Nonrelativistic zitterbewegung in two-band systems

L. Ferrari and G. Russo
Dipartimento di Fisica dell'Università, Gruppo Nazionale di Struttura della Materia and Centro Universitario di Struttura della Materia Unitá di Bologna, Bologna I 40126, Italy
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The notion of zitterbewegung and the resulting formalism, originally proposed for relativistic quantum dynamics, is applied to describe the acceleration of a nonrelativistic electron moving in a crystal, due to the periodic force experienced. A general linear-combination-of-atomic-orbitals (LCAO) approach is developed for multiband systems, and the special case of two-band systems is studied in detail. It is shown that the zitterbewegung determines the minimum spatial extension of localized wave packets formed by a combination of Bloch functions belonging to a single band, in a manner that depends strongly on the relative parity of the orbitals entering the LCAO bands. In the case of two orbitals with opposite parity, one is able to extend the notion of effective mass to deep defect levels, and to estimate the width of the tails of localized states in glassy semiconductors, as a function of the separation between the mobility edges.

I. INTRODUCTION

Since the original work of Schrödinger,[1] the "zitterbewegung" (trembling motion) has been currently referred to as a relativistic quantum effect leading a Dirac electron to oscillate around the center-of-mass trajectory, even in the absence of external fields. According to the quantum field theories, however, such a trembling motion should not be a real effect, but only a curious mathematical consequence of the single-particle picture of the Dirac equation. Thus the physical relevance of the zitterbewegung in relativistic quantum dynamics is a controversial point that we do not discuss further here.[2] We simply stress that the zitterbewegung is not a relativistic concept in itself, but can be applied to any free-particle Hamiltonian giving rise to a self-acceleration. Let, for example,

$$\underline{H}=\{H_{\alpha\beta}(\mathbf{P})\}$$

be a matrix Hamiltonian whose elements $H_{\alpha\beta}(\mathbf{P})$ depend only on the momentum $\mathbf{P}$. The matrix acts on a finite-dimensional space of vectors describing an "internal" phase space. If for the velocity operator $\underline{\mathbf{V}}=\mathrm{grad}_{\mathbf{P}}\underline{H}$ one has

$$[\underline{H},\underline{\mathbf{V}}]\neq 0 ,$$

a nonvanishing self-acceleration exists, due to the transitions among the "internal" eigenstates. The resulting fluctuations around the uniform motion are what we may call a zitterbewegung, in a generalized sense. An example has been recently given[3] for a nonrelativistic chain, leading to a Dirac-like wave equation. In this and in other cases, such as polyacteylene[4] and graphite,[5] the zitterbewegung might appear as a consequence of the pseudorelativistic form of the wave equation. In contrast, we will now show that the zitterbewegung is a general real effect for a nonrelativistic particle moving in a crystal, as a consequence of interband transitions. The main point is the role of the *acceleration* in the Bloch formalism. By means of Bloch's theorem, it is possible to treat a particle accelerated by a periodic (in space) force as a freelike particle, characterized by a well-defined wave vector $\mathbf{k}$ (ranging in the first Brillouin zone) and momentum $\hbar\mathbf{k}$. The general form of the Hamiltonian in the k representation reads, after diagonalization, as

$$\underline{H}(\mathbf{k})=\sum_b E_b(\mathbf{k})(\mathbf{k})\underline{P}_b(\mathbf{k}) ,$$

where $\underline{P}_b(\mathbf{k})=|\mathbf{k},b\rangle\langle b,\mathbf{k}|$ is the projector on the Bloch state $|\mathbf{k},b\rangle$, with wave vector $\mathbf{k}$, in the bth band, and $E_b(\mathbf{k})$ is the corresponding energy. In principle, a nonsingular periodic potential yields an *infinite* number of bands, though one may refer to few or one of them, under suitable approximations. Once the Hamiltonian is expressed as a function of the momentum $\hbar\mathbf{k}$, one is *formally* left with a freelike particle, even if the dependence on $\mathbf{k}$ is not quadratic. However, it should be clear that the Bloch formalism cannot really eliminate the acceleration, but only express it in a different form. The crucial point for the acceleration is the band multiplicity discussed above. We first notice that the Hamiltonian $\underline{H}(\mathbf{k})$ now appears as a *diagonal* matrix, with elements $E_b(\mathbf{k})$ depending on the "external" degree of freedom $\mathbf{k}$, and acting on an "internal" space with dimensions fixed by the number of bands involved. Apart from diagonality, this corresponds to the general case, discussed at the very beginning, which may give rise to a self-acceleration. To clarify this point, let us consider the position operator $i\nabla_{\mathbf{k}}$, canonically conjugate to the momentum, and the resulting velocity operator:

$$\underline{v}(\mathbf{k})=\frac{1}{\hbar}\nabla_{\mathbf{k}}\underline{H}=\frac{1}{\hbar}\sum_b\{[\nabla_{\mathbf{k}}E_b(\mathbf{k})]\underline{P}_b(\mathbf{k})+E_b(\mathbf{k})[\nabla_{\mathbf{k}}\underline{P}_b(\mathbf{k})]\} .$$

Due to the second term in brackets, a self-acceleration is found as

$$\underline{a}(\mathbf{k})=\frac{i}{\hbar}[\underline{H},\underline{v}]=\frac{i}{\hbar^2}\sum_{b\neq b'}E_b(\mathbf{k})E_{b'}(\mathbf{k})[\underline{P}_b(\mathbf{k}),\nabla_{\mathbf{k}}\underline{P}_{b'}(\mathbf{k})]\ .$$

The condition $b\neq b'$ in the preceding sum follows from the equation $\underline{P}_b^2=\underline{P}_b$, which yields $(\nabla_{\mathbf{k}}\underline{P}_b)\underline{P}_b=\underline{P}_b(\nabla_{\mathbf{k}}\underline{P}_b)=0$. One of the aims of the calculations in the following sections is to show that, in general, $\underline{P}_b$ does not commute with $\nabla_{\mathbf{k}}\underline{P}_{b'}$ for $b\neq b'$. Therefore it is seen that the acceleration produced by a periodic potential results in a multiband effect which would vanish in the single-band approximation. By means of the Bloch formalism, the effects of the periodic force can be expressed as the self-acceleration of a free particle, due to the transitions among "internal" states, corresponding to the bands. The resulting zitterbewegung is a real effect, just because it follows from a real force.

In order to study the physical consequences of the zitterbewegung in multiband systems, we need to be more specific about the band structure, without losing too much in generality. In Sec. II we develop a linear-combination-of-atomic-orbitals (LCAO) approach to the band calculation, including ionic interactions and overlap integrals to *all* orders. This will make it possible to extend the validity of the next results to a wide class of systems. In Sec. III the self-acceleration and the zitterbewegung, due to interband transitions, are studied for two-band systems. In Sec. IV the zitterbewegung effects are calculated for wave packets formed by a superposition of Bloch states of a single band (equivalent to the positive- and negative-energy solutions in the relativistic theory). In Sec. V the results obtained will be applied to estimate the minimum localization length of defect states in the gap. This provides a definition of effective mass, valid for *deep* levels, and makes it possible to calculate the extension and overlap of tails of localized states in glassy semiconductors.

II. GENERAL LCAO APPROACH TO THE BAND CALCULATION

In the present section we extend to the multiorbital case the LCAO approach developed, for example, by Peierls,[6] for a single orbital and including overlap integrals at any order of approximation. Let

$$\langle\mathbf{r}|n,\alpha\rangle=\Psi_\alpha(\mathbf{r}-\mathbf{R}_n);\quad\alpha=1,2,\ldots,G \tag{1}$$

represent a set of G orbitals, localized around the nth side of a periodic lattice. Let

$$\langle\alpha,n|m,\beta\rangle\equiv S_{\alpha\beta}(\mathbf{R}_n-\mathbf{R}_m) \tag{2}$$

be the resulting overlap integrals, such that $S_{\alpha\beta}(O)=\delta_{\alpha\beta}$, because of the orthonormality of the G orbitals in the same site. The single-particle periodic potential is assumed (but this is not essential) as a superposition of local potentials $V(\mathbf{r}-\mathbf{R}_n)$, so that the Hamiltonian reads

$$H=T+\sum_n V(\mathbf{r}-\mathbf{R}_n)\ , \tag{3}$$

$T=-(\hbar^2/2m)\nabla_{\mathbf{r}}^2$ being the kinetic energy. Expressing the quantum states in the LCAO approximation

$$|\Psi\rangle=\sum_{m,\beta}c_{m\beta}|m,\beta\rangle\ , \tag{4}$$

the time-dependent Schrödinger equation $i\hbar\partial|\Psi\rangle/\partial t=H|\Psi\rangle$ yields, with the aid of Eqs. (2) and (3),

$$i\hbar\sum_{j,\beta}S_{\alpha\beta}(\mathbf{R}_n-\mathbf{R}_j)\frac{\partial c_{j\beta}}{\partial t}=\sum_{j,\beta}\left\langle\alpha,n\left|T+\sum_m V(\mathbf{r}-\mathbf{R}_m)\right|j,\beta\right\rangle c_{j\beta}\ . \tag{5}$$

By means of Eq. (1) and of the periodicity condition, it can be shown that

$$\left\langle\alpha,n\left|T+\sum_m V(\mathbf{r}-\mathbf{R}_m)\right|j,\beta\right\rangle=V_{\alpha\beta}(\mathbf{R}_n-\mathbf{R}_j)\ . \tag{6}$$

Hence Eq. (5) can be cast in the matricial form

$$i\hbar\sum_j\underline{S}(\mathbf{R}_n-\mathbf{R}_j)\frac{\partial}{\partial t}\underline{c}(\mathbf{R}_j)=\sum_j\underline{V}(\mathbf{R}_n-\mathbf{R}_j)\underline{c}(\mathbf{R}_j)\ , \tag{7a}$$

where

$$\underline{c}(\mathbf{R}_j)=\{c_{j\beta};\beta=1,2,\ldots,G\} \tag{7b}$$

is a G-component column matrix, i.e., a vector in a G-dimensional "internal" space (bold symbols are used here only to indicate positions, wave vectors, and velocities). Similarly,

$$\begin{aligned}&\underline{S}(\mathbf{R}_n)=\{S_{\alpha\beta}(\mathbf{R}_n);\alpha,\beta=1,2,\ldots,G\}\ ,\\&\underline{V}(\mathbf{R}_n)=\{V_{\alpha\beta}(\mathbf{R}_n);\alpha,\beta=1,2,\ldots,G\}\ ,\end{aligned} \tag{7c}$$

are $G\times G$ matrices. Expressing Eqs. (2) and (6) in the coordinate representation, the following relations can be obtained, for an *even* local potential $V(\mathbf{r})=V(-\mathbf{r})$:

$$\begin{aligned}&S_{\alpha\beta}(\mathbf{R}_n)=P_\alpha P_\beta S_{\alpha\beta}(-\mathbf{R}_n)=P_\alpha P_\beta S^*_{\beta\alpha}(\mathbf{R}_n)\ ,\\&V_{\alpha\beta}(\mathbf{R}_n)=P_\alpha P_\beta V_{\alpha\beta}(-\mathbf{R}_n)=P_\alpha P_\beta V^*_{\beta\alpha}(\mathbf{R}_n)\ ,\end{aligned} \tag{8}$$

where $P_\alpha=\pm1$ is the spatial parity (that we assume to be defined) of the orbital $\Psi_\alpha(\mathbf{r})$. Passing to the Fourier transforms in the first Brillouin zone Ω_1,

$$\begin{aligned}&\underline{c}(\mathbf{R})=\frac{1}{\Omega_1}\int_{\Omega_1}d\mathbf{k}\underline{\Phi}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{R}}\ ,\\&\underline{S}(\mathbf{R})=\frac{1}{\Omega_1}\int_{\Omega_1}d\mathbf{k}\underline{\Sigma}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{R}}\ ,\\&\underline{V}(\mathbf{R})=\frac{1}{\Omega_1}\int_{\Omega_1}d\mathbf{k}\underline{W}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{R}}\ ,\end{aligned} \tag{9}$$

Eq. (7a) becomes

$$i\hbar\underline{\Sigma}(\mathbf{k})\frac{\partial\underline{\Phi}(\mathbf{k})}{\partial t}=\underline{W}(\mathbf{k})\underline{\Phi}(\mathbf{k})\ . \tag{10}$$

It is an easy matter to show that the matrices $\underline{\Sigma}(\mathbf{k})$ and $\underline{W}(\mathbf{k})$ ($\mathbf{k}\in\Omega_1$) are self-adjoint. We now express their elements in terms of the Fourier transforms $\varphi_\alpha(\mathbf{k})$ and $\mathcal{V}(\mathbf{k})$ ($\mathbf{k}\in\mathbb{R}^2$) of orbitals and local potentials, respectively:

$$\Sigma_{\alpha\beta}(\mathbf{k})=\sum_n e^{i\mathbf{k}\cdot\mathbf{R}_n}S_{\alpha\beta}(\mathbf{R}_n)$$
$$=\Omega_1\sum_n \varphi_\alpha^*(\mathbf{k}-\mathbf{K}_n)\varphi_\beta(\mathbf{k}-\mathbf{K}_n)\ ,$$
$$W_{\alpha\beta}(\mathbf{k})=\sum_n e^{i\mathbf{k}\cdot\mathbf{R}_n}V_{\alpha\beta}(\mathbf{R}_n) \tag{11}$$
$$=\Omega_1\sum_n \varphi_\alpha^*(\mathbf{k}-\mathbf{K}_n)\varphi_\beta(\mathbf{k}-\mathbf{K}_n)\frac{\hbar^2}{2m}(\mathbf{k}-\mathbf{K}_n)^2$$
$$+\frac{\Omega_1^2}{(2\pi)^{3/2}}\sum_{n,m}\varphi_\alpha^*(\mathbf{k}-\mathbf{K}_n)$$
$$\times\varphi_\beta(\mathbf{k}-\mathbf{K}_m)\mathcal{V}(\mathbf{K}_m-\mathbf{K}_n),$$

where $\mathbf{K}_n$ are the reciprocal-lattice vectors. We expect that the overlap-integral matrix $\underline{\Sigma}(\mathbf{k})$ is positive defined for each $\mathbf{k}$, at least in the tight-binding (TB) approximation, in which $\underline{\Sigma}(\mathbf{k})$ equals identity plus small corrections. Indeed, the positivity of the eigenvalues of $\underline{\Sigma}(\mathbf{k})$ can be shown rigorously in the two-band case ($\alpha,\beta=1,2$) by calculating the trace and the determinant according to the first Eq. (11). This makes it possible to choose a nonsingular, self-adjoint matrix $\underline{\rho}(\mathbf{k})$, such that

$$\underline{\rho}^2(\mathbf{k})=\underline{\Sigma}(\mathbf{k})\ . \tag{12}$$

Setting

$$\underline{u}(\mathbf{k})=\underline{\rho}(\mathbf{k})\underline{\Phi}(\mathbf{k})\ , \tag{13a}$$
$$\underline{\varepsilon}(\mathbf{k})=\underline{\rho}^{-1}(\mathbf{k})\underline{W}(\mathbf{k})\underline{\rho}^{-1}(\mathbf{k})\ , \tag{13b}$$

Eq. (10) can be cast in the form

$$i\hbar\frac{\partial\underline{u}(\mathbf{k})}{\partial t}=\underline{\varepsilon}(\mathbf{k})\underline{u}(\mathbf{k})\ . \tag{13c}$$

According to Eqs. (11), (12), and (13b), the $G\times G$ matrix $\underline{\varepsilon}(\mathbf{k})$ is self-adjoint, and its diagonalization leads in general to G dispersion relations, from which the bands can be calculated. We stress that the number of bands can be smaller than G, due to the possibility of complex (or degenerate) bands.[7] This point will be reconsidered in the following.

From the properties (8) and from the definitions (9), the following rules can be shown to apply:

$$\Sigma_{\alpha\beta}(\mathbf{k})=P_\alpha P_\beta\Sigma_{\alpha\beta}(-\mathbf{k})\ ,$$
$$W_{\alpha\beta}(\mathbf{k})=P_\alpha P_\beta W_{\alpha\beta}(-\mathbf{k})\ , \tag{14}$$
$$\varepsilon_{\alpha\beta}(\mathbf{k})=P_\alpha P_\beta\varepsilon_{\alpha\beta}(-\mathbf{k})\ .$$

If the orbitals $\Psi_\alpha(\mathbf{r})$ are real, one has the following additional properties:

$$W_{\alpha\beta}(\mathbf{k})=\pm e^{i\theta}|W_{\alpha\beta}(\mathbf{k})|\ ,$$
$$\Sigma_{\alpha\beta}(\mathbf{k})=\pm e^{i\theta}|\Sigma_{\alpha\beta}(\mathbf{k})|\ , \tag{15}$$
$$\varepsilon_{\alpha\beta}(\mathbf{k})=\pm e^{i\theta}|\varepsilon_{\alpha\beta}(\mathbf{k})|\ ,$$
$$\theta=(P_\alpha P_\beta-1)(\pi/4)\ .$$

These last equations mean that the matrix elements indicated are real or pure imaginary, according to whether the orbitals have the same or opposite spatial parity. To show that (14) and (15) hold true for $W_{\alpha\beta}$ and $\Sigma_{\alpha\beta}$ is straightforward. Since, for any two nonsingular matrices satisfying (14) and (15), their product and their inverse satisfy too, the properties transfer to $\varepsilon_{\alpha\beta}$ identically, according to the definition (13b).

We stress that, up to now, the only approximation has been the LCAO expansion (4). Thus Eqs. (11) and (13) formally account for ionic interactions and overlap integrals at any nearest-neighbor order. This generalized LCAO approach provides a direct relationship between the orbitals (atomic or molecular) and the band structure, avoiding any intermediate procedure of orthogonalization, such as the introduction of Wannier functions, or the use of biorthonormal systems.[8] For our present purposes, we need only recall that the effective matrix Hamiltonian $\underline{\varepsilon}(\mathbf{k})$ in Eq. (13c) may give rise to zitterbewegung effects, because of interband transitions, as discussed in Sec. I. This will be explicitly shown in the case of two-band systems.

III. ZITTERBEWEGUNG IN TWO-BAND SYSTEMS

By specializing the preceding formulas to 2×2 matrices ($\alpha,\beta=1,2$), and by choosing real orbitals [Eqs. (15)], one can write

$$\underline{\varepsilon}(\mathbf{k})=E_0(\mathbf{k})\underline{I}+\underline{\Delta}(\mathbf{k})\ , \tag{16a}$$

where $\underline{I}$ is the identity, and

$$\underline{\Delta}(\mathbf{k})=\begin{bmatrix}\varepsilon_0(\mathbf{k}) & \varepsilon_1(\mathbf{k})e^{i\theta}\\ \varepsilon_1(\mathbf{k})e^{-i\theta} & -\varepsilon_0(\mathbf{k})\end{bmatrix}\ . \tag{16b}$$

From the properties (14) and (15), it follows that

$$\varepsilon_0(\mathbf{k})=\frac{[\varepsilon_{11}(\mathbf{k})-\varepsilon_{22}(\mathbf{k})]}{2}=\varepsilon_0(-\mathbf{k})\ ,$$
$$E_0(\mathbf{k})=\frac{[\varepsilon_{11}(\mathbf{k})+\varepsilon_{22}(\mathbf{k})]}{2}=E_0(-\mathbf{k})\ , \tag{16c}$$
$$\varepsilon_1(\mathbf{k})=\pm|\varepsilon_{12}(\mathbf{k})|=P_1P_2\varepsilon_1(-\mathbf{k})\ .$$

Since $\underline{\Delta}^2=(\varepsilon_0^2+\varepsilon_1^2)$, the diagonalization of $\underline{\varepsilon}(\mathbf{k})$ is trivial and leads to the following dispersion relations:

$$E_\pm(\mathbf{k})=E_0(\mathbf{k})\pm\Delta E(\mathbf{k})\ ,$$
$$\Delta E(\mathbf{k})=[\varepsilon_0^2(\mathbf{k})+\varepsilon_1^2(\mathbf{k})]^{1/2}\ , \tag{17a}$$

corresponding to the normalized eigenstates:

$$\underline{u}_+(\mathbf{k})=\frac{1}{(1+x^2)^{1/2}}\begin{bmatrix}1\\ xe^{i\theta}\end{bmatrix};$$
$$\underline{u}_-(\mathbf{k})=\frac{1}{(1+x^2)^{1/2}}\begin{bmatrix}xe^{-i\theta}\\ 1\end{bmatrix}, \tag{17b}$$
$$x(\mathbf{k})=\frac{\Delta E(\mathbf{k})-\varepsilon_0(\mathbf{k})}{\varepsilon_1(\mathbf{k})}\ .$$

We can now calculate the zitterbewegung operator $\underline{\mathbf{Z}}(\mathbf{k})$ following the method in Refs. 1 and 2 (or the alternative approach developed in Ref. 9). From the motion equation in the Heisenberg form, $dA/dt=(i/\hbar)[H,A]$, Eqs. (16) yield

$$\frac{d^2\underline{\mathbf{r}}}{dt^2}=\frac{d\underline{\mathbf{v}}_z}{dt}=\frac{2i}{\hbar}\underline{\Delta}\,\underline{\mathbf{v}}_z\ , \tag{18a}$$

$$\underline{\mathbf{v}}_z=\frac{(\varepsilon_0\mathrm{grad}_{\mathbf{k}}\varepsilon_1-\varepsilon_1\mathrm{grad}_{\mathbf{k}}\varepsilon_0)}{\hbar\Delta E^2}\underline{\Delta}^x\begin{bmatrix}0 & ie^{i\theta}\\ -e^{-i\theta} & 0\end{bmatrix} \tag{18b}$$

for the self-acceleration. Integrating the first Eq. (18a) by means of the second one, and subtracting the part of $\underline{\mathbf{r}}(t)$ proportional to the time, one gets the zitterbewegung component of the position, in the explicit form

$$\underline{\mathbf{Z}}(\mathbf{k})=\frac{\varepsilon_1(\mathbf{k})\mathrm{grad}_{\mathbf{k}}\varepsilon_0(\mathbf{k})-\varepsilon_0(\mathbf{k})\mathrm{grad}_{\mathbf{k}}\varepsilon_1(\mathbf{k})}{2\Delta E^2(\mathbf{k})}\begin{bmatrix}0 & ie^{i\theta}\\ -ie^{-i\theta} & 0\end{bmatrix}, \tag{19}$$

following from Eq. (18b).

IV. EFFECTS OF THE INTERBAND ZITTERBEWEGUNG ON SINGLE-BAND SOLUTIONS

We now consider wave functions $|\Psi_\pm\rangle$ formed only by eigenstates $\underline{u}_\pm(\mathbf{k})$ [Eq. (17b)] belonging to a single band [Eq. (17a)]. As far as the zitterbewegung is concerned, these wave functions are equivalent to the positive- and negative-energy states in relativistic quantum dynamics. In the k representation, one gets

$$\begin{aligned}&\langle\mathbf{k}|\Psi_\pm\rangle=f_\pm(\mathbf{k})\underline{u}_\pm(\mathbf{k});\quad \mathbf{k}\in\Omega_1\ ,\\ &\int_{\Omega_1}|f_\pm(\mathbf{k})|^2d\mathbf{k}=1\ ,\end{aligned} \tag{20}$$

in terms of the probability amplitude $f_\pm(\mathbf{k})$ in the first Brillouin zone Ω_1. A straightforward calculation, based on Eqs. (17) and (19), yields

$$\begin{aligned}\langle\Psi_\pm|\mathbf{r}|\Psi_\pm\rangle&=i\langle\Psi_\pm|\mathrm{grad}_{\mathbf{k}}|\Psi_\pm\rangle\\ &=\int_{\Omega_1}f_\pm^*(\mathbf{k})[i\,\mathrm{grad}_{\mathbf{k}}f_\pm(\mathbf{k})]d\mathbf{k}\\ &\equiv\langle\mathbf{r}_{\mathrm{st}}\rangle\ ,\end{aligned} \tag{21a}$$

where the subscript "st" indicates the standard expression of the mean position operator, without zitterbewegung. Equation (21a) shows a general property of the zitterbewegung, i.e., that it averages out to zero for any positive- or negative-energy solution.[10] In contrast, it can be shown that (see also Ref. 11)

$$\begin{aligned}\langle\Psi_\pm|\mathbf{r}^2|\Psi_\pm\rangle&=\int_{\Omega_1}d\mathbf{k}[-f_\pm^*(\nabla_{\mathbf{k}}^2f_\pm)+\mathbf{Z}^2(\mathbf{k})|f_\pm|^2]\\ &\equiv\langle\mathbf{r}_{\mathrm{st}}^2\rangle+\langle\mathbf{Z}^2\rangle\ ,\end{aligned} \tag{21b}$$

where

$$\mathbf{Z}^2(\mathbf{k})=\frac{[\varepsilon_0(\mathbf{k})\mathrm{grad}_{\mathbf{k}}\varepsilon_1(\mathbf{k})-\varepsilon_1(\mathbf{k})\mathrm{grad}_{\mathbf{k}}\varepsilon_0(\mathbf{k})]^2}{4\Delta E^4(\mathbf{k})} \tag{22}$$

is just the square zitterbewegung operator given by Eq. (19) with the aid of (17a). From Eq. (21b), the root-mean-square deviation of the position reads

$$\delta r=(\delta r_{\mathrm{st}}^2+\langle\mathbf{Z}^2\rangle)^{1/2}\ , \tag{23}$$

showing that the localization length of a wave function, formed by superimposing Bloch solutions of a single band, is determined not only by the Heisenberg principle, but also by the interband zitterbewegung. From Eq. (21b) it follows also that $\langle\mathbf{Z}^2\rangle$ does not depend on time, since the time dependence of $f_\pm$ results in the phase factor $\exp(-iE_\pm t/h)$. For sufficiently long times, the spreading effect on δr_{st} will then dominate in the freely evolving packet. A formal aspect deserving attention is that minimizing the functional (21b) with respect to $f_\pm$ is equivalent to solving the time-independent Schrödinger equation:

$$-\nabla_{\mathbf{k}}^2f_\lambda(\mathbf{k})+\mathbf{Z}^2(\mathbf{k})f_\lambda(\mathbf{k})=\lambda^2f_\lambda(\mathbf{k}) \tag{24}$$

in the k space, where $\mathbf{Z}^2(\mathbf{k})$ plays the role of a "potential." Since $\mathbf{Z}^2(\mathbf{k})=\mathbf{Z}^2(-\mathbf{k})$ [Eqs. (22) and (16c)], the eigensolutions f_λ can be chosen with a definite parity in $\mathbf{k}$. In this case $\langle\mathbf{r}_{\mathrm{st}}\rangle=0$ [Eq. (21a)], and solving Eq. (24) is also equivalent to minimizing the root-mean-square deviation (23). We now apply the preceding method to estimate the minimum localization length δr_m of a wave packet formed by Bloch functions of a single band. From Eqs. (22) and (16c), it follows that in the case (a),

$$P_1=P_2 \tag{25}$$

(orbitals with the same parity), $\mathbf{Z}^2(\mathbf{k})$ has a minimum in $\mathbf{k}=0$, since $\mathbf{Z}^2(0)=0$. It is possible that $\mathbf{Z}^2$ does vanish in other points of Ω_1, and especially at the boundary, as suggested by the one-dimensional example of Fig. 1. Thus the solution of Eq. (24) (with f_λ vanishing at the surface of Ω_1) is far from trivial. However, the order of magnitude of the minimum eigenvalue λ^2 can be estimated as given by the ground state of the potential well around

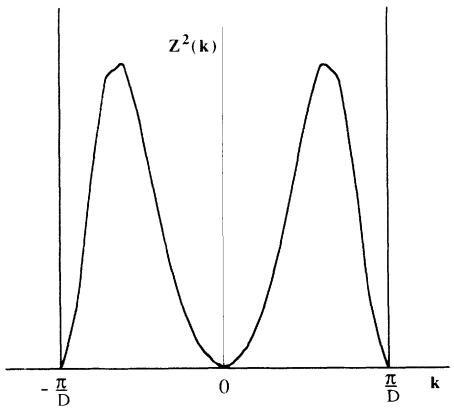

FIG. 1. The square zitterbewegung operator is plotted in arbitrary units against the wave vector k for a one-dimensional system of class (a) (orbitals with the same parity), in the tight-binding, first-nearest-neighbor approximation. Note the parabolic minimum in $k=0$. For further details, see the Appendix.

$\mathbf{k}=0$, in the harmonic approximation. From Eqs. (22) and (16c), one has, to the lowest order in $\mathbf{k}$,

$$\mathbf{Z}^2(\mathbf{k}) \cong \sum_{\eta,\nu,\sigma} \Lambda_{\eta\sigma}\Lambda_{\sigma\nu}k_\eta k_\nu \ , \qquad \Lambda_{\eta\nu}=\left[\frac{\varepsilon_0(\partial_{\eta\nu}\varepsilon_1)-\varepsilon_1(\partial_{\eta\nu}\varepsilon_0)}{2\Delta E^2}\right]_{\mathbf{k}=0} , \tag{26}$$

where k_η ($\eta=1$, 2, and 3) are Cartesian components of $\mathbf{k}$ and $\partial_{\eta\nu}=\partial^2/\partial k_\eta \partial k_\nu$. From the third relation (9) one has, in addition,

$$(\partial_{\eta\nu}W_{\alpha\beta})_{\mathbf{k}=0}=-\sum_n R_{n\eta}R_{n\nu}V_{\alpha\beta}(\mathbf{R}_n) \ , \tag{27}$$

where $R_{n\eta}$ is the ηth component of the lattice vector $\mathbf{R}_n$. In the TB approximation [for which the LCAO expansion (4) is particularly appropriate], let us neglect the overlap integrals and thereby set $\underline{S}(\mathbf{k})\cong\underline{\rho}(\mathbf{k})\cong\underline{I}$, $\underline{\varepsilon}(\mathbf{k})\cong\underline{W}(\mathbf{k})$ [recall Eqs. (12) and (13)]. From Eqs. (16c) it follows that

$$\varepsilon_0(0)\cong-\tfrac{1}{2}\sum_n[V_{11}(\mathbf{R}_n)-V_{22}(\mathbf{R}_n)] \equiv-\tfrac{1}{2}\sum_n \Delta V(\mathbf{R}_N) \ ,$$

$$\varepsilon_1(0)\cong\sum_n V_{12}(\mathbf{R}_n) \ .$$

Thus, from Eq. (27),

$$\Lambda_{\eta\nu}\cong\frac{\sum_{n,j} R_{n\eta}R_{n\nu}[\Delta V(\mathbf{R}_n)V_{12}(\mathbf{R}_j)-\Delta V(\mathbf{R}_j)V_{12}(\mathbf{R}_n)]}{\sum_{n,j}[\Delta V(\mathbf{R}_n)\Delta V(\mathbf{R}_j)+4V_{12}(\mathbf{R}_n)V_{12}(\mathbf{R}_j)]} \ . \tag{28}$$

In the TB approximation, $\Delta V(\mathbf{R}_n)$ and $V_{12}(\mathbf{R}_n)$ vanish exponentially with increasing $|\mathbf{R}_n|$. Hence, in the first nearest-neighbors approximation, the leading term in Eq. (28) becomes

$$\Lambda_{\eta\nu}\cong\frac{\Delta V(\mathbf{D})V_{12}(0)-\Delta V(0)V_{12}(\mathbf{D})}{[\Delta V(0)+\Delta V(\mathbf{D})]^2+4[V_{12}(0)+V_{12}(\mathbf{D})]^2} \times D_\eta D_\nu+\cdots \ , \tag{29a}$$

where $\mathbf{D}$ is the basic lattice vector. By using Eqs. (26) in Eq. (24), δr_m turns out to be given by the square root of the only nonvanishing eigenvalue of the matrix (29a):

$$\delta r_m\cong|\mathbf{D}|\left|\frac{\Delta V(\mathbf{D})V_{12}(0)-\Delta V(0)V_{12}(\mathbf{D})}{[\Delta V(0)+\Delta V(\mathbf{D})]^2+4[V_{12}(0)+V_{12}(\mathbf{D})]^2}\right|^{1/2} . \tag{29b}$$

In fact, matrices in the form (29a) have zero eigenvalue in the subspace orthogonal to the vector $\mathbf{D}$. In the case (b),

$$P_1=-P_2 \tag{30}$$

(orbitals with opposite parity), Eqs. (22) and (16c) lead one to conclude that $\mathbf{k}=0$ corresponds either to a maximum or to a minimum of $\mathbf{Z}^2(\mathbf{k})$, because

$$\mathbf{Z}^2(0)=\sum_\eta\left[\frac{\partial\eta\varepsilon_1}{2\varepsilon_0}\right]^2_{\mathbf{k}=0} \tag{31}$$

is nonzero [unless the odd function $\varepsilon_1(\mathbf{k})$ has vanishing gradient in $\mathbf{k}=0$]. As sketched in the one-dimensional examples of Fig. 2, the behavior of $\mathbf{Z}^2(\mathbf{k})$ may be rather complicated in the case (b) [Eq. (30)], and the preceding method to estimate δr_m is not as suitable as in the case (a) [Eq. (25)]. However, if $\mathbf{Z}^2(0)$ is the absolute minimum in Ω_1 [Fig. 2(a)], Eq. (31) already provides a lower limit to δr_m. If $\mathbf{Z}^2(0)$ is a maximum [Fig. 2(b)], its value corresponds to the height of the "potential" barrier spanning the absolute minima. In this second case, it is perhaps more interesting to study the diverging behavior of the barrier when $\varepsilon_0(0)$ vanishes [Eq. (31)]. Since

$$E_{\text{gap}}(\mathbf{k})=2\Delta E(\mathbf{k}) \tag{32}$$

is the gapwidth [see Eqs. (17)] as a function of $\mathbf{k}$, and since $\varepsilon_1(0)$ vanishes in the case (30), the next calculations will illustrate the effects of the zitterbewegung when the gap in $\mathbf{k}=0$ vanishes, leading the two band to transform into a single degenerate band.[7] In the case (b), [Eq. (30)],

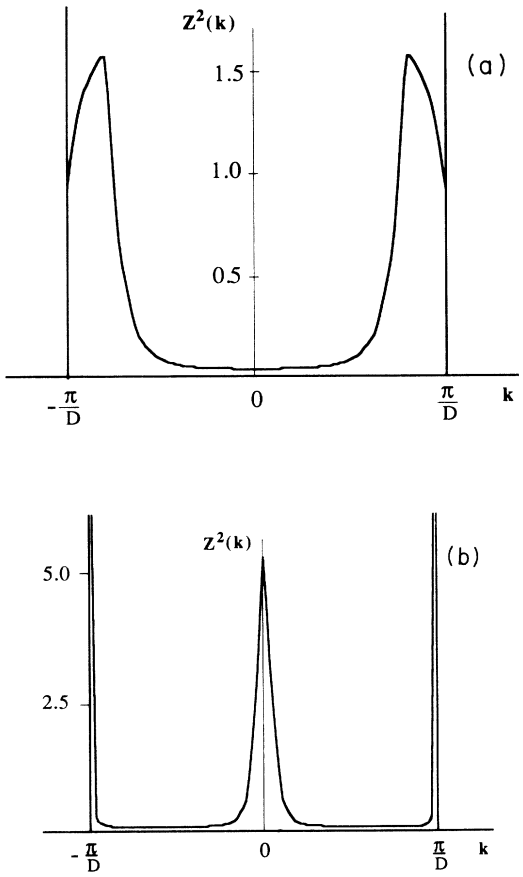

FIG. 2. The square zitterbewegung operator is plotted in units of the square lattice vector D^2 against the wave vector k for a one-dimensional system of class (b) (orbitals with opposite parity), in the same approximations as in Fig. 1. (a) The case of gap and bandwidth comparable in $k=0$. (b) A gap small compared with the bandwidth (see also the Appendix).

Eqs. (16c) yield, to the lower orders in $\mathbf{k}$,

$$\varepsilon_0 \cong \varepsilon_0(0) + \tfrac{1}{2} \sum_{\eta\nu} k_\beta k_\nu (\partial_{\eta\nu}\varepsilon_0)_{\mathbf{k}=0} ,$$
$$\varepsilon_1 \cong \sum_\eta k_\eta (\partial_\eta \varepsilon_1)_{\mathbf{k}=0} . \tag{33}$$

In the limit of small $\varepsilon_0(0)$, one may assume $|\partial_\eta\varepsilon_1\partial_\nu\varepsilon_1| \gg |\varepsilon_0\partial_{\eta\nu}\varepsilon_0|$ in $\mathbf{k}=0$. This condition and the two expressions (33) can be used in Eq. (22) to obtain the leading term of $\mathbf{Z}^2(\mathbf{k})$:

$$\mathbf{Z}^2(\mathbf{k}) \cong \frac{\varepsilon_0^2(0) \sum_\eta (\partial_\eta \varepsilon_1)^2_{\mathbf{k}=0}}{4\left[\varepsilon_0^2(0) + \sum_{\eta\nu} k_\eta k_\nu (\partial_\eta\varepsilon_1 \partial_\nu \varepsilon_1)_{\mathbf{k}=0}\right]^2}$$
$$= \frac{\varepsilon_0^2(0)(\mathrm{grad}_{\mathbf{k}}\varepsilon_1)_0^2}{4[\varepsilon_0^2(0) + k_\parallel^2 (\mathrm{grad}_{\mathbf{k}}\varepsilon_1)_0^2]^2} , \tag{34a}$$

where the subscript "0" means that the gradient of $\varepsilon_1(\mathbf{k})$ (with components $\partial_\eta\varepsilon_1$) is calculated in $\mathbf{k}=0$, and $k_\parallel$ is the projection of $\mathbf{k}$ on the gradient itself. By considering the integral $\int \mathbf{Z}^2(\mathbf{k}) F(\mathbf{k}) d\mathbf{k}$ in a finite region around the origin, for any regular function F, in the limit $\varepsilon_0(0) \to 0$, one gets from Eq. (34a) the following:

$$\mathbf{Z}^2(\mathbf{k}) \to |k_\parallel|^{-1} \delta(k_\parallel) \quad \text{for } \varepsilon_0(0) \to 0 . \tag{34b}$$

In fact,

$$\mathbf{Z}^2(\mathbf{k}) \cong \begin{cases} \mathbf{Z}^2(0) & \text{for } k_\parallel^2 \le \dfrac{1}{\mathbf{Z}^2(0)} , \\ \dfrac{1}{k_\parallel^4 \mathbf{Z}^2(0)} & \text{for } k_\parallel^2 \gg \dfrac{1}{\mathbf{Z}^2(0)} , \end{cases} \tag{34c}$$

with $\mathbf{Z}^2(0)$ given by Eq. (31). Of course, the first condition on $k_\parallel$ in Eq. (34c) refers only to the order of magnitude. By means of Eqs. (34b) and (34c), it can be shown that for small but *finite* $\varepsilon_0(0)$, Eq. (21b) yields

$$\langle \mathbf{Z}^2 \rangle \cong \frac{\pi}{2} |\mathbf{Z}(0)| \int |f_\pm(0, \mathbf{k}_\perp)|^2 d\mathbf{k}_\perp , \tag{35}$$

where the wave vector $\mathbf{k}$ has been expressed as $(k_\parallel, \mathbf{k}_\perp)$, in the components parallel and perpendicular to $(\mathrm{grad}_{\mathbf{k}}\varepsilon_1)_0$. Setting $k_\parallel = 0$ in Eq. (35) is justified if $f_\pm(\mathbf{k})$ is smooth around the origin in a region of order $|\mathbf{Z}(0)|^{-1}$. In particular, from Eqs. (23) and (35), it follows that

$$\delta r^2 \cong \langle \mathbf{Z}^2 \rangle \cong \frac{|\mathbf{Z}(0)|}{k_M} \frac{3\pi}{8} , \tag{36}$$

for any spherical wave packet, localized in k space around the origin, in a region of order $k_M \gg 1/|\mathbf{Z}(0)|$ (this result is independent of the dimensionality of $\mathbf{k}$, apart from a factor).

V. APPLICATIONS

The results obtained in the preceding sections can be regarded as a formal relationship between the crystal band structure [as given by $\varepsilon_0(\mathbf{k})$ and $\varepsilon_1(\mathbf{k})$] and the localization length of states originated by a single band. In the case (a) [Eq. (25)] of orbitals with the same parity, the zitterbewegung "potential" $\mathbf{Z}^2(\mathbf{k})$ in Eq. (24) is parabolically attractive in the origin [Eqs. (26)], and the minimum localization length δr_m can be estimated according to Eq. (29b).

In the case (b) [Eq. (30)] of opposite-parity orbitals [including many semiconducting systems, whose highest bands are formed by bonding (even) and antibonding (odd) orbitals], the zitterbewegung "potential" $\mathbf{Z}^2(\mathbf{k})$ is divergingly repulsive around the origin, at least for vanishing $E_{\mathrm{gap}}(0) = |\varepsilon_0(0)|$ [Eqs. (34)]. In this case Eq. (36) provides an estimate for the localization length of wave packets centered around $\mathbf{k}=0$, with spatial extension $1/k_M$. We are particularly interested in this class of functions, because they include the ground state of most defect spectra. Since $\mathbf{k}$ is limited to the first Brillouin zone, for the minimum localization length of these states, one has

$$\delta r_m^2 \cong |\mathbf{D}|\,|\mathbf{Z}(0)| = \frac{|\mathrm{grad}_{\mathbf{k}}\varepsilon_1|_0}{2E_{\mathrm{gap}}(0)} |\mathbf{D}| , \tag{37a}$$

where $|\mathbf{D}|$ is the basic lattice vector. Equation (37a) shows that δr_m decreases as the inverse square root of the gap. This result has a fairly transparent interpretation. Since δr_m is the minimum localization length for a superposition of single-band Bloch functions, one expects that E_{gap} corresponds to the maximum binding energy of a possible bound state; i.e.,

$$E_{\mathrm{gap}}(0) = \frac{\hbar^2}{2M_{\mathrm{eff}} \delta r_m^2} , \tag{37b}$$

as obtained by applying the Heisenberg principle to a suitably defined particle of effective mass M_{eff}. This evaluation of the binding energy is rigorous if the bound state is hydrogenlike. According to this interpretation, Eqs. (37a) and (37b) provide a definition of the effective mass:

$$M_{\mathrm{eff}} = \frac{\hbar^2}{|\mathrm{grad}_{\mathbf{k}}\varepsilon_1|_0 |\mathbf{D}|} , \tag{37c}$$

for the deepest acceptor/donor state in the gap of the two-band system. For shallow states, in contrast, Kohn's theory predicts the same effective mass as the Bloch states in each band.[12]

A further application of Eqs. (37) is to estimate the tails of localized states[13] in a disordered semiconductor [of class (b)], under Mott's hypothesis of sharp mobility edges E_v, E_c in the valence and conduction band, respectively.[14] By definition, the gap width E_{gap} entering Eq. (37a) separates extended states. If we consider crystals, such that $E_{\mathrm{gap}}(\mathbf{k})$ has a minimum in $\mathbf{k}=0$, we expect that in the glassy phase the gap $E_{\mathrm{gap}}(0)$ spanning the extended states is measured by the distance between the mobility edges [if $E_{\mathrm{gap}}(0)$ were not a minimum, its value would include, totally or in part, the bandwidth of the extended states]. Then we assume that

$$E_{\mathrm{gap}}(0) = E_c - E_v . \tag{38}$$

For the localization length $\lambda_\xi(E)$ of a state with energy E in the gap ($\xi = v, c$ indicates the band which the state

originates from), the following expression is currently assumed:[15]

$$\lambda_\xi(E)=B_\xi/|E-E_\xi| \ , \tag{39}$$

the B_ξ's being phenomenological constants. According to the present results, two energies $E_{1\xi}(\xi=v,c)$ will exist, such that $\lambda_\xi(E_{1\xi})=\delta r_m$. The quantity $|E_{1\xi}-E_\xi|$ now represents the width of the ξ tail in the gap and can be calculated by using Eqs. (38) and (39) in Eq. (37a), with the result that

$$|E_{1\xi}-E_\xi|=\frac{B_\xi}{\hbar}\sqrt{2M_{\rm eff}(E_c-E_v)} \ , \tag{40a}$$

$M_{\rm eff}$ being given by Eq. (37c). Another quantity of interest, in view of a Mott metal-insulator transition, can be calculated from Eq. (40a):

$$E_{1c}-E_{1v}=(E_c-E_v)^{1/2} \times\left[(E_c-E_v)^{1/2}-\frac{(B_c+B_v)\sqrt{2M_{\rm eff}}}{\hbar}\right] , \tag{40b}$$

i.e., the distance between the lower edge E_{1c} of the tail originating from the conduction band and the higher edge E_{1v} of the tail originating from the valence band. The transition of the quantity (40b) from positive to negative values, occurring at a certain critical value of E_c-E_v, marks the onset of the overlap between the tails of localized states, and thus the onset of the metal-insulator transition *à la* Mott.

VI. CONCLUSIONS

In the present paper the notion of zitterbewegung and the resulting formalism, originally proposed for relativistic quantum dynamics,[1,2] have been applied to the interband transition in a crystal. A generalized LCAO approach has been developed for the band calculations, including ionic interactions and overlap integrals at any nearest-neighbor order. Since any intermediate process of orthogonalization has been avoided, the connection between band-structure and LCAO orbitals is straightforward. In particular, we have shown that the parity of the orbitals has important effects on the interband zitterbewegung at small wave vectors. We have studied in detail two-band systems of class (b), i.e., formed by two orbitals with opposite parity [the case (a) of orbitals with the same parity is formally more complicated and, perhaps, less interesting for practical applications]. The main result stands in the formal expression of a fairly simple idea, i.e., that donor/acceptor states can be more sharply localized in a large gap, than in a small one. However, to express this relationship in a quantitative way is not as simple. While setting $E_{\rm gap}\cong\hbar^2/(2M_{\rm eff}\lambda_m^2)$ may look a natural choice, what effective mass $M_{\rm eff}$ is appropriate to determine the minimum localization length λ_m, is a nontrivial question, which we have tried to answer [Eqs. (37)]. The resulting definition of effective mass, valid for deep defect levels, should be of some utility, especially for small-gap semiconductors, in which the distinction between shallow and deep defect states tends to vanish.

A further application of the preceding results has been considered for the tails of localized states in disordered semiconductors. Following Mott's theory of the mobility edges,[14] it has been argued that such tails are limited by two cutoff values of the energy, depending on the difference E_c-E_v of the mobility edges [Eq. (40a)]. The overlap of the two tails is also shown to depend on E_c-E_v [Eq. (40b)]; so that in systems displaying a Mott (metal-insulator) transition, the decrease of the gap between the extended states is now expected to play a crucial role. This agrees with the argument that, even in crystalline systems, zitterbewegung effects (favoring delocalization) are relevant if a metal-insulator transition occurs, from a two-band to a single degenerate-band structure,[7] as remarked in Sec. IV. A special case of this behavior has been studied in Ref. 3 as the "ultrarelativistic" limit of a Dirac-like wave equation.

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APPENDIX

In this Appendix we calculate the zitterbewegung "potential" $\mathbf{Z}^2(\mathbf{k})$ [Eq. (22)] in the one-dimensional case, with a tight-binding, first-nearest-neighbor approximation, so that the overlap-integral matrix given by Eq. (2) becomes

$$\underline{S}(\mathbf{R}_n-\mathbf{R}_j)=\underline{I}\delta_{n,j} \ , \tag{A1}$$

and the Hamiltonian matrix given by Eq. (6) becomes, in turn

$$\underline{V}(\mathbf{R}_n-\mathbf{R}_j)=\underline{V}(0)\delta_{n,j}+\underline{V}(D)\delta_{n+1,j}+\underline{V}(-D)\delta_{n-1,j} \ , \tag{A2}$$

where D is the distance between first-nearest-neighbor sites on the one-dimensional lattice. By means of Eqs. (A1) and (A2), one can invert Eq. (9) and write

$$\underline{\varepsilon}(k)=\underline{W}(k)=\underline{V}(0)+\underline{V}(D)e^{ikD}+\underline{V}(-D)e^{-ikD} \ , \tag{A3}$$

according to the definitions (12) and (13b). From Eqs. (A3) and (16), the general structure of the matrix $\underline{\Delta}$ can be found as

$$\varepsilon_j(k)=\alpha_j+\beta_j\cos kD \quad (j=0,1) \ , \tag{A4a}$$

in the case (a) of orbitals with the same parity. In contrast, the same calculation yields

$$\varepsilon_0(k)=\alpha_0+\beta_0\cos kD \ , \qquad \varepsilon_1(k)=\beta_1\sin kD \ , \tag{A4b}$$

in the case (b) of orbitals with opposite parity. The definitions (22) and (17a) can now be applied to Eqs. (A4a) and (A4b), to obtain

$$Z^2(k)=\frac{(\alpha_0\beta_1-\alpha_1\beta_0)^2\sin^2(kD)}{[(\alpha_0+\beta_0\cos kD)^2+(\alpha_1+\beta_1\cos kD)^2]^2}\frac{D^2}{4} \tag{A5a}$$

in the case (a), and

$$Z^2(k)=\frac{\beta_1^2(\beta_0+\alpha_0\cos kD)^2}{[(\alpha_0+\beta_0\cos kD)^2+\beta_1^2\sin^2(kD)]^2}\frac{D^2}{4} \tag{A5b}$$

in the case (b). Equation (A5a) has been used for Fig. 1 with $\alpha_0=0.5$, $\beta_0=0.2$, $\alpha_1=0.6$, $\beta_1=0.1$ (arbitrary units). Equation (A5b) has been used for Fig. 2(a), with $\alpha_0/\beta_1=2$, $\beta_0/\beta_1=2.5$ (gap and bandwidth comparable at $k=0$), and for Fig. 2(b), with $\alpha_0/\beta_1=0.12$, $\beta_0/\beta_1=0.10$ (gap small compared with the bandwidth at $k=0$). In the last case, the value in $k=\pm\pi/D$ is 625, in units of D^2. This is the reason for the apparent divergence at the boundaries in Fig. 2(b).

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