1), with $s\geqslant 1$. Such terms approach zero as $\Delta \to 0$ and so we do not need to consider them. Thus we write (5.1), when $\Delta \to 0$ as

$$D(E)=\det[\delta_{\mathbf{m}_*,\mathbf{n}_*}-\lambda\sum_{\mathbf{m}_*'}V(\mathbf{m}_*',\mathbf{n}_*)g(\mathbf{m}_*-\mathbf{m}_*') - \sum_{r=1}^{p}\mu_{\mathbf{m}_*}{}^r b_{\mathbf{n}_*}{}^r], \quad (5.3)$$

[27] We assume the $q\mathbf{k}_3$ subband being considered does not touch any other $j\mathbf{k}_3$ subband; if it does we must consider a compound subband, e.g., that formed by all the states of the $q\mathbf{k}_3$ and $(q+1)\mathbf{k}_3$ subbands. The modifications in the argument are obvious and the conclusions essentially unchanged.

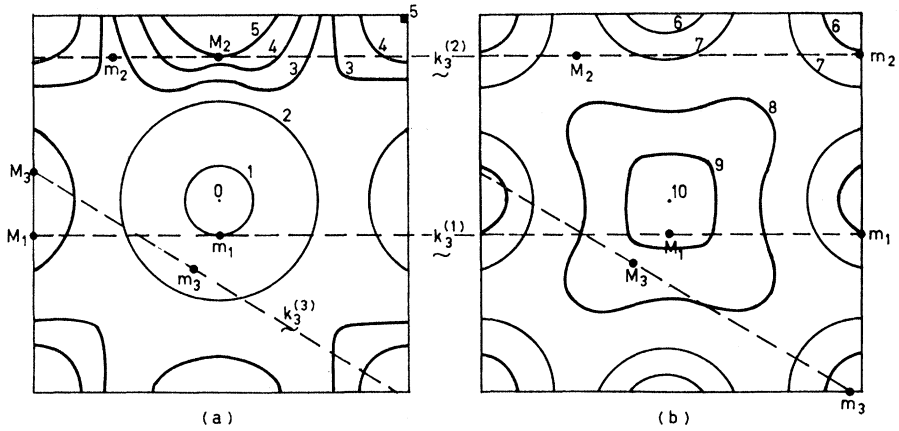

FIG. 2. Illustrating typical degeneracies of energy subband extrema.

where

$$\mu_{\mathbf{m}_*}{}^{r}=\lambda a(\mathbf{k}_*{}^{r})\ \ln\Delta e^{i\mathbf{k}_*{}^{r}\cdot\mathbf{m}_*}$$

and

$$b_{\mathbf{n}_*}{}^{r}=\sum_{\mathbf{m}_*{}'} V(\mathbf{m}_*{}',\mathbf{n}_*)e^{-i\mathbf{k}_*{}^{r}\cdot\mathbf{m}_*{}'}. \tag{5.4}$$

Now for a determinant of any order p we have

$$\det[a_{ij}+\mu\delta_{qi}b_j]=\det a_{ij}+\mu D_q, \tag{5.5}$$

where D_q is $\det a_{ij}$ except for the replacement of the qth row by the row b_j. By repeated application of (5.5) to (5.3), it is easy to show that the highest power of $\ln\Delta$ appearing in the expansion of (5.3) is $(\ln\Delta)^{\nu}$, and it is this term which determines the behavior of $D(E)$ as $\Delta\rightarrow 0$. We note this major departure from the case of the simple models (4.1) and (4.5) where the degeneracy of the subband extrema makes no difference.

In view of this new behavior we must consider what values of ν are likely to arise for crystals of interest. We will not concern ourselves with any accidental degeneracies, but only with those occuring as a result of symmetry. Thus for cubic crystals we generally expect either $\nu=1$ or 4 for a line defect, although if the direction of the defect line is one of low symmetry we may get $\nu=1$ or 2 or just $\nu=1$. For a plane defect in a cubic crystal we expect $\nu=1$ or 2, but if the defect normal is a direction of low symmetry we may just have $\nu=1$. Figure 2 illustrates schematically some of these cases for the first and second conduction bands of a typical metal, which for simplicity we have drawn as if its structure was simple cubic. The solid lines are sections through the center of the Brillouin zone and parallel to a zone face of the constant-energy surfaces whose general shape for various metallic structures is discussed by Harrison,[28] and which for any crystal have characteristics similar to Fig. 2. The broken lines are sections of $\mathbf{k}_3$ subband planes; those labeled $\mathbf{k}_3{}^{(1)}$ and $\mathbf{k}_3{}^{(2)}$ represent two different subbands for a line defect parallel to a cubic axis; the line $\mathbf{k}_3{}^{(3)}$ corresponds to a defect whose direction has low symmetry. From Fig. 2(a) we see that $\mathbf{k}_3{}^{(1)}$ has a nondegenerate minimum m_1 in the first band, but a 4-fold degenerate maximum at points like M_1; the situation for $\mathbf{k}_3{}^{(2)}$ is just the reverse. On the other hand $\mathbf{k}_3{}^{(3)}$ has nondegenerate minimum m_3 and maximum M_3. The same $\mathbf{k}_3$ subbands of the second band are indicated in Fig. 2(b) and we see the degeneracies may be different. The point is, that given the constant-energy surfaces for any crystal, we can determine the subband degeneracies at any points of interest. The general features of phonon constant-energy surfaces are also as in Fig. 2 and the same remarks apply. The constructions for plane defects are as for Fig. 2, except that the broken lines are to be regarded just as lines, not as cross sections of planes.

The proof of existence of bound states and resonances near certain subband edges depends on the nature of the perturbing potential, both its sign and general form, and also on the nature of the subband edge, both its degeneracy and whether a maximum or minimum.

For example, we first consider bound states near a nondegenerate subband extreme at point $\mathbf{k}_3+\mathbf{k}_*$. Then repeated application of (5.5) reduces (5.3) to

$$D(E)=\det[\delta_{\mathbf{m}_*\mathbf{n}_*}-\lambda\sum_{\mathbf{m}_*{}'} V(\mathbf{m}_*{}',\mathbf{n}_*)g(\mathbf{m}_*-\mathbf{m}_*{}')]$$
$$-\sum_{\mathbf{m}_*}\mu_{\mathbf{m}_*}D_{\mathbf{m}_*}, \tag{5.6}$$

where $D_{\mathbf{m}_*}$ is just the determinant appearing as the first term on the right side of (5.6) except that the $\mathbf{m}_*$th row is replaced by the row $b_{\mathbf{n}_*}$.

Now as $\lambda\rightarrow 0$ we expand all determinants in (5.6) as polynomials in λ to get

$$D(E)=1-\lambda\sum_{\mathbf{n}_*,\mathbf{m}_*} V(\mathbf{m}_*,\mathbf{n}_*)g(\mathbf{n}_*-\mathbf{m}_*)+O(\lambda^2)$$
$$-\lambda\ln\Delta\{a(\mathbf{k}_*)\sum_{\mathbf{n}_*,\mathbf{m}_*} V(\mathbf{m}_*,\mathbf{n}_*)e^{i\mathbf{k}_*\cdot(\mathbf{n}_*-\mathbf{m}_*)}+O(\lambda)\}, \tag{5.7}$$

and then keeping λ fixed at some small value and letting the energy approach the $q\mathbf{k}_3$ subband edge so that as $\Delta\rightarrow 0$, we get

$$D(E)\rightarrow 1-\lambda\ln\Delta a_q(\mathbf{k}_*)v_q(\mathbf{k}_*), \tag{5.8}$$

[28] W. A. Harrison, Phys. Rev. 118, 1190 (1960).

where

$$v_q(\mathbf{k}_*)\equiv \sum_{\mathbf{n}_*,\mathbf{m}_*} V_{qq}(\mathbf{m}_*,\mathbf{n}_*)e^{i\mathbf{k}_*\cdot(\mathbf{n}_*-\mathbf{m}_*)}, \quad (5.9)$$

and using the definition (2.6) we readily find that

$$v_q(\mathbf{k}_*)=N_*\int_{N\Omega} V(\mathbf{r})\,|\,b_q(\mathbf{k}_3+\mathbf{k}_*,\mathbf{r})\,|^2 d^3r. \quad (5.10)$$

Suppose now our nondegenerate subband edge is a maximum; then $a_q(\mathbf{k}_*)<0$ and (5.8) has the solution

$$\ln\Delta=[\lambda a_q v_q]^{-1}\to-\infty, \quad \text{if} \quad v_q(\mathbf{k}_*)>0. \quad (5.11)$$

Likewise, if the edge is a minimum (5.8) has a suitable solution when $v_q(\mathbf{k}_*)<0$. Thus if we could, for instance, say that $v_q(\mathbf{k}_*)$ had the same sign for different subbands we could be sure that a good proportion of subbands satisfied (5.8) since, as in Fig. 2, there will always be a good number of subbands with either nondegenerate maxima or minima. Now provided $V(\mathbf{r})$ does not vary too rapidly, we get from (5.10)

$$v_q(\mathbf{k}_*)\simeq\frac{1}{N_3}\int_{N\Omega} V(\mathbf{r})d^3r=\int_{N_*\Omega} V(\mathbf{r})d^3r, \quad (5.12)$$

independent of $q,\mathbf{k}_3$ and $\mathbf{k}_*$. The second integral in (5.12) is over a cell of volume $N_*\Omega$ extending only the distance $\mathbf{a}_3$ in the direction of the (line) defect. This approximation will be reasonable provided the contributions to the integral from regions of positive and negative $V(\mathbf{r})$ do not almost cancel.

Thus for dislocations with appreciable screw component, and also for stacking faults, where we expect $V(\mathbf{r})$ to be substantially one-signed, we have established the existence of bound states near some, but not all, $\mathbf{k}_3$ subbands.

The approximation (5.12) does not decide the issue in cases where $N_3^{-1}\int V(\mathbf{r})d^3\mathbf{r}\simeq 0$, such as for a dislocation of almost purely edge character. However in these cases we can establish the existence of bound states near *degenerate* subband edges. By applying (5.5) successively we find that when $\nu=2$ the leading terms of order $(\ln\Delta)^2$, in (5.3) are

$$\sum_{\mathbf{m}_*,\mathbf{n}_*}{}' \mu_{\mathbf{m}_*}{}^1\mu_{\mathbf{n}_*}{}^2 D_{12}(\mathbf{m}_*,\mathbf{n}_*), \quad (5.13)$$

and when $\nu=4$ the leading terms, of order $(\ln\Delta)^4$, are

$$\sum_{\mathbf{m}_*,\mathbf{m}_*',\mathbf{m}_*'',\mathbf{m}_*'''}{}' \mu_{\mathbf{m}_*}{}^1\mu_{\mathbf{m}_*'}{}^2\mu_{\mathbf{m}_*''}{}^3\mu_{\mathbf{m}_*'''}{}^4 \times D_{1234}(\mathbf{m}_*,\mathbf{m}_*',\mathbf{m}_*'',\mathbf{m}_*'''), \quad (5.14)$$

where the primes on the sums indicate that no two indices are to take the same value, and $D_{qr\cdots}(\mathbf{m}_*,\mathbf{m}_*',\cdots)$ is just the first term of the right side of (5.6) with the $\mathbf{m}_*$th row replaced by the row $b_{\mathbf{n}_*}{}^q$, the $\mathbf{m}_*'$th row by $b_{\mathbf{n}_*}{}^r\cdots$.

Considering just the $\nu=2$ case and using (5.13) we find, corresponding to (5.8), that for small λ, and $\Delta\to 0$,

$$D(E)\to 1+O(\lambda\ln\Delta)+(a\lambda\ln\Delta)^2 \times\sum_{\mathbf{n}_*,\mathbf{n}_*'}{}'\sum_{\mathbf{m}_*,\mathbf{m}_*'}{}'[V(\mathbf{m}_*,\mathbf{n}_*)V(\mathbf{m}_*',\mathbf{n}_*') - V(\mathbf{m}_*,\mathbf{n}_*')V(\mathbf{m}_*',\mathbf{n}_*)]\exp[i\mathbf{k}_*{}^1\cdot(\mathbf{n}_*-\mathbf{m}_*) +i\mathbf{k}_*{}^2\cdot(\mathbf{n}_*'-\mathbf{m}_*')]. \quad (5.15)$$

The $a(\mathbf{k}_*{}^r)$ will be the same for all $r=1,\cdots,\nu$ if the degeneracy is due to crystal symmetry and we put them all equal to a in (5.15). We will be interested in how the sign of the sum in (5.15) depends on the type of perturbation, and to investigate this without excessive labor will assume without discussion that the potential is sufficiently slowly varying to make acceptable the approximation

$$V(\mathbf{m}_*,\mathbf{n}_*)=\delta_{\mathbf{m}_*,\mathbf{n}_*}V(\mathbf{m}_*). \quad (5.16)$$

Using (5.16) we reduce (5.15) to

$$D(E)\to 1+O(\lambda\ln\Delta)+(a\lambda\ln\Delta)^2\{[\sum_{\mathbf{n}_*}V(\mathbf{n}_*)]^2 - |\sum_{\mathbf{n}_*}V(\mathbf{n}_*)e^{i\mathbf{n}_*\cdot(\mathbf{k}_*{}^1-\mathbf{k}_*{}^2)}|^2\}. \quad (5.17)$$

Thus, for a potential with a definite bias towards one sign, when $|\sum_{\mathbf{n}_*}V(\mathbf{n}_*)|\gg|\sum_{\mathbf{n}_*}V(\mathbf{n}_*)e^{i\mathbf{n}_*\cdot(\mathbf{k}_*{}^s-\mathbf{k}_*{}^r)}|$, call this a type-I perturbation, we have $D(E)\to+\infty$ as $\Delta\to 0$, while for a potential giving $\sum_{\mathbf{n}_*}V(\mathbf{n}_*)\simeq 0$, a type-II perturbation, we have $D(E)\to-\infty$, the latter being the case for an edge dislocation. Considering a 4-fold degenerate subband edge, we are led to the same conclusions.

Now suppose the degenerate edge we are considering is the top of the $q\mathbf{k}_3$ subband, and is separated from the bottom of the $(q+1)\mathbf{k}_3$ subband by a finite gap; then by taking $E=\bar{E}$, the middle of this gap, we make all the Green's functions of (5.1) finite, so that we have on expanding (5.1),

$$D(\bar{E})\simeq 1-\lambda\sum_{\mathbf{m}_*,\mathbf{n}_*}V(\mathbf{m}_*,\mathbf{n}_*)G_{\bar{E}}(\mathbf{n}_*-\mathbf{m}_*)>\tfrac{1}{2} \quad (5.18)$$

for λ sufficiently small. Thus for some E between $\bar{E}$ and the top of the $q\mathbf{k}_3$ subband we must have $D(E)=0$ for type-II potentials, which establishes the existence of a bound state near this subband edge. The same argument applies near degenerate minima.

Since the real part of $\mathfrak{D}(E)$ behaves exactly as $D(E)$ when E approaches a subband edge, the above discussion of bound-state energies needs little modification to apply to resonances. Thus if both edges of a given subband are nondegenerate there must be a resonance just inside one of them for a type-I perturbation. However, suppose for instance that the bottom of the sub-band is nondegenerate and the top degenerate; then as we approach the bottom from inside we see

from (5.8) that

$$\mathfrak{R}[\mathfrak{D}(E)]\rightarrow +\infty \times v_q(\mathbf{k}_*).$$

Likewise (5.17) shows that as we approach the top

$$\mathfrak{R}[\mathfrak{D}(E)]\rightarrow +\infty \text{ for type-I perturbations}$$
$$\rightarrow -\infty \text{ for type-II perturbations.}$$

Thus if $v_q(\mathbf{k}_*)>0$ at the nondegenerate minimum, we see that type-II perturbations have scattering resonances in this subband, while if $v_q(\mathbf{k}_*)<0$, type-I perturbations have them. The situation is reversed for subbands with a nondegenerate maximum and a degenerate minimum. If both edges of the subband are degenerate the situation is not quite so clear; however in so far as it is a good approximation to take the coefficient of the $\lambda \ln\Delta$ term in (5.17) as zero for a type-II perturbation we expect this type of potential to yield resonances for such subbands.

In problems associated with the effects of defects on the electrical and optical properties (e.g. carrier mobility, photoconductivity, light absorption, excess carrier lifetimes) of semiconductors, the possibility of resonance scattering and trapping of holes is of interest. The above treatment can be applied to holes simply by changing the sign of each energy eigenvalue in the Green's functions and also of the perturbation potential energy, provided this be electrostatic. Thus if an electron bound state or resonance occurs at an electron energy $E_e=E$, a hole bound state or resonance, respectively, occurs at a hole energy $E_h=-E$. For reasons outlined in Appendix B we do not believe the concept of a hole bound state is very useful; on the other hand the concept of resonance scattering of holes is very important for transport problems. The above argument shows that hole resonance scattering occurs for the same wave vectors $\mathbf{k}_3+\mathbf{k}_*$ in the valence subbands as would electron resonance scattering.

B. Stronger Perturbations

Equations (5.8) and (5.17) establish the existence of bound states and resonances very close to the edges of certain subbands, for very weak perturbations. We now try to see what happens when λ is increased to the value unity which characterizes the perturbation we actually want to study. Intuitively it is hard to imagine such states existing for weak perturbations and completely failing to exist for stronger ones; in fact we would expect more such states to appear as the strength increased. Unfortunately we have not been able to produce anything like a general proof of these propositions.

Nonetheless it is worth observing firstly that both from (5.8) and (5.17) it follows for small λ and Δ that

$$\frac{d\Delta}{d\lambda}=-\frac{\Delta \ln\Delta}{\lambda}, \tag{5.19}$$

so that initial increase of λ certainly moves both bound states and resonances away from the subband edge; however, this is not really of much help since before reaching $\lambda=1$ we generally reach a stage where (5.8) or (5.17) do not apply, for instance when

$$|\lambda a_q(\mathbf{k}_*)v_q(\mathbf{k}_*)|\simeq 1.$$

Secondly we observe that the simple models of Sec. IV, and also variations on them which include the effects of more than one band of the unperturbed crystal, invariably show that on increasing λ from very small values the bound states and resonances move away from band edges to energies respectively well into the gaps between subbands or well into the subband interior.

The difficulty with the general case lies in the complexity of the determinant (5.3) which itself is considerably simpler than the original (2.8). As long as we are only concerned with the *existence* of bound states and resonances rather than their exact positions it seems sufficient to study (5.3) rather than (2.8). We illustrate this for states appearing near a nondegenerate sub-band edge, so that (5.6) applies.

Writing

$$A(\lambda)=\det[\delta_{\mathbf{m}_*\mathbf{n}_*}-\lambda \sum_{\mathbf{m}_*'} V(\mathbf{m}_*',\mathbf{n}_*)g(\mathbf{m}_*-\mathbf{m}_*')], \tag{5.20}$$

and

$$B(\lambda)=a(\mathbf{k}_*)\sum_{\mathbf{m}_*} e^{i\mathbf{k}_*\cdot\mathbf{m}_*}D_{\mathbf{m}*}, \tag{5.21}$$

(5.6) shows that for any value of λ, if there is a bound state or resonance *close to the subband edge* it satisfies

$$\ln\Delta=A(\lambda)/\lambda B(\lambda). \tag{5.22}$$

Now consider $\lambda\gtrless 0$; provided A and B are of opposite signs we see, as in Sec. V A, that (5.22) has a solution for small Δ. Now as λ increases, (5.22) can only have a solution for those λ for which $B(\lambda)\rightarrow 0$ *and* for which A and B are of opposite sign. Suppose then that $A(0)>0$, $B(0)<0$, and denote the zeros of A and B for $0<\lambda<1$ by $\lambda_A^{(i)}$ and $\lambda_B^{(i)}$, where $\lambda_A^{(i)}<\lambda_A^{(j)}$ if $i<j$ and likewise for the $\lambda_B^{(i)}$. Now suppose $\lambda_B^{(1)}<\lambda_A^{(1)}$; then as $\lambda\rightarrow\lambda_B^{(1)}-0$ we see that (5.22) has a solution Δ which gets *smaller* as $\lambda\rightarrow\lambda_B^{(1)}$ and corresponds to the dissappearance of the initial bound state or resonance. On the other hand, if $\lambda_A^{(1)}<\lambda_B^{(1)}<\lambda_A^{(2)}$ then Eq. (5.22) next has a solution only as $\lambda\rightarrow\lambda_B^{(1)}+0$ and this solution Δ increases as λ increases; this corresponds to the emergence of a second bound state or resonance from the subband edge to which the initial state still has not returned. We can see from this, since $\mathfrak{R}[\mathfrak{D}(E)]\rightarrow D(E)$ near a subband edge, that the correspondence between bound and resonant states, remarked on in the discussion of Fig. 1, is preserved. Thus by studying the zeros of $A(\lambda)$ and $B(\lambda)$ as λ varies between 0 and 1 we can ascertain the total number of bound states and resonances to leave a given

sub-band edge. Presumably some progress could be made along these lines for specific values of the $V(\mathbf{m}_*,\mathbf{n}_*)$ but a general treatment appears too difficult. A corresponding procedure for degenerate subband edges is readily obtained.

We finally observe, from the arguments of Sec. IV and the present section, that the bound-state and resonance energies, if they exist, are continuous functions of the parameter $\mathbf{k}_3$, since all matrix elements appearing are continuous functions of $\mathbf{k}_3$. Thus we expect each band, q, of the original crystal to have associated with it a *band* of resonances and a *band* of bound-state energies, the latter not necessarily lying completely in the gaps between allowed bands of the unperturbed crystal.

VI. DISCUSSION

The arguments of Secs. IV and V give excellent reasons to believe that linear defects generally have electron and phonon bound states and scattering resonances associated with a large proportion of sub-bands. For plane defects the same remarks apply concerning bound states, but not resonances. For point defects neither bound states nor resonances need appear.

Our treatment makes evident the dangers of omitting the band structure of the crystal from any problem involving the scattering of phonons, electrons and holes, and therefore excitons, by defects; such omission clearly has special relevance to dislocation scattering, but may be acceptable for point and plane defect scattering. By the same token, the diversity of our results for defects localized in one, two, and three dimensions, respectively, makes evident the difficulties and dangers of trying to deduce, even qualitatively, the properties of crystal defects from one-dimensional models. The forms of the Green's functions indicate that only for a plane defect can we expect a one-dimensional model to give reliable information; this is comforting support for the one-dimensional treatments used to establish the existence of Tamm states at the finite surfaces of crystals, to which our treatment does not apply. Koutecky[29] has used a very similar treatment to study states at the surface of a semi-infinite crystal; being expanded in terms of Wannier functions, and hence ultimately Bloch functions, his surface-state wave functions satisfy the periodic boundary conditions applied to the unperturbed crystal, as indeed do the wave functions discussed in the present paper. While this situation is acceptable for the representation of a fault in the interior of a real (finite) crystal, the use of such wave functions to discuss finite crystal surfaces seems to be contrary to the spirit in which periodic boundary conditions are usually accepted.

The bound-state energies are seen, from (5.8) and (5.17), to be nonanalytic functions of the perturbation-strength parameter λ for small λ, so one cannot treat these states by perturbation theory. Likewise, the the existence of scattering resonances for line defects clearly invalidates the usual Born-approximation perturbation approach[30] to dislocation scattering. It is known[15,30–33] that such treatments of electron and phonon scattering by dislocations greatly underestimate the measured effects, whereas such marked discrepancies do not appear to exist between experiment and perturbation treatments of point- and plane-defect scattering. The following paper discusses these points in more detail, and we show there that a resonance-scattering mechanism is capable of producing dislocation scattering effects of the right order of magnitude.

The existence of localized states associated with edge dislocations in semiconductors was predicted on the basis of the well-known "dangling bond" model by Shockley,[34] and the theory developed by Read.[35,36] A great deal of experimental work has subsequently been carried out and the importance of such states on optical absorption, photoconductance and carrier recombination properties is well established. The theory of Shockley and Read treats the dislocation as a row of localized (in *three* dimensions) acceptor sites; the possibility of these single levels broadening into a one-dimensional band,[10] as is our conclusion in Sec. V, has often been discussed in the literature. Recent experiments[37] have observed more than one dislocation level, and indeed[38,39] appear to show the existence of a band of dislocation levels in the forbidden gap; furthermore it has become apparent[40] that such states are associated with screw as well as edge dislocations so that the states are apparently not specifically associated with dangling bonds. With the fairly large quantity of experimental data accumulating, the need for a quantitative theory of dislocation bound states in semiconductors is apparent, and the methods of the present paper would seem to afford a likely line of investigation. In accordance with the above discussion, the one-dimensional model of Heine[40] would apply better to a discussion of plane-defect bound states; his paper gives several references bearing on the observation of donor and acceptor levels associated with grain boundaries.

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The effect of scattering resonances on electron and hole mobilities seems to afford another interesting line of investigation, and the resonance scattering of excitons is of interest with regard to optical absorption.

Finally we remark that in most of the above-mentioned problems we will be interested in the *occupation* of the localized levels, and so will generally have to take some account of interactions between the trapped electrons, which we have ignored in the one-electron treatment developed so far. We have not yet tried to tackle this problem. Read's treatment,[35,36] which regards the trapped electrons as discrete charges, obviously needs modification to apply to the states we wish to consider, but nonetheless probably gives roughly the right answers. The modification of the perturbation due to the space-charge region formed when the dislocation line becomes charged also needs to be treated in a self-consistent manner. The use of a one-electron picture, with many-body effects being taken into account by means of some sort of self-consistent one-electron Hamiltonian is apparently basic to the concept of bound states, which cannot be properly defined for a many-electron system when the totality of single-electron wave functions is synthesized into a determinantal wave function.[41,42]

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APPENDIX A

We first establish the forms (3.3), (3.7), and (5.2) as the energy approaches a subband maximum or minimum from outside the subband. Secondly we consider the energy approaching a value corresponding to a saddle point of $E_{0q}(\mathbf{k}_3;\mathbf{k}_*)$ and show that in this case the Green's functions remain finite, so that resonances are not associated with these saddle points.

Using (3.1) in (2.7), we have

$$G_{E,q}(\mathbf{n}_*-\mathbf{m}_*)=\sigma_*\int\frac{e^{i\mathbf{k}_*\cdot(\mathbf{n}_*-\mathbf{m}_*)}}{E-E_{0,q}(\mathbf{k}_3;\mathbf{k}_*)}d^2k_*. \quad \text{(A1)}$$

Now the neglect of higher than quadratic terms of (3.2) is a good approximation up to some (small) value κ_M *independent* of $\Delta\equiv\mathcal{E}_B(\mathbf{k}_3)-E$. Thus we break up the integral (A1),

$$G_{E,q}(\mathbf{n}_*-\mathbf{m}_*)=-\sigma_*\int_{S_M}\frac{e^{i\mathbf{k}_*\cdot(\mathbf{n}_*-\mathbf{m}_*)}}{\Delta+\sum a_{ij}\kappa_i\kappa_j}d^2\kappa+I_M, \quad \text{(A2)}$$

where the first integral is over the area of the circle of radius κ_M (or, if the subband minimum is degenerate, is the sum of integrals over segments of such circles) and centered at the subband minimum (or minima, if degenerate). I_M is the integral over the remainder of the subband, and clearly

$$|I_M|\leqslant\sigma_*A_q(\mathbf{k}_3)/\delta_M, \quad \text{(A3)}$$

where $A_q(\mathbf{k}_3)$ is the total area, in $\mathbf{k}_*$ space, of the $q\mathbf{k}_3$ subband, and δ_M is the minimum value of $|\sum a_{ij}\kappa_i\kappa_j|$ for $|\kappa_i|\geq\kappa_M$. Because of the definite character of the quadratic form for a subband maximum or minimum $\delta_M>0$ and so (A3) provides a definite upper bound for $|I_M|$. The form (3.3) then follows in a very straightforward manner; the results (3.7) and (5.2) likewise follow by expanding the exponential in (A2). The corresponding behavior of the Green's functions $\mathcal{G}_{E,q}(\mathbf{m}_*-\mathbf{n}_*)$ as E approaches a subband maximum or minimum (absolute or local) from inside the subband can be determined in the same way, the integrals existing as principal values.

Near a saddle point, (2.11) takes the form

$$\mathcal{G}_{E,q}(\mathbf{n}_*-\mathbf{m}_*)=-\sigma_*P\int_{S_M}\frac{e^{i\mathbf{k}_*\cdot(\mathbf{n}_*-\mathbf{m}_*)}d^2\kappa}{\Delta-(a_1{}^2\kappa_1{}^2-a_2{}^2\kappa_2{}^2)}+\mathcal{I}_M, \quad \text{(A4)}$$

and we can show $|\mathcal{I}_M|$ is bounded independent of Δ by considering higher terms than quadratic in the expansion of $E_0(\mathbf{k}_3;\mathbf{k}_*)$. Expanding the exponential in the integral yields

$$\mathcal{G}_{E,q}(\mathbf{n}_*-\mathbf{m}_*)=\mathcal{I}_M+e^{i\mathbf{k}_*{}^{(s)}\cdot(\mathbf{n}_*-\mathbf{m}_*)}\sum_{n=0}^{\infty}\Delta^{2n}I_{2n}(\Delta), \quad \text{(A5)}$$

where $\mathbf{k}_3+\mathbf{k}_*{}^{(s)}$ is the position of the saddle point (again, if this is degenerate minor alterations which do not change our conclusions must be made), and $I_{2n}(\Delta)$ is of the form

$$I_{2n}(\Delta)=\int_0^{2\pi}d\phi\int_0^{\kappa M}d\kappa\frac{\kappa^{2n-1}P_n(\cos^2\phi)}{(\Delta/\kappa^2+a_2{}^2)-(a_1{}^2+a_2{}^2)\cos^2\phi}. \quad \text{(A6)}$$

Here $P_n(\cos^2\phi)$ is an nth degree polynomial in $\cos^2\phi$, with its coefficients independent of Δ.

We prove that $\mathcal{G}_{E,q}(\mathbf{n}_*-\mathbf{m}_*)$ remains finite as $\Delta\to0$, i.e., as E approaches the saddle-point energy, by showing that

$$\lim_{\Delta\to0}I_{2n}(\Delta)=I_{2n}(0), \text{ a finite constant.} \quad \text{(A7)}$$

We will need the result

$$\int_0^{2\pi}\frac{d\phi}{1-b^2\cos^2\phi}=0, \quad b^2>1, \quad \text{(A8)}$$

[41] W. Kohn and C. Majumdar, Phys. Rev. **138**, A1617 (1965).
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which is readily verified by separating into partial fractions and realizing that

$$\frac{1}{(b^2-1)^{1/2}}\frac{d}{d\phi}\ln\frac{b+\cos\phi+(b^2-1)^{1/2}\sin\phi}{1+b\cos\phi}=\frac{1}{1+b\cos\phi}. \quad \text{(A9)}$$

Now writing

$$[a+b\cos^2\phi]^{-1}\cos^2\phi=b^{-1}\{1-a[a+b\cos^2\phi]^{-1}\},$$

we see that, as $\Delta\to 0$, any $\cos^2\phi$ terms in P_n can only yield terms which behave as $A+BI_0(\Delta)$, A and B being independent of Δ. The same reduction applied successively to higher terms of P_n yields the same result, so the proof of (A7) reduces to showing that $I_0(\Delta)$ remains finite as $\Delta\to 0$.

Now using (A8) in (A6), we get

$$I_0(\Delta)=\int_0^{(a_1^{-1}\vee\Delta)}\frac{d\kappa}{\kappa(a_2^2+\Delta/\kappa^2)}\times\int_0^{2\pi}d\phi\left[1-\frac{a_2^2+a_1^2}{a_2^2+\Delta/\kappa^2}\cos^2\phi\right]^{-1}. \quad \text{(A10)}$$

The result

$$\int_0^{2\pi}\frac{d\phi}{1-a^2\cos^2\phi}=\frac{2\pi}{(1-a^2)^{1/2}},\quad a^2<1 \quad \text{(A11)}$$

is well known, and using it in (A10) we get finally

$$I_0(\Delta)=\frac{2\pi}{a_1a_2}\arctan\frac{a_2}{a_1}, \quad \text{(A12)}$$

so that $I_0(\Delta)=I_0(0)$ independent of Δ, which establishes (A7), and so establishes that $\mathcal{G}_{E,q}(\mathbf{m}_*-\mathbf{n}_*)$ remains finite as E approaches a saddle-point energy.

APPENDIX B

At the risk of appearing pedantic we wish to briefly discuss the following point. In semiconductor transport theory the concept of holes in the valence band behaving as positively charged electrons is well known. Since free holes in this sense are such a useful concept, it seems reasonable to ask whether it is meaningful to speak of a localized hole state about a defect in the same way as we speak of localized electron states. Such states arise from the equations of Secs. IV and V if we make the usual electron $\to$ hole correspondence of changing the sign of the perturbation potential energy and the energy eigenvalues; in fact, we fine hole bound states at hole energies $E_h=-E_e$, where E_e is an electron bound state. Having posed the question, the purpose of this appendix is to point out that such states do not appear to be a useful concept. The hole concept is justified in transport problems since one can ignore the effects of a *full* valence band of electrons on the grounds that they cannot absorb energy continuously from small electric or thermal field gradients; this does not apply to the finite energy transitions involved in occupying bound states, so the effects of the electrons must be taken into account, thus robbing the hole concept of its significance. The only sense in which we should speak of a hole being trapped by a defect level is when we mean the evacuation by an electron of a level it previously occupied, and its subsequent fall to the valence band; this is in fact the sense in which the term is used in the literature on traps and recombination centers. Our treatment of scattering resonances applies equally well to electrons and holes in conduction problems.