Effects of the nonrelativistic *Zitterbewegung* on the electron-phonon interaction in two-band systems

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(Received 17 January 1991; revised manuscript received 13 June 1991)

The effects of the nonrelativistic *Zitterbewegung* (trembling motion), originated by interband transitions, on the electron-phonon interaction is considered. It is shown that the one-phonon matrix elements of *intraband* transitions are damped with respect to the single-band case. In two-band systems, the lowest-order damping is equivalent to a Debye-Waller factor, with the decay length given by the spatial amplitude of the *Zitterbewegung*. Two-band systems whose Hamiltonian becomes Dirac-like along a certain direction (defined as *pseudorelativistic*) are discussed. They show an extreme effect in the zero-gap limit, i.e., the total suppression of one-phonon processes, closely related to the divergence of the *Zitterbewegung* amplitude near the Γ point.

I. INTRODUCTION

In two recent papers,[1,2] which we shall refer to as papers I and II, respectively, the authors studied some pseudorelativistic aspects of the quantum theory of crystals, with special reference to the two-band case. In paper I the Hamiltonian of a linear chain is expanded on a basis of atomic orbitals with *opposite* parity, placed in alternate sites. It is shown that the resulting two-band Hamiltonian becomes Dirac-like, and that the band picture can be expressed in analogy with relativistic concepts, such as *rest mass, Compton wavelength,* and *Zitterbewegung.* In paper II, a more systematic study is performed in arbitrary dimension and for different parity relations, showing that in the multiband case the electron quasivelocity (defined as the gradient of the Hamiltonian with respect to the quasimomentum) does *not* commute with the Hamiltonian, even though the quasimomentum does. Thus, a sort of "self-acceleration" arises, in the Bloch formalism, which leads the particle to oscillate around the average trajectory, in close analogy with the *Zitterbewegung* (trembling motion) in the relativistic quantum theory.[3] Similar results have been obtained independently by other authors,[4] in a slightly different context. These effects are small in the standard case of bandwidth comparable with the gap. They become increasingly important for vanishing gap, i.e., when the spectrum tends to a *single degenerate* band, a limit which we call "ultrarelativistic," since in the example of paper I the velocity of the electron along the chain tends to a limiting value, independent of the wave vector, just like an ultrarelativistic massless particle. In paper II the rigid-lattice theory of the nonrelativistic *Zitterbewegung* is illustrated in general and applications are performed to the localization length of defect states. The aim of the present paper is to discuss the effects of the *Zitterbewegung* on the electron-phonon interaction. We use a linear combination of atomic orbitals (LCAO) formalism, developed in paper II, which is independent both of the internal symmetries of the orbitals and of the lattice symmetries.

In Sec. II we recall some basic results and generalize to the *polyatomic* case the expression of the two-band *Zitterbewegung* operator obtained in paper II for *monatomic* systems. In Sec. III we study the problem of the electron-phonon interactions in multiband systems, by using our LCAO formalism. We show that a multiband effect is present even in the *intraband* processes of electron-phonon scattering. This results in a *damping* of the one-phonon matrix element, with respect to the single-band case. To the lowest order in the momentum transfer and in the interband coupling, the damping effect is quadratic in a characteristic wavelength, which turns out to be the spatial extension of the *Zitterbewegung.*

In Sec. IV we consider the electron-phonon interactions in systems whose Hamiltonian becomes Dirac-like along a certain direction, which we call *pseudorelativistic.* These systems are the generalization of the one-dimensional chain studied in paper I, and are defined as "class (b) systems" in paper II. The energy-momentum conservation and the selection rules obtained from the results of Sec. III are analyzed in this special case for arbitrary momentum transfer. We define two regimes, "ultrasonic" and "subsonic," according to whether the limiting velocity of the pseudorelativistic electron does or does not exceed the sound velocity. In the supersonic regime electrons interacting with *soft* phonons can undergo both interband and intraband transitions. In contrast, in the subsonic regime, only interband transitions are allowed. Due to the selection rules, the rate of one-phonon pro-

cesses always vanishes, in the "ultrarelativistic" zero-gap limit, whereas the *Zitterbewegung* becomes divergingly large near the Γ point.

II. BAND STRUCTURE AND *ZITTERBEWEGUNG* IN CRYSTALS

Let us first recall some results of paper II, using the same symbols adopted therein. Matrices will be indicated by underlined characters, and vectors in the direct or reciprocal space by bold characters. In Sec. II of paper II the single-particle Hamiltonian

$$H=T+\sum_n V(\mathbf{r}-\mathbf{R}_n) \tag{1}$$

of a periodic lattice $\{\mathbf{R}_n\}$ (T is the kinetic energy) is expanded on a basis of localized atomic orbitals $\langle \mathbf{r}|n,\alpha\rangle=\Psi_\alpha(\mathbf{r}-\mathbf{R}_n)$ $(\alpha=1,2,\ldots,G)$, forming an orthonormal set of G elements in each site. This amounts to introduce a $G\times G$ potential matrix

$$\underline{V}(\mathbf{R}_n-\mathbf{R}_m)=\{\langle \alpha,n|H|m,\beta\rangle\} \tag{2a}$$

acting on a G-dimensional space of column matrices

$$\underline{c}(\mathbf{R}_j)=\{c_\alpha(\mathbf{R}_j)\}\ , \tag{2b}$$

whose elements $c_\alpha(\mathbf{R}_j)$ are the projections of the quantum state on the αth orbitals of the jth site. Since the $\Psi_\alpha(\mathbf{r}-\mathbf{R}_n)$'s are *not* assumed to be Wannier functions, a further overlap matrix

$$\underline{S}(\mathbf{R}_n-\mathbf{R}_m)=\{\langle \alpha,n|m,\beta\rangle\} \tag{2c}$$

has to be introduced, accounting for the overlap integrals. By taking the space Fourier transforms of the matrices Eqs. (2),

$$\begin{aligned}\underline{\Phi}(\mathbf{k})&=\sum_n \underline{c}(\mathbf{R}_n)e^{i\mathbf{k}\cdot\mathbf{R}_n}\ ,\\ \underline{W}(\mathbf{k})&=\sum_n \underline{V}(\mathbf{R}_n)e^{i\mathbf{k}\cdot\mathbf{R}_n}\ ,\\ \underline{\Sigma}(\mathbf{k})&=\sum_n \underline{S}(\mathbf{R}_n)e^{i\mathbf{k}\cdot\mathbf{R}_n}\ ,\end{aligned} \tag{3}$$

defined in the first Brillouin zone Ω_1, the eigenvalue equation reads

$$\underline{\varepsilon}(\mathbf{k})\underline{u}(\mathbf{k})=E_u\underline{u}(\mathbf{k}) \tag{4a}$$

with

$$\underline{\varepsilon}=\underline{\rho}^{-1}\underline{W}\underline{\rho}^{-1},\quad \underline{\rho}^2=\underline{\Sigma},\quad \underline{u}=\underline{\rho}\underline{\Phi}\ , \tag{4b}$$

where $\underline{\varepsilon},\underline{\rho},\underline{W}$ are self-adjoint. For *real* orbitals[5] of *well-defined* parity and for an *even* potential $V(\mathbf{r})=V(-\mathbf{r})$ in Eq. (1), one derives the following rule: *Each matrix element* $A_{\alpha\beta}(\mathbf{k})$ ($\underline{A}=\underline{W},\underline{\Sigma},\underline{\varepsilon}$) is *odd (even) in* $\mathbf{k}$ *and pure imaginary (real) if the two orbitals* α,β *have opposite (identical) spatial parity.* This rule applies, for example, to *monatomic* systems, for which the $\mathbf{R}_n$'s may be chosen to coincide with the *atomic* sites. Let us consider an extension to systems whose unit cell contains more atomic or molecular centers, so that the site potential

$$V(\mathbf{r}-\mathbf{R}_n)=\sum_{\mathbf{d}} V_{\mathbf{d}}(\mathbf{r}-\mathbf{R}_n-\mathbf{d})$$

results from the contributions $V_{\mathbf{d}}$ of different potentials (possibly spherically symmetrical with respect to the points $\mathbf{R}_n+\mathbf{d}$). In this case, one has to relax the assumption of a well-defined spatial parity, with respect to the sites $\{\mathbf{R}_n\}$, since one has to include odd and even contributions, both from the potentials $V_{\mathbf{d}}(\mathbf{r}-\mathbf{R}_n-\mathbf{d})$, and from the orbitals $\Psi_{\mathbf{d}\alpha}(\mathbf{r}-\mathbf{R}_n-\mathbf{d})$. However, the definitions (3) and the equations (4) still hold true, and the matrix element rule turns out to be

$$A_{\alpha\beta}(\mathbf{k})=A^*_{\alpha\beta}(-\mathbf{k})=A_{\beta\alpha}(-\mathbf{k})\quad (\underline{A}=\underline{\rho},\underline{W},\underline{\varepsilon})\ , \tag{5}$$

which actually expresses the time-reversal symmetry. From Eq. (5), the imaginary part $\mathrm{Im}[\underline{A}(\mathbf{k})]$ is an *odd* function of $\mathbf{k}$, so that one has in particular, to the lowest nonvanishing order in $\mathbf{k}$,

$$\mathrm{Im}\,(\underline{\varepsilon})\cong\sum_{\eta=1}^{3} k_\eta\left[\frac{\partial\,\mathrm{Im}\,(\underline{\varepsilon})}{\partial k_\eta}\right]_{\mathbf{k}=0}\ .$$

Thus a power expansion of the Bloch Hamiltonian $\underline{\varepsilon}(\mathbf{k})=\underline{\varepsilon}(\mathbf{P}/\hbar)$ may contain a term linear in the quasimomentum $\mathbf{P}=\hbar\mathbf{k}$, of the form $\underline{C}\mathbf{P}$. It is this term that, in the long-wavelength limit, leads the Hamiltonian to assume a relativistic form, if the $G\times G$ matrices $\underline{C}_1,\underline{C}_2,\underline{C}_3$, and $\underline{\varepsilon}(0)$ have suitable commutation relations, reminiscent of a Pauli or Clifford algebra. We stress that the origin of the $\underline{C}\mathbf{P}$ contribution is related to the existence of terms having *opposite* spatial parity, and represents an *interband* interaction. In fact, the LCAO representation of $\mathrm{Im}[\underline{\varepsilon}(\mathbf{k})]$ is an antisymmetric matrix, which thereby couples only different orbitals. In the present section we do not consider the effects of the relativistic form of the Hamiltonian on the electron-phonon scattering, leaving the discussion to Sec. IV.

In the case of two arbitrary orbitals ($G=2$), not necessarily of well-defined spatial parity, the Hamiltonian Eq. (4a) reads

$$\begin{aligned}\underline{\varepsilon}(\mathbf{k})&=E_0(\mathbf{k})\underline{I}+\underline{\Delta}(\mathbf{k})\\ &=E_0(\mathbf{k})\underline{I}+\begin{bmatrix}\varepsilon_0(\mathbf{k}) & \varepsilon_1(\mathbf{k})e^{i\theta(\mathbf{k})}\\ \varepsilon_1(\mathbf{k})e^{-i\theta(\mathbf{k})} & -\varepsilon_0(\mathbf{k})\end{bmatrix}\ ,\end{aligned} \tag{6}$$

where $\underline{I}$ is the identity matrix, ε_0, ε_1, and θ are real, and $\varepsilon_1\sin\theta$ is an *odd* function of $\mathbf{k}$, because of the rule (5). The calculations performed in Sec. III of paper II can be applied to Eq. (6), which yields the following expressions for the eigenvalues E_u in Eq. (4a):

$$E_u=E_0\pm E=E_0\pm\sqrt{\varepsilon_0^2+\varepsilon_1^2}\ . \tag{7a}$$

The corresponding eigenvectors are

$$\underline{u}_+=\frac{1}{\sqrt{1+x^2}}\begin{bmatrix}1\\ xe^{-i\theta}\end{bmatrix},\quad \underline{u}_-=\frac{1}{\sqrt{1+x^2}}\begin{bmatrix}-x\\ e^{-i\theta}\end{bmatrix}\ , \tag{7b}$$

with

$$x=\frac{E-\varepsilon_0}{\varepsilon_1}\ . \tag{7c}$$

In paper II, one calculates the *Zitterbewegung* operator $\underline{Z}(\mathbf{k})$ describing the "trembling motion" of a charge in a crystal due to interband transitions in the case of orbitals of well-defined parity. The same method (for an alternative derivation, see Ref. 4), can also be applied to the Hamiltonian (7a), valid in the general case, with the result

$$\underline{Z}(\mathbf{k})=\frac{1}{2E^2}\left[(\varepsilon_1\partial\varepsilon_0-\varepsilon_0\partial\varepsilon_1)\begin{bmatrix}0 & ie^{i\theta}\\ -ie^{-i\theta} & 0\end{bmatrix}+\varepsilon_0\varepsilon_1\partial\theta\begin{bmatrix}0 & e^{i\theta}\\ e^{-i\theta} & 0\end{bmatrix}\right], \tag{8}$$

where the symbol $\partial\ldots$, applied to a scalar function of $\mathbf{k}$, indicates the gradient in $\mathbf{k}$ (and is thereby a *vector* in the reciprocal space). The difference between Eq. (8) of the present paper and Eq. (19) in paper II results in the second term in large parentheses, proportional to $\partial\theta$. In fact, for orbitals of well-defined parity, the phase θ may be 0 or $\pi/2$ (if the two orbitals have the same or the opposite parity, respectively), but is independent of $\mathbf{k}$ in any case.

III. ELECTRON-PHONON INTERACTION IN TWO-BAND SYSTEMS

In the present section we extend to the multiband case the standard single-band formalism for the electron-phonon interaction, developed in textbooks.[6] This will be done by using the generalized LCAO approach outlined in Sec. II. The coordinate representation of the electron-phonon interaction reads, for *one-phonon* processes,

$$w_{\rm ph}(\mathbf{r})=\frac{i}{(2\pi)^{3/2}}\sum_{\mathbf{n}}\int_{\Omega_1}d\mathbf{k}\,e^{-i(\mathbf{k}+\mathbf{K}_n)\cdot\mathbf{r}}(\mathbf{k}+\mathbf{K}_n)\times\mathbf{A}(\mathbf{k})\mathcal{V}(\mathbf{k}+\mathbf{K}_n)\,, \tag{9}$$

where $\{\mathbf{K}_m\}$ are the reciprocal-lattice vectors, Ω_1 is the first Brillouin zone, and $\mathcal{V}(\mathbf{k})$ and $\mathbf{A}(\mathbf{k})$ are, respectively, the Fourier transform of the site potential $V(\mathbf{r})$ and of the lattice displacements. Let $\varphi_\alpha(\mathbf{k})$ be the Fourier transform of the α orbital (localized in the coordinate origin). The rates of one-phonon processes depend on the matrix elements between the Bloch eigenstates $|\mathbf{k},\sigma\rangle$, with wave vector $\mathbf{k}$ and belonging to the band (or branch) σ. Let σ label the eigensolutions $\underline{u}_\sigma(\mathbf{k})$ of Eq. (4a) ($\sigma=\pm$ for two-band systems). Because of the third relation (4b) and of the first relation (3), the coordinate representation of the Bloch functions reads

$$\langle\mathbf{r}|\mathbf{k},\sigma\rangle=\frac{1}{\sqrt{N}}\sum_n[\underline{\Psi}(\mathbf{r}-\mathbf{R}_n)]^\dagger\underline{\rho}^{-1}(\mathbf{k})\underline{u}_\sigma(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{R}_n}\,, \tag{10}$$

where N is the number of sites and the symbol $\underline{\Psi}(\mathbf{r}-\mathbf{R}_n)$ stands for the *column* matrix formed by the G orbitals in the nth site ($\dagger$ indicates the adjoint, i.e., the *row* matrix formed by the complex conjugates of the G orbitals).[7] By constructing $\langle\sigma',\mathbf{k}'|\mathbf{k},\sigma\rangle$ from Eq. (10), it can be seen that the matrix $\underline{\rho}^{-1}$ accounts for the overlap integrals [see the second relation (4b) and the second relation (3)], in such a way that the orthonormality relations are satisfied, i.e., $\langle\sigma',\mathbf{k}'|\mathbf{k},\sigma\rangle=\Xi_1\delta(\mathbf{k}-\mathbf{k}')\delta_{\sigma\sigma'}$ (Ξ_1 being the volume of the first Brillouin zone). By means of Eqs. (9) and (10), the matrix element of the electron-phonon interaction, connecting a state with wave vector $\mathbf{k}$, in the band (or branch) σ, to one with wave vector $\mathbf{k}'$ in the band (or branch) σ', becomes

$$\langle\sigma,\mathbf{k}|w_{\rm ph}|\mathbf{k}',\sigma'\rangle=\frac{i\Xi_1^2}{(2\pi)^{3/2}}\sum_{s,m}\underline{u}_\sigma^\dagger(\mathbf{k})\underline{\rho}^{-1}(\mathbf{k})\underline{\varphi}(\mathbf{k}+\mathbf{K}_s+\mathbf{K}_m;\mathbf{k}'+\mathbf{K}_m)\times\underline{\rho}^{-1}(\mathbf{k}')\underline{u}_{\sigma'}(\mathbf{k}')(\mathbf{k}-\mathbf{k}'+\mathbf{K}_s)\,\mathbf{A}(\mathbf{k}-\mathbf{k}')\mathcal{V}(\mathbf{k}-\mathbf{k}'+\mathbf{K}_s)\,, \tag{11a}$$

where the $G\times G$ matrix $\underline{\varphi}$ is defined as

$$\varphi_{\alpha\beta}(\mathbf{k};\mathbf{k}')=\varphi_\alpha^*(\mathbf{k})\varphi_\beta(\mathbf{k}') \tag{11b}$$

for $\mathbf{k}$ and $\mathbf{k}'$ fulfilling the condition

$$\mathbf{k}-\mathbf{k}'+\mathbf{K}_s\in\Omega_1\,. \tag{11c}$$

The terms of the sum in Eq. (11a) may correspond to *normal* ($\mathbf{K}_s=0$) or to *umklapp* ($\mathbf{K}_s\neq0$) processes. If the orbitals $\Psi_\alpha(\mathbf{r})$ have a localization length sufficiently small, compared with the First-nearest-neighbor (FNN) distance, the overlap integrals can be neglected ($\underline{\rho}=\underline{I}$), and the Fourier transform $\varphi_\alpha(\mathbf{k})$ varies smoothly, in the first Brillouin zone. Hence, from Eqs. (11b) and (11c), it follows that the matrix $\underline{\varphi}$ in Eq. (11a) is almost independent of $\mathbf{k}$ and $\mathbf{k}'$. If one considers normal processes, the sum in "m" can be approximated by the integral in $\mathbf{k}$ (over the whole space) of two orthonormal functions φ_α and φ_β, which yields $\Sigma_m\underline{\varphi}(\mathbf{k}+\mathbf{K}_m;\mathbf{k}'+\mathbf{K}_m)\cong\underline{I}/\Xi_1$. In this case, Eq. (11a) becomes

$$\langle\sigma,\mathbf{k}|w_{\rm ph}|\mathbf{k}',\sigma'\rangle\simeq\frac{i\Xi_1}{(2\pi)^{3/2}}\underline{u}_\sigma^\dagger(\mathbf{k})\underline{u}_{\sigma'}(\mathbf{k}')(\mathbf{k}-\mathbf{k}')\times\mathbf{A}(\mathbf{k}-\mathbf{k}')\mathcal{V}(\mathbf{k}-\mathbf{k}')\,. \tag{12}$$

The single-band case, obtained by setting $\underline{u}_\sigma=\underline{u}_{\sigma'}=1$, corresponds to the standard matrix element depending only on the *transferred* wave vector $\mathbf{q}=\mathbf{k}'-\mathbf{k}$.[6] The multiband effect results in the scalar product of the energy eigenvectors [Eq. (4a)], in the initial and final state. If $\underline{u}_\sigma(\mathbf{k})\neq\underline{u}_{\sigma'}(\mathbf{k}')$, not only an *interband* coupling is produced for $\sigma\neq\sigma'$, but the *intraband* coupling itself ($\sigma=\sigma'$) tends in general to *decrease* in modulus,

with respect to the single-band case, since $|\underline{u}_\sigma^\dagger(\mathbf{k})\underline{u}_\sigma(\mathbf{k}')| \le |\underline{u}_\sigma^\dagger(\mathbf{k})\underline{u}_\sigma(\mathbf{k})| = 1$. We can now connect the damping of the electron-phonon coupling to *Zitterbewegung* considered in Sec. II. For the sake of brevity, we drop the band index σ in $\underline{u}$ and use the same convention as in Sec. II concerning the derivatives in $\mathbf{k}$. Thus $\partial\underline{u}$ is the k gradient of $\underline{u}$ (vector in k space) and $\partial\partial'\underline{u}$ is the Hessian (tensor of rank 2) of the second derivatives. Since $\underline{u}_\sigma^\dagger(\mathbf{k})\underline{u}_\sigma(\mathbf{k})=1$, it follows that $(\partial\underline{u}^\dagger)\underline{u}+\underline{u}^\dagger(\partial\underline{u})=0$ and $(\partial\partial'\underline{u}^\dagger)\underline{u}+\underline{u}^\dagger(\partial\partial'\underline{u}) +(\partial\underline{u}^\dagger)(\partial'\underline{u})+(\partial'\underline{u}^\dagger)(\partial\underline{u})=0$. With the aid of these relations, an expansion to the lowest nonvanishing order in the transferred wave vector $\mathbf{q}=\mathbf{k}'-\mathbf{k}$ gives

$$|\underline{u}^\dagger(\mathbf{k})\underline{u}(\mathbf{k}')|^2 \simeq 1-(\partial\underline{u}^\dagger\cdot\mathbf{q})(\partial\underline{u}\cdot\mathbf{q})-(\underline{u}^\dagger\partial\underline{u}\cdot\mathbf{q})^2 \ . \tag{13}$$

An application of the general Eq. (13) to any one of the matrices $\underline{u}_\pm$ in the two-band case, Eqs. (7) yields

$$\begin{aligned}|\underline{u}^\dagger(\mathbf{k})\underline{u}(\mathbf{k}')|^2 &\simeq 1-\frac{1}{4E^4}[(\varepsilon_1\partial\varepsilon_0-\varepsilon_0\partial\varepsilon_1)\cdot\mathbf{q}]^2 \\ &\quad+(\partial\theta\cdot\mathbf{q})^2\frac{\varepsilon_1^2}{4E^2} \\ &=1-(\underline{Z}\cdot\mathbf{q})^2-\frac{(\partial\theta\cdot\mathbf{q})^2}{4}\left[\frac{\varepsilon_1}{E}\right]^4 ,\end{aligned} \tag{14}$$

where the second equality is obtained by using Eq. (8). From Eq. (14) it is seen that the two-band structure damps the electron-phonon coupling for *intraband* processes by an amount that, to the lowest order in $\mathbf{q}$, equals the square product between the momentum transfer and the *Zitterbewegung* displacement, plus a term proportional to the *fourth* power in the ratio between the interband coupling ε_1 and the gapwidth $2E$ [see Eq. (7a)]. However, Eq. (14) shows that $(\underline{Z}\cdot\mathbf{q})^2$ already includes the contributions proportional to $(\varepsilon_1/2E)^2$, so that the last term in Eq. (14) is a higher-order correction that can be neglected in the limit of small transferred wave vectors *and* small interband couplings.

It was mentioned in paper II that the *Zitterbewegung* in multiband systems is a description of a *true* physical process, related to the periodic (in space) force experienced by the particle in the lattice. Now we have a further indication that the term "trembling motion" is to be taken literally, at least in a perturbative description. In fact, the damping term $(\underline{Z}\cdot\mathbf{q})^2$ is reminiscent of the lowest-order correction due to a Debye-Waller factor, if $|\underline{Z}|$ would measure the amplitude of the oscillations performed by the pointlike target, exchanging a momentum $\mathbf{q}$ with a scattering wave. Hence, as far as the interaction with soft phonons is concerned, in the limit of small interband coupling, the "trembling motion" of the electron around its center of mass is quite similar to a real harmonic oscillation.[8] This analogy is less appropriate for large interband couplings, i.e., in the limit of vanishing gap. As we shall see in the following section, in this case one cannot use a perturbative approach, and the effect of the *Zitterbewegung* may be so large as to suppress all one-phonon processes.

IV. ELECTRON-PHONON INTERACTION AND *ZITTERBEWEGUNG* IN THE PRESENCE OF A PSEUDORELATIVISTIC DIRECTION

We now apply some results of Secs. II and III to the study of one-phonon *normal* processes in crystals [denoted "class (b)" in paper II], formed by two orbitals having *opposite* and well-defined parity. These are characterized by a pseudorelativistic direction, along which the Hamiltonian becomes Dirac-like in the long-wavelength limit. To see this, we set $\theta=-\pi/2$ in Eq. (6), on account of the matrix element rule mentioned in Sec. II. Then we expand to first order in $\mathbf{k}$, and use the Pauli matrices $\underline{\sigma}_\mu$ ($\mu=1,2,3$) to represent the 2×2 matrix $\underline{\Delta}$ in Eq. (6) (without any relation with the electron's spin). This yields

$$\underline{\varepsilon}-E_0(0)\underline{I}\cong MC^2\underline{\sigma}_3+\mathbf{P}\cdot\mathbf{C}\underline{\sigma}_2 \ , \tag{15a}$$

where

$$\mathbf{P}=\hbar\mathbf{k}, \quad \mathbf{C}\equiv\frac{(\partial\varepsilon_1)_0}{\hbar}, \quad M\equiv\frac{\varepsilon_0(0)}{C^2} \ . \tag{15b}$$

Equations (15) show that in a lattice of *arbitrary* dimension, the opposite-parity condition for the pair of orbitals in each site leads the Hamiltonian to become Dirac-like in the long-wavelength limit, with a limiting velocity $\mathbf{C}$ proportional to the gradient $(\partial\varepsilon_1)_0$, calculated in $\mathbf{k}=0$. Equations (15) imply that the current associated to the pseudorelativistic Hamiltonian is directed along $\mathbf{C}$. Thus we expect a strong anisotropic behavior of the electric conductivity, whenever long-wavelength electrons dominate the charge transport. It is possible to show that, in the tight-binding approximation with only first-nearest-neighbor (FNN) interaction, the expression for the pseudorelativistic velocity is

$$\mathbf{C}\cong-\sum_{\mathbf{D}}\mathbf{D}\Big/\hbar[V_{12}(\mathbf{D})-E_{\mathrm{at}}S_{12}(\mathbf{D})] \ , \tag{16}$$

where $\{\mathbf{D}\}$ are the vectors connecting a given site to its FNN's, E_{at} is the twofold-degenerate atomic level in each site, and the matrix elements between the two orbitals 1 and 2 in the FNN sites can be calculated according to Eqs. (2a)–(2c). The existence of a special direction, like $\mathbf{C}/C$, means that some kind of anisotropy has been implicitly introduced. This anisotropy, due to the interaction between s- and p-like bands, has been actually observed and studied theoretically in zero-gap materials like α-Sn and HgSe.[9] In Fig. 1 we sketch a model lattice of class (b), whose pseudorelativistic direction $\mathbf{C}/C$ originates from the application of a shear stress. The model is made by planar structures, with sites occupied by s-p orbitals (solid circles and open ellipses, respectively), the latter being responsible for the interplanar coupling. Figure 1(a) shows the unstressed lattice, with the p orbitals orthogonal to the planes. In this case, both $V_{12}(\mathbf{D})$ and $S_{12}(\mathbf{D})$ entering Eq. (16) vanish for parity reasons and $\mathbf{C}=0$. Figure 1(b) shows the effect of a shear stress along the planes, leading the p orbitals to form an angle $\theta_D\neq\pi/2$ with the planes in the direction of the applied stress. In this case one has nonvanishing contributions $V_{12}(\mathbf{D})$ and

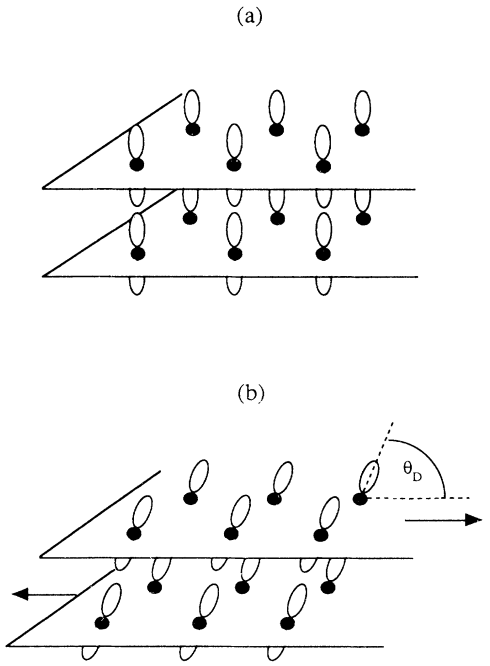

FIG. 1. A sketch of a model lattice with a pseudorelativistic direction. Planar structures, with sites occupied by s orbitals (solid circles) and p orbitals (open ellipses) are coupled with one another mainly by the p orbitals. In the unstressed lattice (a) the p orbitals are orthogonal to the planes. A stress along the planes (b) forces the symmetry axis of the p orbitals to form an angle $\theta_D \neq \pi/2$ with the planes. Arrows indicate the direction of the resulting pseudorelativistic velocity.

$S_{12}(\mathbf{D})$, proportional to cos θ_D [see Eq. (A2) of Ref. 5], giving rise to a pseudorelativistic velocity, in the direction of the applied stress. Each chain of inclined p orbitals realizes a one-dimensional system quite similar to the one studied in paper I.

Equations (15) are a special case of Eq. (6), so that, by means of Eqs. (7), one readily gets two energy bands and two dispersion relations

$$\pm E = \pm\sqrt{M^2C^4+(\mathbf{C}\cdot\mathbf{P})^2}\ , \tag{17a}$$

in the long-wavelength limit and with a suitable choice of the energy origin. The two eigenstates $\underline{u}_\pm$ in the bands are[10]

$$\underline{u}_+ = \frac{1}{\sqrt{1+x^2}}\begin{bmatrix}1\\ ix\end{bmatrix},\quad \underline{u}_- = \frac{1}{\sqrt{1+x^2}}\begin{bmatrix}-ix\\ -1\end{bmatrix},$$
$$x = \frac{E-MC^2}{\mathbf{P}\cdot\mathbf{C}}\ . \tag{17b}$$

One may restrict the analysis to *absorption* processes, since the emission is obviously symmetrical. From Eq. (17a), the energy-momentum conservation for the absorption of one *soft* longitudinal phonon of momentum $\mathbf{Q}$ (in arbitrary dimension) and velocity V_s, leads to the following equations:

$$\pm\sqrt{M^2C^4+(\mathbf{P}\cdot\mathbf{C})^2}+V_sQ = \pm\sqrt{M^2C^4+(\mathbf{P}\cdot\mathbf{C}+\mathbf{Q}\cdot\mathbf{C})^2}$$
(intraband), (18a)

$$-\sqrt{M^2C^4+(\mathbf{P}\cdot\mathbf{C})^2}+V_sQ = \sqrt{M^2C^4+(\mathbf{P}\cdot\mathbf{C}+\mathbf{Q}\cdot\mathbf{C})^2}$$
(interband), (18b)

where $Q=|\mathbf{Q}|$ is the modulus of the phonon momentum. We refer to soft phonons since their energy is V_sQ only in a suitable long-wavelength limit. In Eq. (18a) it is possible to select the positive sign without loss of generality, because the other case reduces to the former, with the substitutions $\mathbf{P}+\mathbf{Q}\to\mathbf{P}'$, $\mathbf{Q}\to-\mathbf{Q}'$. By squaring Eqs. (18) and solving with respect to Q, one gets the two conditions

$$|\cos\phi| \le \frac{V_s}{C}\quad \text{(interband)}, \tag{19a}$$

$$|\cos\phi| \ge \frac{V_s}{C}\quad \text{(intraband)}, \tag{19b}$$

for the angle ϕ between the velocity $\mathbf{C}$ and the phonon momentum $\mathbf{Q}$. In the "ultrasonic" regime $C > V_s$ the conditions (19) can both be satisfied. In contrast the "subsonic" regime $C < V_s$ leads to a vanishing of the *intraband* transitions.

Let us now consider the "ultrarelativistic" zero-gap limit $M\to 0$, which yields $E=|\mathbf{P}\cdot\mathbf{C}|$ [second Eq. (17a)] and leads to a single degenerate band. As suggested by the example in paper I, this limit is realized for the model system in Fig. 1, when the symmetry axis of the odd-parity orbital forms a critical angle with the planes, depending on the FNN distance in the planes themselves. In the ultrarelativistic limit, the third equation (17b) yields $x=\mathbf{P}\cdot\mathbf{C}/|\mathbf{P}\cdot\mathbf{C}|$, so that, from the first two equations (17b)

$$[\underline{u}_\pm(\mathbf{P})]^\dagger \underline{u}_\mp(\mathbf{P}') = \frac{1}{2}\left[1-\frac{(\mathbf{P}\cdot\mathbf{C})(\mathbf{P}'\cdot\mathbf{C})}{|\mathbf{P}\cdot\mathbf{C}||\mathbf{P}'\cdot\mathbf{C}|}\right],$$
$$[\underline{u}_\pm(\mathbf{P})]^\dagger \underline{u}_\pm(\mathbf{P}') = \frac{1}{2}\left[1+\frac{(\mathbf{P}\cdot\mathbf{C})(\mathbf{P}'\cdot\mathbf{C})}{|\mathbf{P}\cdot\mathbf{C}||\mathbf{P}'\cdot\mathbf{C}|}\right]. \tag{20}$$

Recalling Eq. (12) ($\sigma=\pm$), Eqs. (20) imply that, in the ultrarelativistic limit, interband or intraband transitions are forbidden, according to whether the projections of $\mathbf{P}$ and $\mathbf{P}'$ on $\mathbf{C}$ have the same or the opposite sign, respectively. Thus, in addition to the conditions (19), one has also to impose that the quantity $(\mathbf{P}\cdot\mathbf{C})(\mathbf{P}\cdot\mathbf{C}+\mathbf{Q}\cdot\mathbf{C})$ is *negative* for *interband* transitions and *positive* for *intraband* transitions. For this to occur, one needs

$$|\cos\phi| \ge \frac{V_s}{C}\quad \text{(interband)}, \tag{21a}$$

$$|\cos\phi| \le \frac{V_s}{C}\quad \text{(intraband)}. \tag{21b}$$

Since the inequalities (19) and (21) cannot be satisfied simultaneously (apart from the limiting case $V_s=C$), it is seen that the vanishing of the gap in a crystal of class (b), with a pseudorelativistic direction, leads to the suppres-

sion of *all* electron-phonon processes, involving a single soft phonon. Unlike the case of small interband coupling (Sec. III), the vanishing of the gapwidth makes the right-hand side members of Eqs. (20) not expandable in a power series of $\mathbf{P}'-\mathbf{P}$. In the same limit, Eq. (34b) of paper II shows that $\mathbf{Z}^2(\mathbf{k})$ tends to $\delta(k_c)/k_c$, δ being the Dirac function, and k_c being the component of $\mathbf{k}$ parallel to the pseudorelativistic velocity $\mathbf{C}$. We can thus relate the singular behavior of Eqs. (20), and the resulting conditions (21), to the singularity of the *Zitterbewegung* in $\mathbf{k}=\mathbf{0}$, in the limit of vanishing gapwidth. The electron-phonon interaction for zero-gap semiconductors has been studied in a different formalism, for example in Ref. 11. It is theoretically suggested, and experimentally verified[12] that the electron-phonon coupling is in general softened in these materials. For class (b) systems, this may result in the suppression of one-phonon processes and in a divergingly large amplitude of the *Zitterbewegung* near the Γ point.

V. CONCLUSIONS

The present paper is on the same line as paper II and Ref. 4, in which interband transitions in multiband crystals are interpreted as a nonrelativistic *Zitterbewegung* in the Bloch formalism. The origin of this effect is the true force experienced by the particle in the crystal, which is periodical in space in the rigid-lattice approximation. The present paper approaches the next step of the problem, i.e., the effects of the *Zitterbewegung* on the electron-phonon interaction. The main result obtained for two-band systems is that, in the limit of small transferred wave vectors and small interband couplings, the *Zitterbewegung* behaves like a *harmonic oscillation* of the electron, around its center of mass.[8] In fact, the resulting damping on the electron-phonon coupling is reproducible, to first order, by a Debye-Waller factor. This result is general and independent of the form of the two-band Hamiltonian. However, one may suspect that the *Zitterbewegung* is more relevant if the Bloch Hamiltonian has a pseudorelativistic form. Thus we focus our attention on the existence of terms in the Hamiltonian of the form $\underline{C}\mathbf{P}$ (i.e., linear in the quasimomentum $\mathbf{P}$). The $\underline{C}\mathbf{P}$ terms may be responsible for pseudorelativistic effects, which are relevant for the physics of narrow-gap semiconductors.[13] In particular, some crystals, defined as "class (b)" in paper II, are shown to display a Dirac-like behavior in the long-wavelength limit, along a special "pseudorelativistic" direction. These are characterized by the fact that the band structure originates from the mixing of opposite-parity orbitals. A model system is envisaged in Fig. 1, whose pseudorelativistic behavior originates from an applied stress. The most relevant result obtained for class (b) crystals is the suppression of one-phonon processes in the zero-gap (ultrarelativistic) limit,[11] an effect that is closely related to the divergingly large amplitude of the *Zitterbewegung* near the Γ point.

ACKNOWLEDGMENTS

We thank Dr. P. Kocevar for a valuable discussion. We thank also Dr. S. V. Vonsovsky and Dr. Svirsky for providing us with their paper (Ref. 4). This work was partially supported by the Italian Ministry of Education.

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