Exact solutions for a quasi-one-dimensional Coulomb-type potential

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(Received 12 December 1990)

We present a quasi-one-dimensional model with a Coulomb-type perturbation defined on a discrete lattice that can be reduced to an exactly solvable Hamiltonian in the case of a narrow-band system. Due to the long-range character of the perturbation potential, a series of infinitely many discrete levels appears in the band gap of the host crystal. Although the physical situation is completely different, a close mathematical analogy with the so-called Stark-ladder problem is shown to exist. In this context, we give a canonical transformation that allows a simple and elegant derivation of the Stark-ladder levels.
MS code no. BZ4206 1990 PACS number(s): 73.20.Dx, 03.65.Ge

I. INTRODUCTION

The influence of perturbation potentials on the electronic structure in otherwise perfectly ordered crystals has been the object of numerous theoretical investigations in the past. The characteristic properties of the perturbations discussed in the literature are spread as wide as solid-state physics itself. Namely, charge impurities and external fields, structural defects, superlattices, quasiperiodic, and randomly fluctuating potentials (this list is by far not exhaustive) gave reason to detailed analysis.

Focusing our interest to the first group of perturbations cited above (charge impurities), we mention some particularly successful theoretical models: the theory of shallow impurity states in semiconductors based on the effective-mass approximation,[1] the Stark-ladder states in the presence of an external electric field,[2,3] the so-called one-band–one-site approximation,[4] and the Fano problem.[5] Wagner and Vazquez-Marquez[6] recently reviewed some exactly solvable models related to those of Refs. 4 and 5. Ifantis[7] discussed exact solutions of a one-dimensional (1D) one-sided Coulomb potential embedded in a host crystal with a maximally simplified band structure (one-band approximation with a cosine dispersion).

In this work we discuss a quasi-1D model that is reducible to an analytically diagonalizable Hamiltonian in the case of a narrow-energy-band system (one-band approximation). Its predominant feature is the generalization of Ifantis's results to a band with *arbitrary* energy dispersion. The perturbation consists of a one-sided (dielectrically screened) Coulomb potential and refers most naturally to the following physical realization: A point charge is placed at one end of a half-infinite 1D isolating crystal. Due to the dielectric nature of the host crystal, the perturbation is of long-range type and completely alters the unperturbed electronic structure.

The paper is organized as follows. In Sec. II we introduce an artificial potential which is identical to the one-sided (repulsive) Coulomb potential described above for lattice sites with positive site index n. For negative n we prolong the potential *antisymmetrically,* i.e., in the vicinity of $n=0$, the potential changes abruptly from an attractive to a repulsive Coulomb potential.

In the case of a crystal with narrow energy bands the total Hamiltonian corresponding to a particular energy band and the artificial potential is exactly diagonalized in Sec. III.

Section IV is entirely devoted to the calculation of the Green's function associated with the model Hamiltonian. We completely characterize the discrete spectrum and demonstrate, by calculating explicitly the density of states, the existence of extended states.

We draw the reader's attention to the fact that in Secs. II, III, and IV we formulate the problem in three dimensions with the artificial potential acting only in one specific direction and leaving the transverse directions unaffected. This 3D generalization does not touch the essence of the article and it hardly complicates the mathematical analysis. However, it will enable us to compare the solutions of our model with the 3D Stark-ladder representation (see Sec. VI).

In Sec. V we reduce the main results to the purely 1D case and treat in detail a particular unperturbed energy band (cosine band). We rederive the results of Ifantis,[7] who analyzed this simplified model by means of classical functional analysis.

Finally, in Sec. VI we show a close mathematical analogy between our Coulomb-type eigenstates and the Stark-ladder levels arising when an electric field is applied to the solid. As a matter of fact, it will be demonstrated that the Stark-ladder eigenstates can be derived following step by step the calculations in Secs. II and III. It is to be emphasized that the two models in discussion are the only ones allowing an exact and algebraic diagonalization of a zero-order energy band with *general* dispersion perturbed by "long-range" potentials.

As an alternative way to diagonalize the Stark-ladder Hamiltonian, we present a simple canonical transformation that has (to our knowledge) not been reported on before.

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II. HAMILTONIAN

The single-particle Hamiltonian of our 3D model reads

$$H = H^0 + V_{\text{ext}}(\mathbf{r}) ,$$
$$H^0 = -\frac{\hbar^2\nabla^2}{2m_e} + V_L(\mathbf{r}) , \tag{2.1}$$
$$V_{\text{ext}}(\mathbf{r}) = \frac{\alpha c}{r_3 - r_3^0} ,$$

where m_e is the electronic mass in the vacuum and $V_L(\mathbf{r})$ is the periodic 3D lattice potential, i.e., $V_L(\mathbf{r}+\boldsymbol{\rho}) = V_L(\mathbf{r})$ with $\boldsymbol{\rho} = l\mathbf{a} + m\mathbf{b} + n\mathbf{c}$. $\mathbf{a},\mathbf{b},\mathbf{c}$ are the primitive lattice vectors (we suppose for simplicity that the host crystal has orthorhombic symmetry) of length a,b,c, respectively, and l,m,n range through all integral values. The quasi-1D artificial Coulomb-type perturbation $V_{\text{ext}}(\mathbf{r})$ acts only in the $\mathbf{c}$ direction ($r_3 = \mathbf{r}\cdot\mathbf{c}/c$) and changes abruptly from an attractive to a repulsive "Coulomb" potential at the plane $r_3 = r_3^0$. $\alpha > 0$ is a constant measuring the strength of $V_{\text{ext}}(\mathbf{r})$.

The wave functions may be expanded in the Bloch base associated with H^0 as follows:

$$|\Phi(E)\rangle = \sum_{\mathbf{k},\lambda} \xi_{\mathbf{k}}^{\lambda}(E)|\mathbf{k}\lambda\rangle , \tag{2.2}$$

where E is the exact eigenenergy and $|\mathbf{k}\lambda\rangle$ is the Bloch state with band index λ and wave vector $\mathbf{k}$ associated with the energy band $\varepsilon_{\mathbf{k}}^{\lambda}$. Introducing the expansion of the wave function into the Schrödinger equation we get

$$(E - \varepsilon_{\mathbf{k}}^{\lambda})\xi_{\mathbf{k}}^{\lambda}(E) = \sum_{\mathbf{k}',\lambda'} W_{\mathbf{k}\mathbf{k}'}^{\lambda\lambda'} \xi_{\mathbf{k}'}^{\lambda'}(E) , \tag{2.3}$$

with

$$W_{\mathbf{k}\mathbf{k}'}^{\lambda\lambda'} = \langle \mathbf{k}\lambda | V_{\text{ext}} | \mathbf{k}'\lambda' \rangle . \tag{2.4}$$

Since $V_{\text{ext}}(\mathbf{r})$ leaves the degrees of freedom perpendicular to the $\mathbf{c}$ direction unaffected, Bloch states with $\mathbf{k}_\perp \neq \mathbf{k}'_\perp$ are uncoupled. Here we used the abbreviation $\mathbf{k} = (\mathbf{k}_\perp, k_3)$ with $\mathbf{k}_\perp = \mathbf{k}\cdot\mathbf{a}/a + \mathbf{k}\cdot\mathbf{b}/b$ and $k_3 = \mathbf{k}\cdot\mathbf{c}/c$. For *narrow* energy bands the Schrödinger equation (2.3) can be reduced to an exactly solvable problem that has, to our knowledge, not been discussed before. To illuminate the approximation involved we introduce the Wannier functions (WF's)

$$\varphi^{\lambda}(\mathbf{r} - \boldsymbol{\rho}) = N^{-3/2} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\boldsymbol{\rho}} \langle \mathbf{r} | \mathbf{k}\lambda \rangle \tag{2.5}$$

associated with the lattice site $\boldsymbol{\rho}$ and the band λ (N^3 is the total number of lattice sites). We get for the kernel of the eigenvalue equation

$$W_{\mathbf{k}\mathbf{k}'}^{\lambda\lambda'} = N^{-3} \sum_{\boldsymbol{\rho},\boldsymbol{\rho}'} e^{i(\mathbf{k}'\cdot\boldsymbol{\rho}' - \mathbf{k}\cdot\boldsymbol{\rho})} \int d^3r\, \varphi^{\lambda}(\mathbf{r} - \boldsymbol{\rho})^* \frac{\alpha c}{r_3 - r_3^0} \times \varphi^{\lambda'}(\mathbf{r} - \boldsymbol{\rho}') . \tag{2.6}$$

In the case of narrow energy bands the WF's are strongly localized and the one-site terms with $\boldsymbol{\rho} = \boldsymbol{\rho}'$ dominate. Therefore we set

$$\varphi^{\lambda}(\mathbf{r} - \boldsymbol{\rho})^* \frac{\alpha c}{r_3 - r_3^0} \varphi^{\lambda'}(\mathbf{r} - \boldsymbol{\rho}') \approx \delta_{\boldsymbol{\rho}\boldsymbol{\rho}'} \varphi^{\lambda}(\mathbf{r} - \boldsymbol{\rho})^* \frac{\alpha c}{\rho_3 - r_3^0} \varphi^{\lambda'}(\mathbf{r} - \boldsymbol{\rho}) . \tag{2.7}$$

Note that this approximation automatically inhibits band mixing. The dominant part of the kernel reads

$$W_{\mathbf{k}\mathbf{k}'}^{\lambda\lambda'} = \delta_{\lambda\lambda'} \delta_{\mathbf{k}_\perp \mathbf{k}'_\perp} W(k_3 - k'_3) , \tag{2.8}$$

with

$$W(k_3 - k'_3) = \frac{\alpha}{N} \sum_n \frac{e^{-i(k_3 - k'_3)nc}}{n - \nu} , \tag{2.9}$$

and $n = \rho_3/c$, $\nu = r_3^0/c$. In Appendix A, we show that for ν a noninteger (in the following we suppose $0 < \nu < 1$), $W(k_3 - k'_3)$ is in essence equal to the step function. It is this property of the kernel that allows an analytic solution of the remaining eigenvalue problem. Since any physically meaningful function of $\mathbf{k}$ is periodic in reciprocal space,[3] Eq. (2.3) must be supplemented by the boundary conditions

$$\xi_{\mathbf{k}+\mathbf{G}}^{\lambda}(E) = \xi_{\mathbf{k}}^{\lambda}(E) , \tag{2.10}$$

where $\mathbf{G}$ is any reciprocal lattice vector. The boundary conditions imposed on $\xi_{\mathbf{k}}^{\lambda}(E)$ give rise to quantization of energy: For the $\mathbf{c}$ direction (where the crystal is supposed to be infinitely extended) we obtain a nontrivial eigenvalue equation with an infinite number of discrete energy levels, as will be shown in Sec. III. To each level corresponds a 2D energy band due to the transverse degrees of freedom of the system ($\mathbf{k}_\perp$ still is a good quantum number).

III. SOLUTION OF SCHRÖDINGER EQUATION

As stated in Sec. II, the boundary conditions in $\mathbf{k}$ space for the state vector amplitude $\xi_{\mathbf{k}}^{\lambda}(E)$ give rise to a nontrivial eigenvalue equation in the $\mathbf{c}$ direction which explicitly reads

$$\xi_{\mathbf{k}_\perp k_3 + 2\pi/c}^{\lambda}(E) = \xi_{\mathbf{k}_\perp k_3}^{\lambda}(E) . \tag{3.1}$$

In the case of a narrow band λ, the solution of the Schrödinger equation can be achieved by the following procedure: First, calculate the quantity $W(k_3 - k'_3)$; second, solve Eq. (2.3) treating the energy E as a parameter; and third, determine the allowed energies by condition (3.1).

The first step consists in calculating the sum in Eq. (2.9). Throughout the paper we will suppose that $N \gg 1$, therefore we treat k_3 as a continuous variable (whereas $\mathbf{k}_\perp$ is treated as a discrete variable for convenience, but this point is not essential). We get (see Appendix A)

$$W(k_3 - k'_3) = -\frac{\alpha\pi}{N} e^{-i(k_3 - k'_3)\nu c} \times \left[2i\Theta(k_3 - k'_3) + \frac{e^{-i\nu\pi}}{\sin\nu\pi} \right] , \tag{3.2}$$

where we used the step-function symbol in the following sense:

$$\Theta(x)=\begin{cases}1, & x>0\\ \frac{1}{2}, & x=0\\ 0, & x<0\ .\end{cases}$$

Equivalently, we can write

$$\frac{d}{dk_3}[e^{i(k_3-k_3')\nu c}W(k_3-k_3')]=-\frac{2\pi i\alpha}{N}\delta(k_3-k_3')\ . \tag{3.3}$$

The second step takes advantage of the very special form of Eq. (3.3). Multiplying Eq. (2.3) by $\exp(ik_3\nu c)$ and deriving with respect to k_3 yields

$$\frac{d}{dk_3}[(E-\varepsilon_{\mathbf{k}}^{\lambda})e^{ik_3\nu c}\xi_{\mathbf{k}}^{\lambda}(E)]=-ic\alpha e^{ik_3\nu c}\xi_{\mathbf{k}}^{\lambda}(E)\ , \tag{3.4}$$

where we have replaced the summation over k_3 by integration over the first Brillouin zone. Integration of Eq. (3.4) yields

$$\xi_{\mathbf{k}}^{\lambda}(E)=\frac{N_E}{E-\varepsilon_{\mathbf{k}}^{\lambda}}\exp\left[-ik_3\nu c-ic\alpha\int_{-\pi/c}^{k_3}\frac{dk_3'}{E-\varepsilon_{\mathbf{k}_\perp k_3'}^{\lambda}}\right]\ . \tag{3.5}$$

N_E is a normalization constant that will be specified later [see Eq. (3.8)]. Finally, we determine the allowed energy values by condition (3.1). We find

$$\exp\left[-2\pi i\left[\nu+\frac{c\alpha}{2\pi}\int_{-\pi/c}^{\pi/c}\frac{dk_3}{E-\varepsilon_{\mathbf{k}_\perp k_3}^{\lambda}}\right]\right]=1\ , \tag{3.6}$$

or equivalently,

$$\alpha\int_{-\pi/c}^{\pi/c}\frac{dk_3}{E-\varepsilon_{\mathbf{k}_\perp k_3}^{\lambda}}=\frac{2\pi}{c}(p-\nu)\ , \tag{3.7}$$

with p an integer number. Equations (3.5) and (3.7) constitute the main results of this work. For each eigenvalue $E_{p\mathbf{k}_\perp}^{\lambda}$ solution of Eq. (3.7) (p and $\mathbf{k}_\perp$ being fixed quantum numbers and λ the band index) the corresponding eigenvector is given by Eqs. (3.5) and (2.2) and reads

$$|\Phi(E_{p\mathbf{k}_\perp}^{\lambda})\rangle=\sum_{\mathbf{k}',\lambda'}\xi_{\mathbf{k}'}^{\lambda'}(E_{p\mathbf{k}_\perp}^{\lambda})|\mathbf{k}'\lambda'\rangle\ ,$$

$$\xi_{\mathbf{k}'}^{\lambda'}(E_{p\mathbf{k}_\perp}^{\lambda})=\delta_{\lambda\lambda'}\delta_{\mathbf{k}_\perp\mathbf{k}_\perp'}\frac{N_{p\mathbf{k}_\perp}^{\lambda}}{E_{p\mathbf{k}_\perp}^{\lambda}-\varepsilon_{\mathbf{k}'}^{\lambda}}\times\exp\left[-ik_3'\nu c-ic\alpha\int_{-\pi/c}^{k_3'}\frac{d\kappa_3}{E_{p\mathbf{k}_\perp}^{\lambda}-\varepsilon_{\mathbf{k}_\perp\kappa_3}^{\lambda}}\right]\ , \tag{3.8}$$

$$N_{p\mathbf{k}_\perp}^{\lambda}=\left[\frac{Nc}{2\pi}\int_{-\pi/c}^{\pi/c}\frac{d\kappa_3}{(E_{p\mathbf{k}_\perp}^{\lambda}-\varepsilon_{\mathbf{k}_\perp\kappa_3}^{\lambda})^2}\right]^{-1/2}\ .$$

In the following, we will suppress the band index λ. We now want to prove that for arbitrary p and $\mathbf{k}_\perp$ fixed, there exists a unique real solution $E_{p\mathbf{k}_\perp}$. To this end, for $\mathbf{k}_\perp$ fixed we divide the spectrum in three parts: (i) $E<E_{\min}(\mathbf{k}_\perp)$, (ii) $E>E_{\max}(\mathbf{k}_\perp)$, and (iii) $E_{\min}(\mathbf{k}_\perp)<E<E_{\max}(\mathbf{k}_\perp)$, where $E_{\min}(\mathbf{k}_\perp)=\min_{k_3}\varepsilon_{\mathbf{k}}$, $E_{\max}(\mathbf{k}_\perp)=\max_{k_3}\varepsilon_{\mathbf{k}}$ (the minimum and the maximum are taken in the interval $k_3\in[-\pi/c,\pi/c]$).

Let us first consider the following function:

$$f_{k_3}(E,\mathbf{k}_\perp)=\int_{-\pi/c}^{k_3}\frac{dk_3'}{E-\varepsilon_{\mathbf{k}_\perp k_3'}}\ , \tag{3.9}$$

as well as its derivative with respect to E

$$\frac{d}{dE}f_{k_3}(E,\mathbf{k}_\perp)=-\int_{-\pi/c}^{k_3}\frac{dk_3'}{(E-\varepsilon_{\mathbf{k}_\perp k_3'})^2}\ . \tag{3.10}$$

Inserting Eq. (3.9) in the eigenvalue equation (3.7) we get

$$\alpha f_{\pi/c}(E,\mathbf{k}_\perp)=\frac{2\pi}{c}(p-\nu)\ . \tag{3.11}$$

(i) For $E<E_{\min}(\mathbf{k}_\perp)$ and "smooth" dependence of $\varepsilon_{\mathbf{k}}$ on k_3, $f_{\pi/c}(E,\mathbf{k}_\perp)$ is an analytic function of E, monotonically decreasing and behaves asymptotically as (see Ref. 8, Appendix A therein)

$$f_{\pi/c}(E,\mathbf{k}_\perp)\to\begin{cases}0 & \text{for } E\to-\infty\\ -\infty & \text{for } E\to E_{\min}(\mathbf{k}_\perp)\ .\end{cases} \tag{3.12}$$

Consequently, for $0<\nu<1$ and $\alpha>0$ there exists a unique real solution for any integer $p\le 0$ and $E_{\min}(E,\mathbf{k}_\perp)$ is an accumulation point of eigenvalues.

(ii) For $E>E_{\max}(\mathbf{k}_\perp)$ similar conclusions hold: $f_{\pi/c}(E,\mathbf{k}_\perp)$ is analytic, monotonically decreasing, and behaves asymptotically as

$$f_{\pi/c}(E,\mathbf{k}_\perp)\to\begin{cases}0 & \text{for } E\to+\infty\\ +\infty & \text{for } E\to E_{\max}(\mathbf{k}_\perp)\ .\end{cases} \tag{3.13}$$

There exists a unique real solution for any integer $p\ge 1$ and $E_{\max}(\mathbf{k}_\perp)$ is an accumulation point of eigenvalues. Note that the existence of bound states arising from repulsive potentials is a well-known feature in solid-state physics. These levels are due to the fact that effective masses are negative at the upper-energy-band edges. This implies that potentials which act repulsively on quasiparticles with positive masses become attractive when the effective masses are negative.

(iii) For $E_{\min}(\mathbf{k}_\perp)<E<E_{\max}(\mathbf{k}_\perp)$ the energy E lies within the unperturbed band (for $\mathbf{k}_\perp$ fixed) and the integrand's denominator vanishes at some definite points. Due to this singular behavior there exist no real solutions to Eq. (3.11). This can be seen as follows: Much as in the theory of Green's functions,[8] the analytic continuation $f_{\pi/c}(z,\mathbf{k}_\perp)$ has a branch cut on the real axis in the interval $E_{\min}(\mathbf{k}_\perp)<E<E_{\max}(\mathbf{k}_\perp)$. Its side limits are defined by

$$f_{\pi/c}^{\pm}(E,\mathbf{k}_\perp)=\lim_{\delta\to 0^+}f_{\pi/c}(E\pm i\delta,\mathbf{k}_\perp)\ . \tag{3.14}$$

We get

$$f_{\pi/c}^{\pm}(E,\mathbf{k}_\perp)=f_1(E,\mathbf{k}_\perp)\mp if_2(E,\mathbf{k}_\perp)\ , \tag{3.15}$$

with

$$f_1(E,\mathbf{k}_\perp)=P\int_{-\pi/c}^{\pi/c}\frac{dk_3}{E-\varepsilon_{\mathbf{k}}}\ ,$$

$$f_2(E,\mathbf{k}_\perp)=\begin{cases}\pi\int_{-\pi/c}^{\pi/c}dk_3\delta(E-\varepsilon_{\mathbf{k}})\ , \\ \qquad\qquad E_{\min}(\mathbf{k}_\perp)<E<E_{\max}(\mathbf{k}_\perp) \\ 0\ \text{ otherwise}\ .\end{cases} \tag{3.16}$$

Clearly, for E inside the original band, $f_2(E,\mathbf{k}_\perp)$ is nonzero, and there do not exist any real solutions to Eq. (3.11). However, this fact does not exclude eigenvalues belonging to the continuous spectrum of H. We will demonstrate in Sec. IV that the Green's function $G(z)$ corresponding to H has simple poles at the points $z=E_{p\mathbf{k}_\perp}\forall p,\forall\mathbf{k}_\perp$, i.e., Eq. (3.11) determines only the discrete eigenvalues of H. Therefore information about the continuous spectrum of H, if it exists, must be extracted from the analytic properties of $G(z)$. As a matter of fact, we will show that $G(z)$ has a branch cut on the real axis and that the continuous spectra of H^0 and H coincide.

To conclude this section, we attract the reader's attention to the fact that the wave functions in Eq. (3.8) remain well defined in the limit $\nu\to 0$ for all $p\neq 0$ [note that for $p=\nu=0$ Eq. (3.11) yields unphysical solutions with $E=\pm\infty$, which have to be excluded]. We will now demonstrate that for $\nu=0$ all the eigenfunctions vanish at $n=0$.

Consider the expansion of the state vector in the WF representation

$$\langle\mathbf{r}|\Phi(E_{p\mathbf{k}_\perp})\rangle=\sum_\rho\eta_\rho(E_{p\mathbf{k}_\perp})\varphi(\mathbf{r}-\boldsymbol{\rho})\ ,$$

with

$$\eta_\rho(E_{p\mathbf{k}_\perp})=N^{-3/2}\sum_{\mathbf{k}'}e^{i\mathbf{k}'\cdot\rho}\xi_{\mathbf{k}'}(E_{p\mathbf{k}_\perp})\ . \tag{3.17}$$

Using Eq. (3.8) we get

$$\eta_\rho(E_{p\mathbf{k}_\perp})=\frac{e^{i\mathbf{k}_\perp\cdot\boldsymbol{\rho}_\perp}}{N}\frac{\sqrt{N}c}{2\pi}\int_{-\pi/c}^{\pi/c}dk_3e^{ik_3nc}\xi_{\mathbf{k}}(E_{p\mathbf{k}_\perp})\ , \tag{3.18}$$

with $\boldsymbol{\rho}_\perp=l\mathbf{a}+m\mathbf{b}$. Equation (3.18) reflects just the fact that the wave function factorizes in a plane wave along the $\boldsymbol{\rho}_\perp$ direction and a nontrivial part along the $\mathbf{c}$ direction. Next, note that $\xi_{\mathbf{k}}$ can be rewritten as

$$\xi_{\mathbf{k}}(E_{p\mathbf{k}_\perp})=i\frac{N_{p\mathbf{k}_\perp}}{c\alpha}e^{-ik_3vc}\frac{\partial}{\partial k_3}\times\exp\left[-ic\alpha\int_{-\pi/c}^{k_3}\frac{d\kappa_3}{E_{p\mathbf{k}_\perp}-\varepsilon_{\mathbf{k}_\perp\kappa_3}}\right]\ . \tag{3.19}$$

Introducing Eq. (3.19) into (3.18) and performing a partial integration, we get finally

$$\eta_\rho(E_{p\mathbf{k}_\perp})=\frac{e^{i\mathbf{k}_\perp\boldsymbol{\rho}_\perp}}{N}\frac{cN_{p\mathbf{k}_\perp}}{2\pi\alpha}\sqrt{N}(n-\nu)\times\int_{-\pi/c}^{\pi/c}dk_3\exp[ik_3(n-\nu)c-ic\alpha f_{k_3}(E_{p\mathbf{k}_\perp},\mathbf{k}_\perp)]\ . \tag{3.20}$$

In Eq. (3.20) we have used definition (3.9). Since

$$|\eta_\rho(E_{p\mathbf{k}_\perp})|\le N^{-1/2}\frac{N_{p\mathbf{k}_\perp}}{\alpha}|n-\nu|\ , \tag{3.21}$$

we can conclude that for $\nu=0$ (and $p\neq 0$)

$$\eta_\rho(E_{p\mathbf{k}_\perp})|_{n=\nu=0}=0\ . \tag{3.22}$$

IV. GREEN'S FUNCTION

This section is entirely devoted to the study of the time-independent Green's function (GF) of the system Hamiltonian (2.1) in the case of a narrow band λ with band dispersion $\varepsilon_{\mathbf{k}}^{\lambda}$ (the band index will be suppressed). All the mathematical tools used in this section can be found in Economou's treatise on GF's.[8] We define the GF $G(z)$ and $G^0(z)$ corresponding to $H=H^0+V_{\text{ext}}$ and H^0, respectively, as

$$G(z)=(z-H)^{-1}\ , \tag{4.1}$$

$$G^0(z)=(z-H^0)^{-1}=\sum_{\mathbf{k}}\frac{|\mathbf{k}\rangle\langle\mathbf{k}|}{z-\varepsilon_{\mathbf{k}}}\ . \tag{4.2}$$

For reasons of mathematical simplicity we first calculate the so-called t matrix $T(z)$ defined by

$$T(z)=V_{\text{ext}}G(z)(z-H^0)\ . \tag{4.3}$$

G, G^0, and T are related by the following standard formulas:

$$G=G^0+G^0V_{\text{ext}}G\ , \tag{4.4}$$

$$T=V_{\text{ext}}+V_{\text{ext}}G^0T\ , \tag{4.5}$$

$$G=G^0+G^0TG^0\ . \tag{4.6}$$

Starting from Eq. (4.5), a calculation similar to the one that led to the expression for the state vector's amplitude [Eq. (3.5)] yields the GF in $\mathbf{k}$ representation (for details see Appendix B)

$$T_{\mathbf{k}\mathbf{k}'}(z)=\frac{2\pi i\alpha}{N}\delta_{\mathbf{k}_\perp\mathbf{k}_\perp'}e^{i\{(k_3'-k_3)vc+c\alpha[f_{k_3'}(z,\mathbf{k}_\perp)-f_{k_3}(z,\mathbf{k}_\perp)]\}}\times[(1-e^{2\pi iv+c\alpha f_{\pi/c}(z,\mathbf{k}_\perp)})^{-1}-\Theta(k_3-k_3')]\ , \tag{4.7}$$

where the function $f_{k_3}(E,\mathbf{k}_\perp)$ is defined in Eq. (3.9). Again, we supposed that $N\gg 1$, i.e., sums over k_3 are replaced by integrals multiplied by $Nc/2\pi$.

According to Eq. (4.6) the matrix elements of the corresponding GF are given by

$$G_{\mathbf{k}\mathbf{k}'}(z)=G^0_{\mathbf{k}\mathbf{k}'}(z)+\frac{T_{\mathbf{k}\mathbf{k}'}(z)}{(z-\varepsilon_{\mathbf{k}})(z-\varepsilon_{\mathbf{k}'})}\ , \tag{4.8}$$

where

$$G^0_{\mathbf{k}\mathbf{k}'}(z)=\frac{2\pi}{Nc}\frac{1}{z-\varepsilon_{\mathbf{k}}}\delta_{\mathbf{k}_\perp\mathbf{k}_\perp'}\delta(k_3-k_3')\ . \tag{4.9}$$

Equation (4.9) follows from Eq. (4.2). We remind the reader of the fact that k_3 is treated as a continuous vari-

able, whereas $\mathbf{k}_\perp$ denotes the discrete transversal components of $\mathbf{k}$. With this in mind we write

$$\langle \mathbf{k}|\mathbf{k}'\rangle = \frac{2\pi}{Nc}\delta_{\mathbf{k}_\perp\mathbf{k}'_\perp}\delta(k_3-k'_3) \tag{4.10}$$

instead of $\langle \mathbf{k}|\mathbf{k}'\rangle = \delta_{\mathbf{k}\mathbf{k}'}$ if k_3 also were a discrete variable.

The knoweldge of the density of states (DOS) is particularly important in the analysis of the spectrum of H. For this purpose we consider the side limits $G^+(E)$ and $G^-(E)$ of the GF and their difference $G^\Delta(E)$,

$$G^\pm(E) = \lim_{\delta\to 0^+} G(E\pm i\delta) , \tag{4.11}$$

$$G^\Delta(E) = G^+(E) - G^-(E) \tag{4.12}$$

[with analogous definitions of $G^{0+}(E)$, $G^{0-}(E)$, and $G^{0\Delta}(E)$]. These quantities allow us to calculate the DOS per state $|\mathbf{k}\rangle$ $\rho_{\mathbf{k}}(E)$ and $\rho^0_{\mathbf{k}}(E)$ associated with H and H^0, respectively,

$$\rho_{\mathbf{k}}(E) = i(2\pi)^{-1}G^\Delta_{\mathbf{k}\mathbf{k}}(E) , \tag{4.13a}$$

$$\rho^0_{\mathbf{k}}(E) = i(2\pi)^{-1}G^{0\Delta}_{\mathbf{k}\mathbf{k}}(E) , \tag{4.13b}$$

as well as the total DOS $D(E)$ and $D^0(E)$,

$$D(E) = \sum_{\mathbf{k}} \rho_{\mathbf{k}}(E) = i(2\pi)^{-1}\sum_{\mathbf{k}} G^\Delta_{\mathbf{k}\mathbf{k}}(E) , \tag{4.14a}$$

$$D^0(E) = \sum_{\mathbf{k}} \rho^0_{\mathbf{k}}(E) = i(2\pi)^{-1}\sum_{\mathbf{k}} G^{0\Delta}_{\mathbf{k}\mathbf{k}}(E) . \tag{4.14b}$$

Let us define the two following quantities with obvious significance:

$$\Delta\rho_{\mathbf{k}}(E) = \rho_{\mathbf{k}}(E) - \rho^0_{\mathbf{k}}(E) , \tag{4.15a}$$

$$\Delta D(E) = D(E) - D^0(E) . \tag{4.15b}$$

According to Eqs. (4.8), (4.12), and (4.13) they are given by

$$\Delta\rho_{\mathbf{k}}(E) = -\frac{\alpha}{N}\left[\frac{(1-e^{2\pi i\nu+ic\alpha f^+_{\pi/c}(E,\mathbf{k}_\perp)})^{-1}-\frac{1}{2}}{(E+i0^+-\varepsilon_{\mathbf{k}})^2} - \frac{(1-e^{2\pi i\nu+f^-_{\pi/c}(E,\mathbf{k}_\perp)})^{-1}-\frac{1}{2}}{(E-i0^+-\varepsilon_{\mathbf{k}})^2}\right] , \tag{4.16a}$$

$$\Delta D(E) = \sum_{\mathbf{k}} \Delta\rho_{\mathbf{k}}(E) . \tag{4.16b}$$

Here we used $\Theta(0)=\frac{1}{2}$ [compare with Eq. (A7)]. In the following, we give a complete characterization of the solutions associated with the discrete spectrum (eigenvalues, degree of degeneracy, eigenvectors, DOS) and we calculate explicitly the DOS of the continuous spectrum of H.

A. Discrete spectrum

As is well known, each pole of the GF on the real axis corresponds to a discrete eigenvalue of H, the residue of the GF at this pole determining the degree of degeneracy of the eigenvalue as well as the projector on the associated eigenspace.

The poles of the GF are given by the equation

$$1-e^{2\pi i\nu+ic\alpha f_{\pi/c}(E,\mathbf{k}_\perp)}=0 . \tag{4.17}$$

Recalling the definition of $f_{\pi/c}(E,\mathbf{k}_\perp)$ [Eq. (3.9)], we see that Eqs. (3.11) and (4.17) are identical. Note that the zeros of the denominator in the second term of the right-hand side (rhs) of Eq. (4.8) do not give rise to discrete levels, but rather contribute to the branch cut of $G(z)$ (see below).

The degree of degeneracy $d_{p\mathbf{k}_\perp}$ of the eigenvalue $E_{p\mathbf{k}_\perp}$ solution of Eq. (4.17) can be calculated as follows (Tr is the trace):

$$d_{p\mathbf{k}_\perp} = \mathrm{Tr}\,\mathrm{Res}[G(z),E_{p\mathbf{k}_\perp}] . \tag{4.18}$$

$\mathrm{Res}[f(z),z_0]$ means taking the residue of $f(z)$ at the point z_0. Let us first calculate the residue of $G_{\mathbf{k}'\mathbf{k}''}(z)$ at $z=E_{p\mathbf{k}_\perp}$:

$$\mathrm{Res}[G_{\mathbf{k}'\mathbf{k}''}(z),E_{p\mathbf{k}_\perp}] = \lim_{z\to E_{p\mathbf{k}_\perp}}(z-E_{p\mathbf{k}_\perp})G_{\mathbf{k}'\mathbf{k}''}(z)$$

$$= \left[-\frac{2\pi}{Nc}\delta_{\mathbf{k}'_\perp\mathbf{k}_\perp}\delta_{\mathbf{k}''_\perp\mathbf{k}_\perp}\frac{\exp[ic(k''_3\nu+\alpha f_{k''_3}-k'_3\nu-\alpha f_{k'_3})]}{(z-\varepsilon_{\mathbf{k}''})(z-\varepsilon_{\mathbf{k}'})}\left[\frac{d}{dz}f_{\pi/c}\right]^{-1}\right]_{z=E_{p\mathbf{k}_\perp}} . \tag{4.19}$$

Introducing Eq. (4.19) into Eq. (4.18) we get

$$d_{p\mathbf{k}_\perp} = \sum_{\mathbf{k}'}\mathrm{Res}[G_{\mathbf{k}'\mathbf{k}'}(z),E_{p\mathbf{k}_\perp}] = 1 , \tag{4.20}$$

i.e., all the eigenvalues are nondegenerate. Consequently, the projecter $P_{p\mathbf{k}_\perp}$ on the eigenspace associated with $E_{p\mathbf{k}_\perp}$ is one dimensional and may be expressed as

$$P_{p\mathbf{k}_\perp} = |\Phi(E_{p\mathbf{k}_\perp})\rangle\langle\Phi(E_{p\mathbf{k}_\perp})| . \tag{4.21}$$

Its matrix elements read

$$\langle \mathbf{k}'|P_{p\mathbf{k}_\perp}|\mathbf{k}''\rangle = \xi_{\mathbf{k}'}(E_{p\mathbf{k}_\perp})\xi^*_{\mathbf{k}''}(E_{p\mathbf{k}_\perp}) , \tag{4.22}$$

where we used definition (2.2). According to the theory of GF's, we have

$$\langle \mathbf{k}'|P_{p\mathbf{k}_\perp}|\mathbf{k}''\rangle = \mathrm{Res}[G_{\mathbf{k}'\mathbf{k}''}(z), E_{p\mathbf{k}_\perp}] \ . \tag{4.23}$$

Comparing Eq. (4.23) with (4.22) and (4.19), we get as a result

$$\xi_{\mathbf{k}'}(E_{p\mathbf{k}_\perp}) = \delta_{\mathbf{k}'_\perp \mathbf{k}_\perp} \frac{N_{p\mathbf{k}_\perp}}{E_{p\mathbf{k}_\perp} - \varepsilon_{\mathbf{k}'}} \times \exp[-ik'_3 \nu c - ic\alpha f_{k'_3}(E_{p\mathbf{k}_\perp}, \mathbf{k}_\perp)] \ , \tag{4.24}$$

with

$$N_{p\mathbf{k}_\perp} = \left[\frac{Nc}{2\pi} \int_{-\pi/c}^{\pi/c} \frac{dk_3}{(E_{p\mathbf{k}_\perp} - \varepsilon_{\mathbf{k}})^2} \right]^{-1/2} . \tag{4.25}$$

As expected, this expression for the amplitude of the state vector is identical to Eq. (3.8). We recall [see the discussion of Eq. (3.11)] that for $\mathbf{k}_\perp$ fixed, we have $E_{p\mathbf{k}_\perp} < E_{\min}(\mathbf{k}_\perp)$ for $p \le 0$ and $E_{p\mathbf{k}_\perp} > E_{\max}(\mathbf{k}_\perp)$ for $p > 0$. Therefore the integrals in Eqs. (4.24) and (4.25) are well defined and real, i.e., $\xi_{\mathbf{k}'}(E_{p\mathbf{k}_\perp})$ is normalized to unity with $N_{p\mathbf{k}_\perp}$ playing the role of a normalizing factor.

To close this first subsection we calculate $\Delta\rho_{\mathbf{k}}(E)$. We have from Eq. (4.16a)

$$\Delta\rho_{\mathbf{k}}(E) = -\frac{\alpha}{N}(E - \varepsilon_{\mathbf{k}})^{-2}[(1 - e^{2\pi i\nu + ic\alpha f^+_{\pi/c}})^{-1} - (1 - e^{2\pi i\nu + ic\alpha f^-_{\pi/c}})^{-1}] \ . \tag{4.26}$$

Both terms on the rhs of Eq. (4.26) have simple poles at $E = E_{p\mathbf{k}_\perp}$, $\forall p$. A careful evaluation yields for $E \approx E_{p\mathbf{k}_\perp}$ (i.e., $|E - E_{p\mathbf{k}_\perp}| \ll |E - E_{p\pm 1\mathbf{k}_\perp}|$)

$$(1 - e^{2\pi i\nu + ic\alpha f^{\pm}_{\pi/c}(E,\mathbf{k}_\perp)})^{-1} = \left[-ic\alpha \frac{d}{dE} f_{\pi/c}(E, \mathbf{k}_\perp) \right]^{-1}_{E = E_{p\mathbf{k}_\perp}} \times \left[\frac{PP_E}{E - E_{p\mathbf{k}_\perp}} \mp i\pi\delta(E - E_{p\mathbf{k}_\perp}) \right] \tag{4.27}$$

(PP_E is the principal part with respect to integration over E), where account has been taken of the eigenvalue equation (4.17). Introducing Eq. (4.27) in (4.26) and using (4.24) and (4.25) we get

$$\Delta\rho_{\mathbf{k}}(E) = |\xi_{\mathbf{k}}(E)|^2 \delta(E - E_{p\mathbf{k}_\perp}), \quad E \approx E_{p\mathbf{k}_\perp} \ . \tag{4.28}$$

Repeating the argument for arbitrary p yields finally

$$\Delta\rho_{\mathbf{k}}(E) = \sum_p |\xi_{\mathbf{k}}(E_{p\mathbf{k}_\perp})|^2 \delta(E - E_{p\mathbf{k}_\perp}) \ . \tag{4.29}$$

The change of the total density of states $\Delta D(E)$ associated with only the discrete spectrum is obtained from Eq. (4.16b), namely

$$\Delta D(E) = \sum_{p\mathbf{k}_\perp} \delta(E - E_{p\mathbf{k}_\perp}) \ . \tag{4.30}$$

These results are easily interpreted: Eq. (4.28) represents the contribution of the exact state $|\Phi(E_{p\mathbf{k}_\perp})\rangle$ to the occupation of state $|\mathbf{k}\rangle$ and Eq. (4.29) sums up the contributions from all the discrete levels with $\mathbf{k}_\perp$ fixed. Finally, integration of Eq. (4.30) over E yields the total number of discrete levels produced by the Coulomb-type potential. It is of course not surprising that this number diverges since we have supposed in our calculations that the crystal has infinite extension in the **c** direction.

B. Continuous spectrum

It is a general result of the theory of GF that the continuous spectrum of H [denoted by $\sigma_c(H)$ as opposed to $\sigma_c(H^0)$, the continuous spectrum of H^0] gives rise to a branch cut of $G(z)$ along the real z axis. We now want to show that $G(z)$ indeed has a branch cut [and therefore that $\sigma_c(H)$ exists] by calculating explicitly the total DOS.

We start with summing up expression (4.16a) over k_3 with $\mathbf{k}_\perp$ fixed. Using definition (3.15) and its derivative with respect to E [for the sake of brevity we suppress the arguments E and $\mathbf{k}_\perp$ in $f_{\pi/c}(E, \mathbf{k}_\perp)$ in our formulas],

$$\frac{d}{dE} f^{\pm}_{\pi/c} = \frac{d}{dE} f_1 \mp i \frac{d}{dE} f_2 = -\int_{-\pi/c}^{\pi/c} \frac{dk_3}{(E \pm i0 \pm \varepsilon_{\mathbf{k}})^2} \ , \tag{4.31}$$

we get

$$\sum_{k_3} \Delta\rho_{\mathbf{k}}(E) = \frac{c\alpha}{2\pi} \left[(1 - e^{2\pi i\nu + ic\alpha f^+_{\pi/c}})^{-1} \frac{d}{dE} f^+_{\pi/c} - (1 - e^{2\pi i\nu + ic\alpha f^-_{\pi/c}})^{-1} \frac{d}{dE} f^-_{\pi/c} + i \frac{df_2}{dE} \right] . \tag{4.32}$$

Introducing the equality

$$\frac{e^{-2\pi i\nu - ic\alpha f^{\pm}_{\pi/c}}}{e^{-2\pi i\nu - ic\alpha f^{\pm}_{\pi/c}} - 1} \frac{d}{dE} f^{\pm}_{\pi/c} = \frac{i}{c\alpha} \frac{d}{dE} \ln(e^{-2\pi i\nu - ic\alpha f^{\pm}_{\pi/c}} - 1) \tag{4.33}$$

in Eq. (4.32) we get

$$\sum_{k_3} \Delta\rho_{\mathbf{k}}(E) = \frac{c\alpha}{2\pi} \frac{d}{dE} \left[\frac{i}{c\alpha} \ln \frac{e^{-2\pi i\nu - ic\alpha f^+_{\pi/c}} - 1}{e^{-2\pi i\nu - ic\alpha f^-_{\pi/c}} - 1} + i f_2 \right] . \tag{4.34}$$

Separating the argument of the logarithm in real part x and imaginary part y where

$$x=\frac{e^{-c\alpha f_2}}{\cosh(c\alpha f_2)-\cos(2\pi\nu+c\alpha f_1)}\times[1-\cos(2\pi\nu+c\alpha f_1)\cosh(c\alpha f_2)]\ ,$$

$$y=-\frac{e^{-c\alpha f_2}}{\cosh(c\alpha f_2)-\cos(2\pi\nu+c\alpha f_1)}\times\sin(2\pi\nu+c\alpha f_1)\sinh(c\alpha f_2)\ ,$$

we rewrite Eq. (4.34) using

$$\ln(x+iy)=\tfrac{1}{2}\ln(x^2+y^2)+i[\arctan(y/x)+2\pi s] \tag{4.35}$$

(s is an arbitrary integer number). As expected, the imaginary part in Eq. (4.34) vanishes and we have

$$\sum_{k_3}\Delta\rho_{\mathbf{k}}(E)=\frac{1}{2\pi}\frac{d}{dE}\arctan\left[\frac{\sin(2\pi\nu+c\alpha f_1)\sinh(c\alpha f_2)}{1-\cos(2\pi\nu+c\alpha f_1)\cosh(c\alpha f_2)}\right]. \tag{4.36}$$

From Eqs. (4.15b) and (4.16b) we get for the total DOS

$$D(E)=D^0(E)+\sum_{\mathbf{k}_\perp}\sum_{k_3}\Delta\rho_{\mathbf{k}}(E)\ . \tag{4.37}$$

It is important to note that due to the transversal energy dispersion (with quantum numbers $\mathbf{k}_\perp$) there are infinitely many discrete levels degenerated with "band" (or extended) states. This gives rise to relaxation or broadening of the discrete levels in the presence of any additional perturbation term in the Hamiltonian which couples the degenerated states. There exist many theoretical investigations on this topic, one of the most elegant exact treatments was given by Fano.[5]

V. EXPLICIT RESULTS FOR THE 1D COSINE BAND

As an illustration of the results exposed in this work, we consider a simple one-dimensional Hamiltonian with nearest-neighbor interactions as the nonperturbed part:

$$H=H^0+V_{\text{ext}}\ ,$$
$$H^0=\sum_n\frac{B}{2}(|n+1\rangle\langle n|+\text{H.c.})=\sum_k\varepsilon_k|k\rangle\langle k|\ , \tag{5.1}$$
$$V_{\text{ext}}=\sum_n\frac{\alpha}{n-\nu}|n\rangle\langle n|$$

where

$$|k\rangle=N^{-1/2}\sum_n e^{iknc}|n\rangle\ ,$$
$$\varepsilon_k=B\cos kc\ . \tag{5.2}$$

$|n\rangle$ is a shorthand notation for the WF at the lattice site n for the particular band considered. A very similar version of this particular problem has been studied by Ifantis.[7] It consists of a half-infinite chain with lattice sites $x=sa$ for $s=0,1,2,\ldots,\infty$ (a is the lattice constant), nearest-neighbor interactions (the bandwidth is set equal to 2) and a point charge of weight b at site $x=0$. It was shown that the point spectrum associated with the homogeneous boundary conditions (vanishing wave function at $x=0$ and ∞) is given by

$$\varepsilon_p=\begin{cases}[1+(b/ap)^2]^{1/2}, & b>0 \quad (5.3a)\\ -[1+(b/ap)^2]^{1/2}, & b<0\ , \quad (5.3b)\end{cases}$$

where $p=1,2,\ldots,\infty$. For the repulsive potential ($b>0$) the corresponding eigenfunctions were explicitly calculated in local representation.

We will now show that for $\nu=0$ (i) the point spectrum of our Hamiltonian (5.1) is identical to the composed spectrum (5.3a) and (5.3b) (where b/a has to be replaced by α/B and ε_p by E_p/B) and (ii) the respective wave functions are identical.

The applications of the formulas in Secs. II–IV to the 1D case are straightforward. According to Eq. (3.8) the discrete level eigenfunctions are given by

$$|\Phi(E_p)\rangle=\sum_k\xi_k(E_p)|k\rangle\ ,$$
$$\xi_k(E_p)=\frac{N_p}{E_p-\varepsilon_k}\exp[-ik\nu c-ic\alpha f_k(E_p)]\ , \tag{5.4}$$

with

$$N_p=\left[\frac{Nc}{2\pi}\int_{-\pi/c}^{\pi/c}\frac{d\kappa}{(E_p-\varepsilon_\kappa)^2}\right]^{-1/2}, \tag{5.5}$$

$$f_k(E)=\int_{-\pi/c}^{k}\frac{d\kappa}{E-\varepsilon_\kappa}\ . \tag{5.6}$$

The corresponding eigenvalues E_p are solutions of Eq. (3.11), which reduces to

$$\alpha f_{\pi/c}(E_p)=\frac{2\pi}{c}(p-\nu)\ . \tag{5.7}$$

The function $f^{\pm}_{\pi/c}(E)=f_1\pm if_2$ is readily calculated (see Ref. 8, p. 81) and reads

$$f_1=\begin{cases}+\frac{2\pi}{c}(E^2-B^2)^{-1/2} & \text{for } E>B\\ -\frac{2\pi}{c}(E^2-B^2)^{-1/2} & \text{for } E<-B\\ 0 \text{ for } |E|<B\ ,\end{cases}$$
$$f_2=\begin{cases}\frac{2\pi}{c}(B^2-E^2)^{-1/2} & \text{for } |E|<B\\ 0 \text{ for } |E|>B\ .\end{cases} \tag{5.8}$$

This yields for the allowed energies

$$E_p=\begin{cases}\left[B^2+\left[\dfrac{\alpha}{p-\nu}\right]^2\right]^{1/2} & \text{for } p=1,2,\ldots,\infty\\ -\left[B^2+\left[\dfrac{\alpha}{p-\nu}\right]^2\right]^{1/2} & \text{for } p=0,-1,\ldots,-\infty\ .\end{cases}\tag{5.9}$$

Comparing Eqs. (5.3) and (5.9) we see that for $\nu=0$ the allowed energies are identical. However, in Eq. (5.9) we must exclude the eigenvalues $E_0=\pm\infty$ for $p=0$ because they are due to the pathological divergency of the potential on site $n=0$. The upper and lower band edges $E_u=B$ and $E_l=-B$ are accumulation points of discrete eigenvalues. The state vector's amplitude $\xi_k(E_p)$ corresponding to the level E_p is given by Eq. (5.4), where N_p and $f_k(E_p)$ explicitly read

$$N_p=\left[N\frac{\pm E_p}{(E_p^2-B^2)^{3/2}}\right]^{-1/2}\tag{5.10}$$

and

$$f_k(E_p)=\frac{2}{c(E_p^2-B^2)^{1/2}}\times\left[\arctan\left[\frac{E_p+B}{(E_p^2-B^2)^{1/2}}\tan(kc/2)\right]\pm\frac{\pi}{2}\right],\qquad |k|<\frac{\pi}{c}\ ,\tag{5.11}$$

where the upper (lower) sign in Eqs. (5.10) and (5.11) must be taken for $p>\nu$ ($p<\nu$). In the following, we demonstrate that our solutions corresponding to positive eigenvalues E_p, with $p=1,2,\ldots,$ are identical to Ifantis's solutions in the repulsive case ($b>0$). The latter amplitudes were calculated in local representation, therefore we need to calculate the Fourier transform of Eq. (5.4). Setting $\nu=0$ and transcribing Eq. (3.20) for the 1D case, the local amplitude $\eta_n(E_p)$ reads

$$\eta_n(E_p)=\sqrt{N}\,\frac{cN_p}{2\pi\alpha}nI_n(E_p)\ ,\tag{5.12}$$

with

$$I_n(E_p)=\int_{-\pi/c}^{\pi/c}dk\,\exp[iknc-ic\alpha f_k(E_p)]\ .\tag{5.13}$$

$I_n(E_p)$ is calculated in Appendix C. We get, for $p=1,2,\ldots,$

$$I_n(E_p)=\begin{cases}\dfrac{2\pi}{c}\dfrac{(\lambda_p)^{p-n}}{n}\displaystyle\sum_{m=0}^{p-1}\left[-\frac{2\alpha}{Bp}\right]^{m+1}\binom{p}{p-m-1}\frac{1}{m!}\times\dfrac{n(n+1)\cdots(n+m)}{(\lambda_p)^{m+1}}, & n\geq 0\\ 0, & n<0\ ,\end{cases}\tag{5.14}$$

where

$$\lambda_p=\left[E_p+\frac{\alpha}{p}\right]\Big/B\ .\tag{5.15}$$

Introducing Eqs. (5.10) and (5.14) in (5.12) we get as a result

$$\eta_n(E_p)=\begin{cases}C_p(\lambda_p)^{-n}\displaystyle\sum_{m=0}^{p-1}\left[-\frac{2\alpha}{Bp}\right]^m\binom{p}{p-m-1}\frac{1}{m!}\times\dfrac{n(n+1)\cdots(n+m)}{(\lambda_p)^{m+1}}, & n\geq 0\\ 0, & n<0\ ,\end{cases}\tag{5.16}$$

where C_p is a normalization constant given by

$$C_p=-\frac{2\alpha}{Bp^2}\left[\frac{\alpha}{pE_p}\right]^{1/2}(\lambda_p)^p\ .\tag{5.17}$$

Equation (5.16) for $n>0$ is identical to Ifantis's (non-normalized) solution, except for the normalization constant C_p. Since we started from normalized amplitudes $\xi_k(E_p)$ in k space, $\eta_n(E_p)$ are also normalized, i.e.,

$$\sum_n|\eta_n(E_p)|^2=1,\quad p=1,2,\ldots,\infty\ .\tag{5.18}$$

Finally we remark that $\eta_n(E_p)$ are exponentially localized in the region where the potential is positive (repulsive), i.e., $n>0$, and zero for $n\leq 0$ [consistent with Eq. (3.22)]. By similar considerations one can show that for $p=-1,-2,\ldots,-\infty$ the particle is exponentially localized in the region where the potential is negative (attractive), i.e., $n<0$, and has zero probability of being in the region $n\geq 0$. This latter property is quite natural, whereas the former result is remarkable: It implies that the quasi-1D Coulomb-type potential wall is perfectly impenetrable for the particle moving on the lattice. However, this opaqueness is due to the fact that transfer integrals other than between nearest neighbors have been neglected. Since the wave function associated with a discrete level vanishes at $n=0$, the particle is forced to localize at one *or* the other side of the potential barrier.

Finally, we attract the reader's attention to the fact that from Eqs. (4.16b), (4.30), and (4.36) we have

$$\Delta D(E)=\begin{cases}0, & |E|<B\\ \displaystyle\sum_p\delta(E-E_p), & |E|>B\end{cases}\tag{5.19}$$

and

$$D(E)=\begin{cases}D^0(E), & |E|<B\\ \displaystyle\sum_p\delta(E-E_p), & |E|>B\ .\end{cases}\tag{5.20}$$

This means that for $|E|<B$ the DOS remains *unaltered* by the artificial perturbation. Note that Eq. (5.19) apparently violates the sum rule

$$\int_{-\infty}^{\infty} dE\, D(E) = \int_{-\infty}^{\infty} dE\, D^0(E) , \tag{5.21}$$

which states that the total number of available states is unaffected by the perturbation. This discrepancy is explained by noting that the crystal has been supposed to be of infinite extension. Therefore it does not make much sense to compare the rhs with the left-hand side of Eq. (5.21) since both quantities are infinite.

VI. MATHEMATICAL ANALOGY WITH STARK-LADDER PROBLEM

Although the physical situations are different, in this section we point out the rather close mathematical analogy that exists between our model representing the Coulomb-type perturbation (2.1) and the so-called Stark-ladder system first described by Wannier,[2,3,9–11] representing the much simpler situation of an applied electric field. For this system Wannier predicted theoretically that the symmetry-breaking field creates quantized electronic states with equidistant energy levels (Stark-ladder levels) given by

$$\bar{E}_{p\mathbf{k}_\perp} = eFcp + \frac{c}{2\pi}\int_{-\pi/c}^{\pi/c} dk_3 \varepsilon_{\mathbf{k}} , \tag{6.1}$$

where p is an integer, $-e$ the electronic charge, $F=|\mathbf{F}|$ the electric field (it is supposed that $\mathbf{F}\|\mathbf{c}$), $\varepsilon_{\mathbf{k}}$ the zero-order energy-band dispersion (interband transitions are not taken into account and the band index λ is suppressed), c the lattice spacing in the $\mathbf{c}$ direction, and $\mathbf{k}_\perp$ denotes the transverse components of $\mathbf{k}$ vectors in the first Brillouin zone.

We stress that the analogy between the two completely different physical situations is of purely mathematical nature. Following step by step the calculations in Secs. II and III, we rederive the energies and wave functions of the Stark-ladder levels. Starting from the Hamiltonian

$$\begin{aligned} H &= H + \bar{V}_{\text{ext}}(\mathbf{r}) , \\ H^0 &= \frac{-\hbar^2\nabla}{2m_e} + V_L(\mathbf{r}) , \\ \bar{V}_{\text{ext}}(\mathbf{r}) &= eFr_3 , \end{aligned} \tag{6.2}$$

where $\bar{V}_{\text{ext}}(\mathbf{r})$ is the potential energy of the electron in the external electric field $\mathbf{F}$ applied along the $\mathbf{c}$ axis (all the other symbols are the same as in Sec. II), in analogy to Eq. (2.9) we rewrite the perturbation in Fourier space

$$\begin{aligned} \bar{W}(k_3-k_3') &= \frac{\Delta}{N}\sum_n n e^{-i(k_3-k_3')nc} \\ &= \frac{2\pi}{Nc}\frac{i\Delta}{c}\frac{\partial}{\partial k_3}\delta(k_3-k_3') . \end{aligned} \tag{6.3}$$

$\Delta = eFc$ is the potential-energy difference over one lattice cell. This expression is much simpler than the corresponding expression for the Coulomb-type perturbation [Eq. (3.2)]. Therefore the solutions can be found straightforwardly. The Schrödinger equation (3.4) becomes

$$(E-\varepsilon_{\mathbf{k}})\bar{\xi}_{\mathbf{k}_\perp k_3}(E) = \frac{i\Delta}{c}\frac{\partial}{\partial k_3}\bar{\xi}_{\mathbf{k}_\perp k_3}(E) \tag{6.4}$$

and is solved by

$$\bar{\xi}_{\mathbf{k}_\perp k_3}(E) = \bar{N}_E \exp\left[-\frac{ic}{\Delta}\int_{-\pi/c}^{k_3} dk_3'(E-\varepsilon_{\mathbf{k}_\perp k_3'})\right] . \tag{6.5}$$

According to Eq. (3.1) the eigenvalue equation reads

$$\exp\left[2\pi i\left[-\frac{c}{2\pi\Delta}\int_{-\pi/c}^{\pi/c} dk_3(E-\varepsilon_{\mathbf{k}})\right]\right] = 1, \tag{6.6}$$

which yields

$$\bar{E}_{p\mathbf{k}_\perp} = p\Delta + \frac{c}{2\pi}\int_{-\pi/c}^{\pi/c} dk_3 \varepsilon_{\mathbf{k}} . \tag{6.7}$$

Therefore the eigenstates of the Stark-ladder levels associated with $\bar{E}_{p\mathbf{k}_\perp}$ are given by

$$\begin{aligned} |\bar{\Phi}(\bar{E}_{p\mathbf{k}_\perp})\rangle &= \sum_{\mathbf{k}'} \bar{\xi}_{\mathbf{k}'}(\bar{E}_{p\mathbf{k}_\perp})|\mathbf{k}'\rangle , \\ \bar{\xi}_{\mathbf{k}'}(\bar{E}_{p\mathbf{k}_\perp}) &= \delta_{\mathbf{k}_\perp\mathbf{k}_\perp'}\bar{N}_{p\mathbf{k}_\perp} \\ &\quad\times\exp\left[-\frac{ic}{\Delta}\int_{-\pi/c}^{k_3'} d\kappa_3(\bar{E}_{p\mathbf{k}_\perp}-\varepsilon_{\mathbf{k}_\perp\kappa_3})\right] , \\ \bar{N}_{p\mathbf{k}_\perp} &= \bar{N} = \frac{1}{\sqrt{N}} . \end{aligned} \tag{6.8}$$

Note the remarkable mathematical resemblance between Eqs. (3.8) and (6.8). However, the physical properties of the levels found in the two models are completely different.

(i) The Stark-ladder energies are equidistant (with spacing Δ) *independently* of the dispersion $\varepsilon_{\mathbf{k}}$, whereas the Coulomb-type state energies depend on $\varepsilon_{\mathbf{k}}$ in a nontrivial way.

(ii) In the case of the Stark-ladder system, the quantization condition (3.1) gives rise to discrete levels only, signifying that the electric field completely breaks up the continuous spectrum of H^0 associated with the degree of freedom in the $\mathbf{c}$ direction. In contrast, Eq. (3.1) yields also continuous eigenvalues in the case of the Coulomb-type field.

(iii) The Stark-ladder states are regularly localized (i.e., the mean positions forming a "lattice"), their mean-squared position being determined by—roughly speaking—the ratio of the unperturbed bandwidth to Δ. The Coulomb-type states are localized essentially in the well (on the barrier) with diverging extensions as their energies tend to the lower (upper) band edge.

To conclude this section, we demonstrate how the Stark-ladder energies can be derived by means of a simple canonical transformation. For a thorough treatise on canonical transformations in solid-state physics we refer the reader to the book by Wagner.[12] We rewrite the Hamiltonian (6.2) in the WF representation corresponding to a particular band with energy dispersion $\varepsilon_{\mathbf{k}}$ (one-band approximation):

$$\bar{H}=H^0+\bar{V}_{\text{ext}} ,$$
$$H^0=\sum_{\rho,\rho'} t_{\rho'}|\rho+\rho'\rangle\langle\rho| , \tag{6.9}$$
$$\bar{V}_{\text{ext}}=\sum_{\rho} n\Delta|\rho\rangle\langle\rho| ,$$

where

$$|\rho\rangle=N^{-3/2}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\rho}|\rho\rangle ,$$
$$t_\rho=N^{-3}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\rho}\varepsilon_{\mathbf{k}} .$$

Consider the unitary transformation

$$T:\bar{H}=e^{-S}\bar{H}e^{S} \tag{6.10}$$

defined by

$$S=-\sum_{\substack{\rho,\rho' \\ (n'\neq 0)}} \frac{t_{\rho'}}{n'\Delta}|\rho+\rho'\rangle\langle\rho| , \tag{6.11}$$

with

$$\rho=\rho_\perp+n\mathbf{c} ,$$
$$\rho'=\rho'_\perp+n'\mathbf{c} .$$

The relevant commutators are

$$[\bar{V}_{\text{ext}},S]=-H^0+\sum_{\substack{\rho,\rho' \\ (n'=0)}} t_{\rho'}|\rho+\rho'\rangle\langle\rho| ,$$
$$[[\bar{V}_{\text{ext}},S],S]=0 , \tag{6.12}$$
$$[H^0,S]=0 ,$$

and we obtain

$$T:\bar{H}=\bar{V}_{\text{ext}}+\sum_{\substack{\rho,\rho' \\ (n'=0)}} t_{\rho'}|\rho+\rho'\rangle\langle\rho| . \tag{6.13}$$

Since the summation over ρ' must be carried out for $n'=0$, the effect of the transformation is to uncouple crystal planes perpendicular to the direction of the applied electric field (i.e., with different index n). Diagonalization of H is completed by performing a 2D Fourier transform with respect to the latteral degrees of freedom. Introducing

$$|\rho\rangle=\frac{1}{N}\sum_{\mathbf{k}_\perp} e^{-i\mathbf{k}_\perp\rho_\perp}|n,\mathbf{k}_\perp\rangle , \tag{6.14}$$

we find

$$T:\bar{H}=\sum_{n\mathbf{k}_\perp}\bar{E}_{n\mathbf{k}_\perp}|n,\mathbf{k}_\perp\rangle\langle n,\mathbf{k}_\perp| , \tag{6.15}$$

with

$$\bar{E}_{n\mathbf{k}_\perp}=n\Delta+\sum_{\rho'} e^{-i\mathbf{k}_\perp\cdot\rho'_\perp}\delta_{n',0}t_{\rho'} . \tag{6.16}$$

By considering the 3D Fourier transform of $t_{\rho'}$, one can immediately identify Eqs. (6.7) and (6.16). The associated Stark-ladder states are obtained by inversion of the canonical transformation:

$$|\bar{\Phi}(\bar{E}_{n\mathbf{k}_\perp})\rangle=e^{S}|n,\mathbf{k}_\perp\rangle=\frac{1}{N}\sum_{\rho_\perp} e^{i\mathbf{k}_\perp\cdot\rho_\perp}e^{S}|\rho\rangle . \tag{6.17}$$

Comparing Eqs. (6.8) with (6.17), we have

$$\bar{\xi}_{\mathbf{k}'}(\bar{E}_{n\mathbf{k}_\perp})=\frac{1}{N}\sum_{\rho_\perp} e^{i\mathbf{k}_\perp\cdot\rho_\perp}\langle\mathbf{k}'|e^{S}|\rho\rangle . \tag{6.18}$$

VII. CONCLUSION

In this work we discussed the influence of a quasi-1D artificial Coulomb-type perturbation on the single-electron spectrum of a perfect crystalline structure. It was shown that for a system with narrow energy bands the problem can be reduced to an analytically solvable model Hamiltonian which consists of a single band of the perfect crystal in the presence of a nearly antisymmetric Coulomb-type potential. This idealized model has the virtue of being applicable to (narrow) bands with arbitrary energy dispersion and of explicitly taking into account the discrete structure of the lattice. Obviously the physical interest of the presented model lies principally in the half-sided version: a point charge placed at one end of a 1D dielectric crystal.

In the case of nearest-neighbor interactions we have *shown* that the two-sided, artificial potential gives rise to discrete states that are identical to Ifantis's solutions of the corresponding (repulsive or attractive) one-sided model. Whenever more general band dispersions are dominated by nearest-neighbor interactions, we *expect* that our two-sided solutions are still of sufficient relevance for the one-sided type of problem.

However, if next-nearest-neighbor interactions become important, the solutions of the two models differ substantially. Nevertheless, it is still possible to use, by a simple generalization of the Hamiltonian H in Eq. (2.1), the solutions presented in this publication. Since the GF associated with H is explicitly known, we can—by inclusion of an additional term to the Hamiltonian of the form $U|-1\rangle\langle-1|$—calculate the new eigenenergies and eigenfunctions according to the adapted form of Eq. (4.4). Letting U tend to infinity, we again obtain exact levels that are completely localized either in the region $n>0$ or $n<-1$. In Sec. VI, we used a nearly identical mathematical treatment as in Secs. II and III to diagonalize the well-known Stark-ladder Hamiltonian. The reason for this close mathematical similarity lies in the special form of the perturbations: The Fourier transform of the $1/n$ potential (n potential) essentially is the primitive (derivative) of Dirac's δ distribution. As far as we know, these are the only two models with "long-range" perturbation potentials in the presence of a *general* zero-order band dispersion that allow an analytic solution.

ACKNOWLEDGMENTS

The authors would like to thank G. Seibold for a careful reading of the manuscript and G. Zavt for helpful discussions. This work was financially supported by the Deutsche Forschungsgemeinschaft (SFB 329).

APPENDIX A

In the following calculation we suppose that the k_3 values in the first Brillouin zone form a quasicontinuum, i.e., $N \gg 1$. It is then possible to derive and integrate with respect to k_3. According to Eq. (2.9) we consider

$$W(k)=\frac{\alpha}{N}\sum_n \frac{e^{-iknc}}{n-\nu} . \tag{A1}$$

For $k=0$ one obtains

$$W(0)=-\frac{\alpha\pi}{N}\cot(\pi\nu) . \tag{A2}$$

Note that

$$\frac{d}{dk}[e^{ik\nu c}W(k)]=-ic\alpha\frac{1}{N}\sum_n e^{-ik(n-\nu)c}=-\frac{2\pi i\alpha}{N}\delta(k) . \tag{A3}$$

Integration from $-\pi/c$ to k yields

$$W(k)=e^{-ik\nu c}\left[-\frac{2\pi i\alpha}{N}\Theta(k)+W\left[-\frac{\pi}{c}\right]e^{-i\pi\nu}\right] . \tag{A4}$$

We finally need to calculate (see Ref. 13, p. 40)

$$W\left[-\frac{\pi}{c}\right]=\frac{\alpha}{N}\sum_n\frac{(-1)^n}{n-\nu}=-\frac{\alpha}{N}\frac{\pi}{\sin(\pi\nu)} . \tag{A5}$$

This yields the result

$$W(k)=-\frac{\alpha}{N}\pi e^{-ik\nu c}\left[2i\Theta(k)+\frac{e^{-i\pi\nu}}{\sin(\pi\nu)}\right] , \tag{A6}$$

where the singular behavior at $k=0$ [Eq. (A2)] has been taken into account by defining the step function as

$$\Theta(k)=\begin{cases}1, & k>0\\ \frac{1}{2}, & k=0\\ 0, & k<0 .\end{cases} \tag{A7}$$

APPENDIX B

We calculate the matrix elements $T_{\mathbf{k}\mathbf{k}'}(z)$ starting from Eq. (4.5)

$$T_{\mathbf{k}\mathbf{k}'}(z)=\langle\mathbf{k}|V_{\text{ext}}|\mathbf{k}'\rangle+\langle\mathbf{k}|V_{\text{ext}}G^0(z)T(z)|\mathbf{k}'\rangle . \tag{B1}$$

Inserting Eqs. (2.8) and (4.2) yields

$$T_{\mathbf{k}\mathbf{k}'}=\delta_{\mathbf{k}_\perp\mathbf{k}'_\perp}W(k_3-k'_3)+\sum_{k''_3}W(k_3-k''_3)\frac{1}{z-\varepsilon_{\mathbf{k}_\perp k''_3}}T_{(\mathbf{k}_\perp k''_3)(\mathbf{k}'_\perp k'_3)} . \tag{B2}$$

For $N\gg1$ we replace the summation in Eq. (B2) by integration over the first Brillouin zone. Deriving

$$\tilde{T}_{\mathbf{k}\mathbf{k}'}=e^{i(k_3-k'_3)\nu c}T_{\mathbf{k}\mathbf{k}'} \tag{B3}$$

with respect to k_3, we get

$$\frac{\partial}{\partial k_3}\tilde{T}_{\mathbf{k}\mathbf{k}'}=-\frac{2\pi i\alpha}{N}\delta_{\mathbf{k}_\perp\mathbf{k}'_\perp}\delta(k_3-k'_3)-ic\alpha\frac{1}{z-\varepsilon_{\mathbf{k}}}\tilde{T}_{\mathbf{k}\mathbf{k}'} . \tag{B4}$$

Here again we made use of the very special Fourier transform of the perturbation potential [see Eq. (3.3)]. Solving Eq. (B4) for $T_{\mathbf{k}\mathbf{k}'}$ we obtain

$$T_{\mathbf{k}\mathbf{k}'}(z)=e^{-i[k_3\nu+\alpha f_{k_3}(z,\mathbf{k}_\perp)]c}\left[e^{-i\pi\nu}T_{(\mathbf{k}_\perp-\pi/c)\mathbf{k}'}-\frac{2\pi i\alpha}{N}\delta_{\mathbf{k}_\perp\mathbf{k}'_\perp}\int_{-\pi/c}^{k_3}d\kappa_3 e^{i[\kappa_3\nu+\alpha f_{\kappa_3}(z,\mathbf{k}_\perp)]c}\delta(\kappa_3-k'_3)\right] . \tag{B5}$$

The first term on the rhs can be determined by exploiting the fact that $T_{\mathbf{k}\mathbf{k}'}(z)$ must be a periodic function in reciprocal space. By analogy with Eq. (2.10) this prescription reads

$$T_{\mathbf{k}+\mathbf{G}\mathbf{k}'}=T_{\mathbf{k}\mathbf{k}'+\mathbf{G}'}=T_{\mathbf{k}\mathbf{k}'} , \tag{B6}$$

where $\mathbf{G}$ and $\mathbf{G}'$ are reciprocal lattice vectors. In particular, we have

$$T_{(\mathbf{k}_\perp\pi/c)\mathbf{k}'}=T_{(\mathbf{k}_\perp-\pi/c)\mathbf{k}'} . \tag{B7}$$

This yields

$$T_{(\mathbf{k}_\perp\pi/c)\mathbf{k}'}=\frac{2\pi i\alpha}{N}\delta_{\mathbf{k}_\perp\mathbf{k}'_\perp}\times\frac{e^{-\pi i\nu-ic\alpha f_{\pi/c}(z,\mathbf{k}_\perp)}}{e^{-2\pi i\nu-ic\alpha f_{\pi/c}(z,\mathbf{k}_\perp)}-1}F_{k_3}(k'_3) \tag{B8}$$

with

$$F_{k_3}(k'_3)=\int_{-\pi/c}^{k_3}d\kappa_3 e^{i[\kappa_3\nu+\alpha f_{\kappa_3}(z,\mathbf{k}_\perp)]c}\delta(\kappa_3-k'_3) . \tag{B9}$$

Introducing Eq. (B9) into Eq. (B5) we obtain

$$T_{\mathbf{k}\mathbf{k}'}=\frac{2\pi i\alpha}{N}\delta_{\mathbf{k}_\perp\mathbf{k}'_\perp}e^{-i[k_3\nu+\alpha f_{k_3}(z,\mathbf{k}_\perp)]c}\times\left[\frac{F_{\pi/c}(k'_3)}{1-e^{2\pi i\nu+ic\alpha f_{\pi/c}(z,\mathbf{k}_\perp)}}-F_{k_3}(k'_3)\right] . \tag{B10}$$

For $|k_3|,|k'_3|<\pi/c$ we have

$$F_{k_3}(k'_3)=e^{i[k'_3\nu+\alpha f_{k'_3}(z,\mathbf{k}_\perp)]c}\Theta(k_3-k'_3) , \tag{B11}$$

and therefore

$$T_{\mathbf{k}\mathbf{k}'}=\frac{2\pi i\alpha}{N}\delta_{\mathbf{k}_\perp\mathbf{k}'_\perp}e^{i\{(k'_3-k_3)\nu+\alpha[f_{k'_3}(z,\mathbf{k}_\perp)-f_{k_3}(z,\mathbf{k}_\perp)]\}c}\times[(1-e^{2\pi i\nu+ic\alpha f_{\pi/c}(z,\mathbf{k}_\perp)})^{-1}-\Theta(k_3-k'_3)]\ . \tag{B12}$$

If we wish to show that $T_{\mathbf{k}\mathbf{k}'}(z)$ is periodic with respect to k_3 and k'_3, we have to use Eq. (B10) rather than (B12) [note that the $\delta(x)$ distribution must be considered as being periodic in x, consistently with, e.g., Eq. (A3)].

APPENDIX C

We calculate the quantity

$$I_n(E_p)=\int_{-\pi/c}^{\pi/c}dk\,\exp[iknc-ic\alpha f_k(E_p)],\qquad p=1,2,\ldots \tag{C1}$$

in the case of a 1D band dispersion $\varepsilon_k=B\cos kc$, for which

$$f_k(E_p)=\frac{2}{c(E_p^2-B^2)^{1/2}}\times\left[\arctan\left[\frac{E_p+B}{(E_p^2-B^2)^{1/2}}\tan\frac{kc}{2}\right]+\frac{\pi}{2}\right]\ . \tag{C2}$$

Defining

$$\omega_p=\frac{E_p+B}{(E_p^2-B^2)^{1/2}} \tag{C3}$$

and using Eq. (5.9) (setting $\nu=0$), we get

$$I_n(E_p)=(-1)^p\int_{-\pi/c}^{\pi/c}dk\,\exp\left[iknc-2ip\arctan\left[\omega_p\tan\frac{kc}{2}\right]\right]\ . \tag{C4}$$

By performing the variable substitution $z=\exp(-ikc)$ and integrating along the unit circle in mathematically positive sense, Eq. (C3) becomes

$$I_n(E_p)=\frac{(-1)^p}{ic}\oint\frac{dz}{z^{n+1}}\exp\left[-2ip\arctan\left[i\omega_p\frac{z-1}{z+1}\right]\right]\ . \tag{C5}$$

We make use of the functional identity $\arctan(ix)=(i/2)\ln[(1+x)/(1-x)]$ and find

$$I_n(E_p)=\frac{(-1)^p}{ic}\oint\frac{dz}{z^{n+1}}[h_p(z)]^p\ , \tag{C6}$$

where

$$h_p(z)=-\lambda_p\frac{z-(1/\lambda_p)}{z-\lambda_p} \tag{C7}$$

and

$$\lambda_p=\frac{\omega_p+1}{\omega_p-1}\ . \tag{C8}$$

Note that for $p=1,2,\ldots$ we have $\omega_p>1$ and $\lambda_p>1$, therefore $h_p(z)$ has a simple pole outside the unit circle at $z=\lambda_p$. Since for $n<0$ the integrand in Eq. (C6) is analytic inside the unit circle, we conclude immediately that

$$I_n(E_p)=0,\quad n<0,\ p=1,2,\ldots\ . \tag{C9}$$

For $n\geq 0$ we choose to close the integration path at infinity. We get

$$I_n(E_p)=-\frac{(-1)^p}{ic}2\pi i\ \mathrm{Res}\left[\frac{[h_p(z)]^p}{z^{n+1}},z=\lambda_p\right]\ , \tag{C10}$$

where $\mathrm{Res}[f(z),z_0]$ means taking the residue of f at $z=z_0$. A straightforward calculation yields

$$I_n(E_p)=-\frac{2\pi}{c}\frac{(\lambda_p)^{p-n}}{n}\sum_{m=0}^{p-1}\frac{p!n(n+1)\cdots(n+m)}{m!(p-m-1)!(m+1)!}(-1)^m\left[1-\frac{1}{\lambda_p^2}\right]^{m+1}\ . \tag{C11}$$

By some algebraic manipulations Eq. (C8) can be rewritten as

$$\lambda_p=\frac{E_p+\frac{\alpha}{p}}{B} \tag{C12}$$

and also

$$1-\frac{1}{\lambda_p^2}=\frac{2\alpha}{pB}\frac{1}{\lambda_p} \ . \tag{C13}$$

Joining Eqs. (C11)—(C13) and Eq. (C9) we finally get

$$I_n(E_p)=\begin{cases}\dfrac{2\pi}{c}\dfrac{(\lambda_p)^{p-n}}{n}\displaystyle\sum_{m=0}^{p-1}\left[-\frac{2\alpha}{pB}\right]^{m+1}\begin{bmatrix}p\\p-m-1\end{bmatrix}\frac{n(n+1)\cdots(n+m)}{m!(\lambda_p)^{m+1}}, & n\geq 0\\ 0, \quad n<0 \ .\end{cases} \tag{C14}$$

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