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Simple scheme for surface-band calculations. II. The Green's function

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We present a very simple scheme for calculating the Green's function of a semi-infinite surface system described within a localized orbital basis. By generating a series of matching conditions for the Green's function we can calculate its matrix elements much faster than any method currently available. We present the formalism for a specific class of systems and include a simple example to illustrate the use of the technique.

I. INTRODUCTION

In a previous paper[1] (hereafter referred to as I), we introduced a simple and efficient scheme for calculating the surface-energy bands, wave functions and decay lengths for semi-infinite surface systems. These systems were described by Hamiltonians based on localized-orbital representations. The essential idea was to generate matching conditions for the wave function using the transfer-matrix approach.[2-5] The transfer matrix was defined so that it directly linked the wave function on pairs of neighboring layer orbitals. The eigenvalues and eigenfunctions of this transfer matrix provided all the information necessary to calculate the electronic structure of the system.

In this paper we introduce the appropriate extensions needed in order to calculate the matrix elements of the Green's function within this approach. This scheme, in fact, allows one to obtain these matrix elements much faster than any other technique currently available. At present, there are two very popular Green's-function methods[6-11] used in surface calculations that are roughly equivalent in computational time. The "Slater-Koster" method[6-8] obtains the surface Green's function from a knowledge of the bulk Green's function. It has the disadvantage of requiring time-consuming integrations over a large number of $\vec{k}_\perp$'s in order to get accurate results. The "effective-field" method[9-11] obtains the surface Green's function using a continued-fraction approach, where

$$G^s_{00}(E)=[E-H_{00}-H_{01}\Phi(E)]^{-1} \tag{1}$$

and

$$\Phi(E)=[E-H_{00}-H_{01}\Phi(E)]^{-1}H^{+}_{01}\,. \tag{2}$$

Zero labels the surface layer and Φ is called an effective field or sometimes a "transfer matrix" (not to be confused with the transfer matrix T defined in I and in this paper). The disadvantage of this approach is that Φ needs to be calculated self-consistently in general, and this involves many iterations (~50) for convergence. The approach that is presented here enables one to calculate Φ, and hence the Green's function, directly, from a simple diagonalization of the transfer matrix T.

The format of this paper is as follows. In Sec. II we discuss the basic formalism, restricting ourselves to a specific class of surface systems, the extension to more general systems being straightforward. In Sec. III we present a simple model to illustrate the use of this method and choose the same model system as in I. In Sec. IV we present rigorous arguments which justify certain assumptions made in Sec. II. Finally in Sec. V we show how the results of the previous sections, and the method described in I, can be unified.

What emerges then, from the results of I and this paper, is a very efficient general scheme for calculating the elementary excitations at surfaces, where one can *directly* obtain the projected band structure, wave functions, surface bands, decay lengths, *and* Green's-function matrix elements from the eigenanalysis of one simple transfer matrix T.

II. FORMALISM

We begin by considering a bulk crystal. We may think of it as an infinite stack of principal layers. As in I, a principal layer is defined as the smallest group of neighboring atomic layers such that only nearest-neighbor interactions between principal layers exist. The schematic representation of this system for each $\vec{k}_\|$ is shown in Fig. 1. We have assumed here that there are only two types of inequivalent principal layers in the system. (The generalization to many inequivalent principal layers is straightforward and follows arguments similar to those presented in I.) If there are μ layer orbitals in each principal layer, the Bloch state of any orbital ϕ_α in any principle layer l is given by

$$\psi_{l,\alpha}(\vec{k}_\|)=\frac{1}{\sqrt{N_\|}}\sum_{\vec{R}_\|} e^{i\vec{k}_\|\cdot\vec{R}_\|}\,\phi_\alpha(l,\vec{R}_\|)\,, \tag{3}$$

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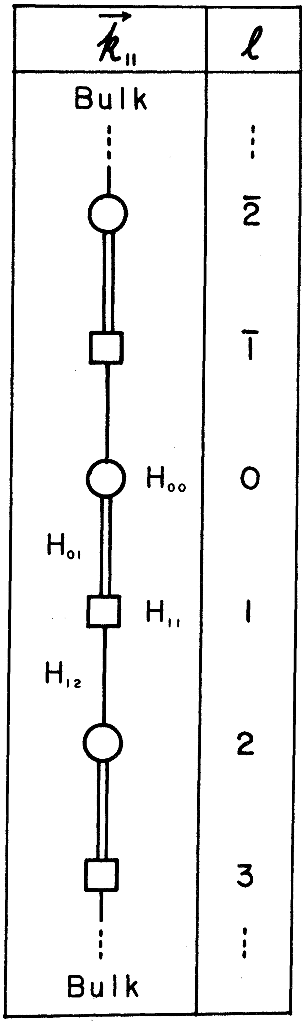

FIG. 1. For each $\vec{k}_{\|}$, a crystal can be represented as an infinite one-dimensional chain of principal layers (l). The circles and squares represent two types of principal layers whose self-interaction matrices are given by H_{00} and H_{11}, respectively. The double and single lines represent the interaction matrices between principal layers.

where $\alpha = 1, 2, \ldots, \mu$ and $\vec{R}_{\|}$ is a lattice vector. The matrix elements of the Green's function are then given by

$$[G_{ll'}(\vec{k}_{\|}, E^+)]_{\alpha\beta} = \left\langle \psi_{l,\alpha}(\vec{k}\ ) \left| \frac{1}{E^+ - H} \right| \psi_{l',\beta}(\vec{k}_{\|}) \right\rangle , \tag{4}$$

where $E^+ = E + i\delta$. We now choose the zeroth principle layer as a reference so that the set of matrix elements $\{G_{0,l};\ -\infty < l < \infty\}$ will satisfy the following equations:

$$(E^+ - H_{00})\, G_{00} - H_{01} G_{10} - H_{12}^{+} G_{\bar{1}0} = 1 \tag{5}$$

with

$$[H_{ll'}(\vec{k}_{\|})]_{\alpha\beta} = \sum_{\vec{R}_{\|}} e^{i\vec{k}_{\|}\cdot\vec{R}_{\|}} \langle \phi_\alpha(l, \vec{0}) | H | \phi_\beta(l', \vec{R}_{\|}) \rangle \tag{6}$$

and

$$\begin{pmatrix} G_{2n,0} \\ G_{2n+1,0} \end{pmatrix} = T^n \begin{pmatrix} G_{1,0} \\ G_{0,0} \end{pmatrix}, \tag{7}$$

$$\begin{pmatrix} G_{2\bar{n},0} \\ G_{2\bar{n}-1,0} \end{pmatrix} = T^{-n} \begin{pmatrix} G_{0,0} \\ G_{\bar{1},0} \end{pmatrix}, \tag{8}$$

with

$$T(\vec{k}_{\|}, E^+) = \begin{pmatrix} H_{01}^{-1}(E^+ - H_{00}) & -H_{01}^{-1} H_{12}^{+} \\ 1 & 0 \end{pmatrix} \times \begin{pmatrix} H_{12}^{-1}(E^+ - H_{11}) & -H_{12}^{-1} H_{01}^{+} \\ 1 & 0 \end{pmatrix}, \tag{9}$$

where the G_{l0}'s and $H_{ll'}$'s are $\mu \times \mu$ matrices and Eq. (9) defines the transfer matrix T. This transfer matrix is slightly different from the one defined in I in that the E^+ are now complex. This is discussed in more detail in Sec. IV. An immediate practical consequence of this, however, is that half the eigenvalues of $T(\vec{k}_{\|}, E^+)$ have modulus less than 1 and half have modulus greater than 1. This is true even for energies in the bulk allowed region.

Consider now $\vec{e}_\beta(\vec{k}_{\|}, E^+)$, $\beta = 1, 2, \ldots, 2\mu$ to be the 2μ-normalized eigenvectors of $T(\vec{k}_{\|}, E^+)$ with respective eigenvalues $\lambda_\beta(\vec{k}_{\|}, E^+)$. Let us assume that $|\lambda_\beta| < 1$ when $1 \leq \beta \leq \mu$ and $|\lambda_\beta| > 1$ for $\mu + 1 \leq \beta \leq 2\mu$. In order for the Green's function to satisfy (7) and (8) and remain normalizable, one must only retain the eigenvalues $|\lambda_\beta| < 1$ when T is diagonalized in (7) and only retain $|\lambda_\beta| > 1$ in (8). This implies that $\binom{G_{2n+1,0}}{G_{2n,0}}$ and $\binom{G_{2\bar{n},0}}{G_{2\bar{n}-1,0}}$ can be expanded in terms of the $\vec{e}_\beta$'s with $1 \leq \beta \leq \mu$ and $\mu + 1 \leq \beta \leq 2\mu$, respectively. In particular, we may write

$$\begin{pmatrix} G_{10} \\ G_{00} \end{pmatrix} = \begin{pmatrix} S_2 \mathcal{G}_1 \\ S_1 \mathcal{G}_1 \end{pmatrix} \tag{10}$$

and

$$\begin{pmatrix} G_{00} \\ G_{\bar{1}0} \end{pmatrix} = \begin{pmatrix} S_4 \mathcal{G}_2 \\ S_3 \mathcal{G}_2 \end{pmatrix} \tag{11}$$

with

$$\begin{aligned} (S_1)_{\alpha\gamma} &= (\vec{v}_\alpha \cdot \vec{e}_\gamma)\,, \\ (S_2)_{\alpha\gamma} &= (\vec{u}_\alpha \cdot \vec{e}_\gamma)\,, \\ (S_3)_{\alpha\gamma} &= (\vec{v}_\alpha \cdot \vec{e}_{\gamma+\mu})\,, \\ (S_4)_{\alpha\gamma} &= (\vec{u}_\alpha \cdot \vec{e}_{\gamma+\mu})\,, \end{aligned} \tag{12}$$

where $\gamma = 1, 2, \ldots, \mu$, and $\vec{u}_\alpha$ and $\vec{v}_\alpha$, $\alpha = 1, 2, \ldots, \mu$

are 2μ-dimensional column vectors with components given by $(\vec{u}_\alpha)_i = \delta_{\alpha, i}$ and $(\vec{v}_\alpha)_i = \delta_{\alpha+\mu, i}$. The $\mu \times \mu$ matrices $\mathscr{G}_1$ and $\mathscr{G}_2$ represent the unknown expansion coefficients. From (10) and (11) these matrices are related by

$$\mathscr{G}_2 = S_4^{-1} S_1 \mathscr{G}_1 , \tag{13}$$

Substituting (10), (11), and (13) into (5) we obtain

$$\mathscr{G}_1 = [(E^+ - H_{00}) S_1 - H_{01} S_2 - H_{12}^+ S_3 S_4^{-1} S_1]^{-1} \tag{14}$$

or

$$G_{00} = [(E^+ - H_{00}) - H_{01} S_2 S_1^{-1} - H_{12}^+ S_3 S_4^{-1}]^{-1} . \tag{15}$$

Equation (15) is isomorphic to the equation one obtains for G_{00} in the effective-field method,[9-11] namely,

$$G_{00} = [(E^+ - H_{00}) - H_{01} \Phi_1 - H_{12}^+ \Phi_2]^{-1} . \tag{16}$$

Thus one immediately identifies the effective fields

$$\Phi_1(\vec{k}_\parallel, E^+) = S_2(\vec{k}_\parallel, E^+) S_1^{-1}(\vec{k}_\parallel, E^+) \tag{17}$$

and

$$\Phi_2(\vec{k}_\parallel, E^+) = S_3(\vec{k}_\parallel, E^+) S_4^{-1}(\vec{k}_\parallel, E^+) . \tag{18}$$

Therefore one is now able to calculate the fields directly by diagonalizing the transfer matrix T rather than performing many iterations as in (2).

The surface Green's function is now obtained at once from

$$G_{00}^{s_1} = [(E^+ - H_{00}) - H_{01} S_2 S_1^{-1}]^{-1} \tag{19}$$

or

$$G_{00}^{s_2} = [(E^+ - H_{00}) - H_{12}^+ S_3 S_4^{-1}]^{-1} , \tag{20}$$

depending on which surface one is interested in. The local density of states is then given in general by

$$n_l(\vec{k}_\parallel, E) = -\frac{1}{\pi} \operatorname{Im}[\operatorname{tr} G_{ll}(\vec{k}_\parallel, E^+)] . \tag{21}$$

III. AN EXAMPLE

Let us consider, as in I, a semi-infinite two-dimensional honeycomb lattice as shown in Fig. 2(a). We assume there is an s orbital on each atom and that they interact only through first-neighbor ($V_1 = -1.0$) and second-neighbor ($V_2 = -0.1$) interactions. It is also assumed that the s orbitals are orthonormal.

Since the atoms interact through second neighbors, each principal layer must contain two atomic layers. This is shown schematically in Fig. 2(b). Note that there is only *one* inequivalent principal layer for the system in this example. Therefore the matrix elements of the Hamiltonian between principal layers must have $H_{00} = H_{11}$ and $H_{01} = H_{12}$. The transfer matrix of Eq. (9) then becomes

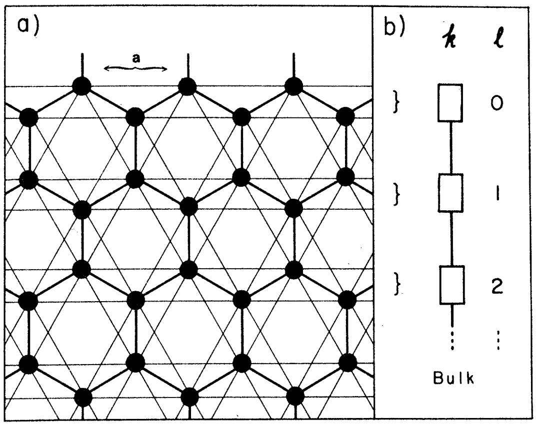

FIG. 2. A semi-infinite two-dimensional honeycomb lattice represented as (a) a system of atoms (black dots) with nearest-neighbor interactions V_1 (thick solid lines) and second-neighbor interactions V_2 (thin solid lines). The atoms along the surface are spaced a distance a apart. (b) A chain of principal layers (l) for each wave vector k in the surface Brillouin zone. Each principal layer (represented as a rectangle) contains two atomic layers as shown.

$$T(k, E^+) = \begin{pmatrix} H_{01}^{-1}(E^+ - H_{00}) & -H_{01}^{-1} H_{01}^+ \\ 1 & 0 \end{pmatrix}^2 \tag{22}$$

with

$$H_{00} = \begin{pmatrix} V_2(\eta + \eta^*) & V_1(1 + \eta) \\ V_1(1 + \eta^*) & V_2(\eta + \eta^*) \end{pmatrix} \tag{23}$$

and

$$H_{01} = \begin{pmatrix} V_2(1 + \eta) & 0 \\ V_1 & V_1(1 + \eta) \end{pmatrix} , \tag{24}$$

where $\eta = e^{ika}$ and a is the lattice constant of the surface line.

The Green's function at any (k, E^+) can now be calculated directly by diagonalizing $T(k, E^+)$. As noted earlier the eigenvalues of T will have the property that two will have modulus less than 1 and two greater than 1. For example, in Table I we list the modulus of these eigenvalues at $k = 0$ for a series of energies with $\delta = 0.01$. We note that in certain regions of energy there are two eigenvalues with modulus very close to 1. These moduli actually approach 1 as $\delta \to 0$ as can be seen in the second panel of Table I where $\delta = 10^{-4}$. These regions of energy define the allowed bulk solutions as in I.

If we label the two eigenvectors of T with modulus less than 1 by $\vec{e}_{\alpha_1}$ and $\vec{e}_{\alpha_2}$ and the other two by $\vec{e}_{\alpha_3}, \vec{e}_{\alpha_4}$, we have from (12)

TABLE I. The moduli of the eigenvalues $\{\lambda_i\}$ of the transfer matrix at $k=0$ are listed for two values of the imaginary part of the energy δ and a series of energies.

	$\delta=0.01$				$\delta=0.0001$			
E	$\lvert\lambda_1(E+i\delta)\rvert$	$\lvert\lambda_2(E+i\delta)\rvert$	$\lvert\lambda_3(E+i\delta)\rvert$	$\lvert\lambda_4(E+i\delta)\rvert$	$\lvert\lambda_1(E+i\delta)\rvert$	$\lvert\lambda_2(E+i\delta)\rvert$	$\lvert\lambda_3(E+i\delta)\rvert$	$\lvert\lambda_4(E+i\delta)\rvert$
−4.0	7262.3125	5.4799	0.1821	0.0001	7262.3125	5.4774	0.1828	0.0001
−3.8	6990.3125	3.3631	0.2975	0.0001	6990.3125	3.3619	0.2977	0.0001
−3.6	6721.9766	1.2077	0.8290	0.0001	6721.9727	1.0062	0.9962	0.0001
−3.4	6457.3165	1.0324	0.9695	0.0001	6457.3125	1.0016	1.00053	0.0001
−3.2	6196.3594	1.0239	0.9780	0.0001	6196.3555	1.00124	1.00078	0.0001
−3.0	5939.1289	1.0198	0.9811	0.0002	5939.1250	1.0007	1.0003	0.0002
−2.8	5685.6406	1.0178	0.9831	0.0002	5685.6328	1.0006	1.0003	0.0002
−2.6	5435.9023	1.0165	0.9843	0.0002	5435.9023	1.0005	1.0002	0.0002
−2.4	5189.9727	1.0160	0.9853	0.0002	5189.9727	1.0005	1.0002	0.0002
−2.2	4947.8516	1.0156	0.9858	0.0002	4947.8516	1.0008	1.0005	0.0002
−2.0	4709.5742	1.0148	0.9854	0.0002	4709.5703	1.0003	1.0000	0.0002
−1.8	4475.1562	1.0149	0.9854	0.0002	4475.1523	1.0002	0.9999	0.0002
−1.6	4244.6328	1.0153	0.9850	0.0002	4244.6250	1.0001	0.9999	0.0002
−1.4	4018.0313	1.0150	0.9839	0.0002	4018.0210	1.0000	0.9996	0.0002
−1.2	3795.3696	1.0178	0.9820	0.0003	3795.3589	0.9998	0.9994	0.0002
−1.0	3576.6851	1.0230	0.9772	0.0003	3576.6743	1.0002	0.9992	0.0003
−0.8	3362.0034	1.1381	0.8785	0.0003	3361.9922	1.0169	0.9830	0.0003
−0.6	3151.3623	2.1865	0.4572	0.0003	3151.3516	2.1860	0.4573	0.0003
−0.4	2944.7891	2.8701	0.3483	0.0003	2944.1773	2.8697	0.3484	0.0003
−0.2	3742.3140	3.3999	0.2941	0.0004	2742.3018	3.3996	0.2941	0.0003
0.0	2543.9687	3.7748	0.2649	0.0004	2543.9557	3.7745	0.2649	0.0004
0.2	2349.7840	3.9731	0.2516	0.0004	2349.7700	3.9740	0.2516	0.0004
0.4	2159.7847	3.9731	0.2517	0.0005	2159.7705	3.9728	0.2517	0.0005
0.6	1973.9981	3.7458	0.2670	0.0005	1973.9829	3.7455	0.2670	0.0005
0.8	1792.4399	3.2668	0.3061	0.0006	1792.4233	3.2666	0.3062	0.0006
1.0	1615.1157	2.4984	0.4003	0.0006	1615.0986	2.4976	0.4004	0.0006
1.2	1442.0156	1.1714	0.8547	0.0007	1441.9961	1.0088	0.9932	0.0007
1.4	1273.1001	1.0323	0.9677	0.0008	1273.0786	0.9999	0.9942	0.0008
1.6	1108.2764	1.0298	0.9708	0.0009	1108.2519	1.0001	0.9996	0.0009
1.8	947.3667	1.0329	0.9691	0.0011	947.3384	1.0007	1.0000	0.0011
2.0	790.0112	1.0392	0.9622	0.0012	789.9775	1.0006	0.9998	0.0012
2.2	635.4756	1.0580	0.9455	0.0015	635.4311	1.0005	0.9994	0.0015
2.4	482.0601	1.4750	0.6757	0.0020	481.9956	1.0716	0.9298	0.0020
2.6	324.6887	13.3688	0.0742	0.0030	324.5581	13.3638	0.0742	0.003
2.8	123.0060	78.0861	0.0123	0.0081	100.2062	95.8268	0.0104	0.0103
3.0	134.4801	126.7525	0.0080	0.0074	130.5884	130.5115	0.0077	0.0077

$$S_1=\begin{bmatrix} e_{\alpha_1,3} & e_{\alpha_2,3} \\ e_{\alpha_1,4} & e_{\alpha_2,4} \end{bmatrix}, \tag{25}$$

$$S_2=\begin{bmatrix} e_{\alpha_1,1} & e_{\alpha_2,1} \\ e_{\alpha_1,2} & e_{\alpha_2,2} \end{bmatrix}, \tag{26}$$

$$S_2=\begin{bmatrix} e_{\alpha_3,3} & e_{\alpha_4,3} \\ e_{\alpha_3,4} & e_{\alpha_4,4} \end{bmatrix}, \tag{27}$$

$$S_4=\begin{bmatrix} e_{\alpha_3,1} & e_{\alpha_4,1} \\ e_{\alpha_3,2} & e_{\alpha_4,2} \end{bmatrix}. \tag{28}$$

Substitution of (25)–(28) into (15) gives the bulk Green's function. Actually in this example $H_{01}S_2S_1^{-1}=H_{01}^{+}S_3S_4^{-1}$ so that

$$G_{00}(k,E^{+})=[(E^{+}-H_{00})-2H_{01}S_2S_1^{-1}]^{-1}. \tag{29}$$

The corresponding local densities of states obtained from (21) are shown in Fig. 3 for a series of energies and surface k points. We note that the density of states at $k=0$ defines band edges which are consistent with the allowed bulk solutions in Table I. The thin solid lines in the E-vs-k plane help define the projected band structure. We also note that at $k\to 2\pi/3a$ the gap becomes zero. At $k=\pi/a$ the off-diagonal elements of the self-interaction (H_{00}) of the principal layers vanish so that the system decouples completely into pairs of atomic layers and the transfer matrix loses meaning. The density of states is then given simply by two delta functions at $E=-2V_2\pm V_1$.

The Green's function for the surface system is

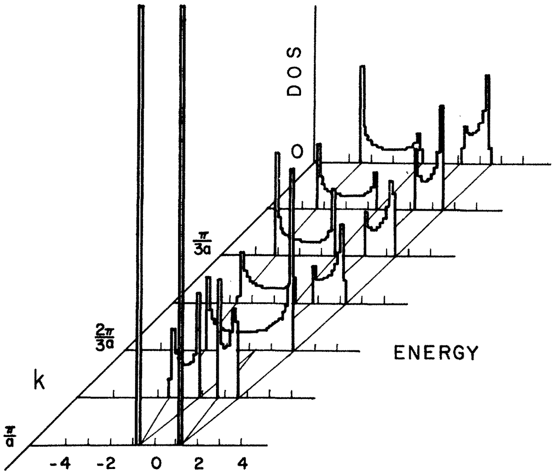

FIG. 3. Local densities of states of a principal layer in the bulk honeycomb lattice as a function of energy and as a function of k parallel to the layer. Each principal layer contains two atomic layers as in the semi-infinite case of Fig. 2. The thin solid curves in the energy–wave-vector plane define the projected band structure.

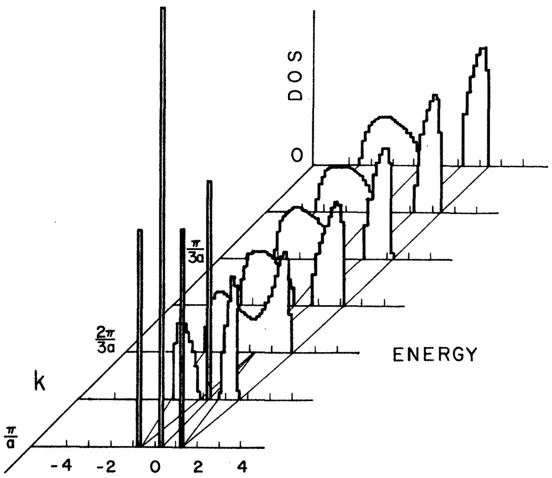

FIG. 4. Local densities of states for the zeroth principal layer of the surface system shown in Fig. 2 as a function of energy and wave vector k in the surface Brillouin zone. A bona fide surface-state band appears for $k \gtrsim 2\pi/3a$ near the zero of energy.

given by Eq. (19). The corresponding local densities of states for the zeroth principal layer (Fig. 2) are shown in Fig. 4. We note, as in I, that a surface-state band appears for $k \gtrsim 2\pi/3a$. This state becomes very localized at the surface principal layer as $k \rightarrow \pi/a$. In fact, this state is entirely localized on the surface *atomic* layer at $k = \pi/a$. In this case the delta functions at $E = -0.8$ and 1.2 are bulklike peaks arising from the second *atomic* layer. We also note that for $k \lesssim \frac{5}{6}\pi/a$ there are relatively strong in-band resonances in the local densities of states. The resonances lie roughly in the middle of the two bands occurring respectively above and below zero energy. These results are similar to those obtained by Foo *et al.*[10] using a honeycomb lattice with three sp^2-like orbitals per site and nearest-neighbor interactions.

IV. ANALYTICAL PROPERTIES OF G AND T

The basic strategy in Sec. II was to first introduce a small imaginary part into the energy, which separated the eigenvalues $\{\lambda_i\}$ of the transfer matrix into two halves with $|\lambda| < 1$ and $|\lambda| > 1$. One then proceeded to construct the bulk Green's function by assuming G_{n0} and $G_{\bar{n}0}$ decay as $n \rightarrow \infty$, and thus choosing each column of the matrices $\left[\begin{smallmatrix} G_{10} \\ G_{00} \end{smallmatrix}\right]$ and $\left[\begin{smallmatrix} G_{00} \\ G_{\bar{1}0} \end{smallmatrix}\right]$ to be a linear combination of eigenvectors of T with $|\lambda| > 1$ and $|\lambda| > 1$, respectively. The combination coefficients were then determined by requiring Eq. (5) to be satisfied. Once the bulk Green's function was obtained, one easily identified the quantities corresponding to the effective fields and surface Green's function.

In this scheme, however, there are two important points that need to be completely justified. The first point is that we need to prove the $G_{n0}(\vec{k}_\parallel, E^+)$ and $G_{\bar{n}0}(\vec{k}_\parallel, E^+)$ decay as $n \rightarrow \infty$. The second point is that in order for Eq. (5) to determine the combination coefficients uniquely, the eigenvalues of T must be divided evenly into groups with $|\lambda| < 1$ and $|\lambda| > 1$. We need to prove that this will always be the case as long as an imaginary part has been introduced into the energy.

To prove the first point, consider the Lehmann representation of the bulk Green's function,

$$G(\vec{k}_\parallel, E^+) = \sum_k \sum_\mu \frac{|\Psi_\mu(k, \vec{k}_\parallel)\rangle\langle\Psi_\mu(k, \vec{k}_\parallel)|}{E^+ - E_\mu(k, \vec{k}_\parallel)}, \tag{30}$$

where the $|\Psi_\mu(k, \vec{k}_\parallel)\rangle$ and $E_\mu(k, \vec{k}_\parallel)$ are eigensolutions of the bulk crystal.

If we take matrix elements of Eq. (30) with the basis functions spanning the principal layers as in (3) and (4) we get

$$\begin{pmatrix} G_{2n+1,1} & G_{2n+1,0} \\ G_{2n,1} & G_{2n,0} \end{pmatrix} = \sum_k \sum_\mu \frac{e^{ikna}}{E - E_\mu(\vec{k})} \begin{pmatrix} \langle 1|\Psi_\mu(\vec{k})\rangle\langle\Psi_\mu(\vec{k})|1\rangle & \langle 1|\Psi_\mu(\vec{k})\rangle\langle\Psi_\mu(\vec{k})|0\rangle \\ \langle 0|\Psi_\mu(\vec{k})\rangle\langle\Psi_\mu(\vec{k})|1\rangle & \langle 0|\Psi_\mu(\vec{k})\rangle\langle\Psi_\mu(\vec{k})|0\rangle \end{pmatrix}, \tag{31}$$

$$\begin{bmatrix} G_{2n+1,1} & G_{2n+1,0} \\ G_{2n,1} & G_{2n,0} \end{bmatrix} = \frac{a}{2\pi} \int_{-\pi/a}^{\pi/a} dk\, e^{ikna} \frac{1}{E^+ - H(e^{ika})} \tag{32}$$

where, for the system shown in Fig. 1, $H(e^{ika})$ is given by

$$H(e^{ika}) = \begin{bmatrix} H_{11} & H_{01}^+ + e^{ika} H_{12} \\ H_{01} + e^{-ika} H_{12}^+ & H_{00} \end{bmatrix} . \tag{33}$$

Now let us make a standard change of variable from k to $\omega \equiv e^{ika}$ in (32). This gives

$$\begin{bmatrix} G_{2n+1,1} & G_{2n+1,0} \\ G_{2n,1} & G_{2n,0} \end{bmatrix} = \frac{1}{2\pi i} \oint_{|\omega|=1} d\omega\, \omega^{n-1} \frac{1}{E^+ - H(\omega)} = \frac{1}{2\pi i} \oint_{|\omega|=1} d\omega\, \omega^{n-1} \frac{\operatorname{adj}[E^+ - H(\omega)]}{\det[E^+ - H(\omega)]} \tag{34}$$

where $\operatorname{adj}(X)$ is the classical adjoint of the matrix X and $X^{-1} \equiv \operatorname{adj}(X)/\det(X)$. By using the identity

$$\det \begin{bmatrix} A & B \\ C & D \end{bmatrix} = \det(CAC^{-1}D - CB) , \tag{35}$$

where A, B, C, D are $\mu \times \mu$ submatrices, one can easily show that

$$\det[\omega - T(E^+)] = \frac{(-\omega)^\mu}{\det(H_{01} H_{12})} \det[E^+ - H(\omega)] , \tag{36}$$

where $T(E^+)$ is for the system shown in Fig. 1 and thus given by

$$T(E^+) = \begin{bmatrix} H_{01}^{-1}(E^+ - H_{00}) H_{12}^{-1}(E - H_{11}) - H_{01}^{-1} H_{12}^+ & -H_{01}^{-1}(E^+ - H_{00}) H_{12}^{-1} H_{01}^+ \\ H_{12}^{-1}(E^+ - H_{11}) & -H_{12}^{-1} H_{01}^+ \end{bmatrix} . \tag{37}$$

Substituting (36) back into (34) we get

$$\begin{bmatrix} G_{2n+1,1} & G_{2n+1,0} \\ G_{2n,1} & G_{2n,0} \end{bmatrix} = \frac{1}{2\pi i} \frac{(-1)^\mu}{\det(H_{01} H_{12})} \oint_{|\omega|=1} d\omega\, \omega^{n-1} \frac{\omega^\mu \operatorname{adj}[E^+ - H(\omega)]}{\det[\omega - T(E^+)]} . \tag{38}$$

Similarly we have

$$\begin{bmatrix} G_{2\bar{n}+1,1} & G_{2\bar{n}+1,0} \\ G_{2\bar{n},1} & G_{2\bar{n},0} \end{bmatrix} = \frac{1}{2\pi i} \frac{(-1)^\mu}{\det(H_{01} H_{12})^*} \oint_{|\omega|=1} d\omega\, \omega^{n-1} \frac{\omega^\mu \operatorname{adj}[E^+ - H(1/\omega)]}{\det[\omega - T^{-1}(E^+)]} . \tag{39}$$

Since $\omega^\mu \operatorname{adj}[E^+ - H(\omega)]$ and $\omega^\mu \operatorname{adj}[E^+ - H(1/\omega)]$ contain only positive powers of ω we may expand them as follows:

$$\omega^\mu \operatorname{adj}[E^+ - H(\omega)] = \sum_{k=0}^{2\mu} \omega^k D_k(E^+) , \tag{40}$$

$$\omega^\mu \operatorname{adj}[E^+ - H(1/\omega)] = \sum_{k=0}^{2\mu} \omega^k D_{2\mu - k}(E^+) , \tag{41}$$

$$D_k(E^+) \equiv \frac{\partial^k}{\partial \omega^k} \bigg|_{\omega=0} \{\omega^\mu \operatorname{adj}[E^+ - H(\omega)]\} . \tag{42}$$

Therefore for $n \geqslant 1$ we have

$$\begin{bmatrix} G_{2n+1,1} & G_{2n+1,0} \\ G_{2n,1} & G_{2n,0} \end{bmatrix} = \frac{(-1)^\mu}{\det(H_{01} H_{12})} \sum_{k=0}^{2\mu} D_k(E^+) \sum_{i;\, |\lambda_i| < 1} \frac{[\lambda_i(E^+)]^{n+k}}{\lambda_i(E^+) \prod_{j \neq i}^{2\mu} [\lambda_i(E^+) - \lambda_j(E^+)]} \tag{43}$$

and

$$\begin{bmatrix} G_{2\bar{n}+1,1} & G_{2\bar{n}+1,0} \\ G_{2\bar{n},1} & G_{2\bar{n},0} \end{bmatrix} = \frac{(-1)^{\mu+1}}{\det(H_{01} H_{12})^*} \sum_{k=0}^{2\mu} D_{2\mu - k}(E^+) \sum_{l;\, |\lambda_l| > 1} \frac{[\lambda_l^{-1}(E^+)]^{n+k}}{\lambda_l^{-1}(E^+) \prod_{j \neq l}^{2\mu} [\lambda_l^{-1}(E^+) - \lambda_j^{-1}(E^+)]} . \tag{44}$$

From (43) and (44) we can see that $G_{n,0}$ and $G_{\bar{n},0}$ should decay as $n \to \infty$.

Let us now turn to the second point. Consider the function

$$\mathcal{F}(\omega, z) \equiv \det(\omega - T(z)), \tag{45}$$

where $T(z)$ is given by (37) with E^{+} replaced by a general complex number z. From (37) it is obvious that $\mathcal{F}$ is an analytic polynomial in both ω and z. Since the coefficient of the term with highest power in ω is unity, we may write $\mathcal{F}$ as

$$\mathcal{F}(\omega, z) = \prod_{i=1}^{2\mu} [\omega - \lambda_i(z)] \tag{46}$$

where the analyticity of $\mathcal{F}$ implies continuity in the $\lambda_i(z)$. We now show in the following argument that the $\lambda_i(z)$ must satisfy $|\lambda_i(z)| \neq 1$ for z not real. Since $H(\omega = e^{i\theta})$ is a Hermitian matrix, its eigenvalues are real and therefore $\det[z - H(\omega = e^{i\theta})] \neq 0$ for z not real. This implies from (36) that $\mathcal{F}(e^{i\theta}, z)$ cannot equal zero for z not real. Thus we conclude that all the $\{\lambda_i(z)\}$ must have the property

$$|\lambda_i(z)| \neq 1 \tag{47}$$

for z off the real axis. We now proceed to show that the set $\{\lambda_i(E)\}$ can be divided equally into two sets with moduli greater and less than 1, respectively. We can easily prove, using arguments similar to those in I that

$$T^{-1}(\vec{k}_{\parallel}, z) = S(\vec{k}_{\parallel}) T^{T}(-\vec{k}_{\parallel}, z) S^{-1}(\vec{k}_{\parallel}) \tag{48}$$

and

$$T^{-1}(\vec{k}_{\parallel}, z) = S(\vec{k}_{\parallel}) T^{+}(\vec{k}_{\parallel}, z^{*}) S^{-1}(\vec{k}_{\parallel}), \tag{49}$$

where

$$S(\vec{k}_{\parallel}) = \begin{bmatrix} 0 & -H_{01}^{-1}(\vec{k}_{\parallel}) \\ H_{10}^{-1}(\vec{k}_{\parallel}) & 0 \end{bmatrix}. \tag{50}$$

If z is on the real axis ($z = E$), Eq. (49) implies that the set $\{\lambda_i(E)\}$ is equal to the set $\{\lambda_j^{*-1}(E)\}$. Thus there are always equal numbers of $\lambda_i(E)$ with modulus greater and less than one. Moreover, if E lies outside the bulk allowed energy region *all* the $\lambda_i(E)$ have modulus greater or less than one.

Since $\{\lambda_i(z)\}$ are continuous and satisfy (47) we must also have an equal number of $\lambda_i(z)$ with modulus greater or less than unity for *z off the real axis*. The proof proceeds by *reductio ad absurdum*. Suppose for some z there are *not* equal number of $\lambda_i(z)$ inside and outside the unit circle. Then we can consider a path connecting this point to another on the real axis outside the bulk allowed energy region. Somewhere along this path eigenvalues $\lambda_i(z)$ must "jump" across the unit circle. This contradicts the continuity of $\lambda_i(z)$ and the analytic nature of $\mathcal{F}$.

V. CONSTRUCTION OF A UNIFIED SCHEME

The present method relies on the eigenanalysis of the transfer matrix $T(\vec{k}_{\parallel}, E^{+})$ with $E^{+} \equiv E + i\delta$. The method described in I relies on $T(\vec{k}_{\parallel}, E)$ where E is purely *real*. Nevertheless, the two schemes can be unified completely in two ways. The first entails *forcing* E in I to have a very small imaginary part δ. The projected band structure, wave function, surface bands, and decay lengths can then be obtained using the same equations as in I with negligible error of the order δ. We note that δ can be chosen as small as one wishes without serious instabilities.

The second is more elegant. It involves setting E^{+} equal to E in the present method. This is exact, as long as we correctly identify which eigenvalues $\{\lambda_i(\vec{k}_{\parallel}, E)\}$ of $T(\vec{k}_{\parallel}, E)$ with modulus *equal* to 1 analytically continue to $\{\lambda_i(\vec{k}_{\parallel}, E^{+})\}$ with modulus *less* than 1. In what follows we discuss this in more detail and illustrate how to construct this "selection procedure" and determine the effective fields for real energies.

For any real energy E *outside* the bulk continuum, the eigenvalues $\{\lambda_i(\vec{k}_{\parallel}, E)\}$ of the transfer matrix are always evenly divided into two groups, with modulus greater and less than one. The Green's function is therefore uniquely defined through Eqs. (10) and (11). A problem arises, however, when E lies *inside* the bulk continuum. In this case there are always an even number of λ's corresponding to Bloch phase factors e^{ika} which have modulus *equal* to one. These λ's correspond to different Riemann sheets which cross at a branch cut for this range of energies. In order to identify the λ's associated with the appropriate Riemann sheet we construct the following selection procedure.

We introduce a small imaginary part $i\delta$ into the energy and examine what happens when we take the limit $\delta \to 0$. From what we learned in Sec. IV, none of the $\{\lambda_i(E + i\delta)\}$ can have modulus 1, and the wave vectors $k(E + i\delta)$ are now complex. Expanding the function $k(E + i\delta)$ around E, we get

$$e^{ik(E+i\delta)a} = e^{ik(E)a} e^{-\delta a(\partial k/\partial E)}. \tag{51}$$

If we let $\lambda = \lambda_I + i\lambda_R$, the $\partial k/\partial E = \lambda_R^{-1} \partial\lambda_I/\partial E$ and the modulus of $e^{ik(E+i\delta)a}$ is

$$|\lambda(E^{+})| = |e^{ik(E+i\delta)a}| = e^{-a\delta\lambda_R^{-1}(\partial\lambda_I/\partial E)}. \tag{52}$$

From (52) we can see that only the $\lambda(E)$ with $\lambda_R^{-1} \partial\lambda_I/\partial E \geqslant 0$ can analytically continue to the $\lambda(E^{+})$ with $|\lambda(E^{+})| < 1$. Therefore, these $\lambda(E)$'s with modulus 1 correspond to the appropriate Riemann sheet for the Green's function in (34). This selection procedure only requires knowledge of $\lambda_R(E)$ and $\partial\lambda_I(E)/\partial E$ at the real energy E.

We can calculate $\partial\lambda_I/\partial E$ exactly using the transfer matrix T by

$$\frac{\partial\lambda(E)}{\partial E}=\left(\vec{e}(\lambda)\cdot\frac{\partial T}{\partial E}\vec{e}(\lambda)\right), \tag{53}$$

where $\vec{e}(\lambda)$ is the corresponding eigenvector with eigenvalue λ, and $\partial T/\partial E$ is given by

$$\frac{\partial T}{\partial E}=\begin{pmatrix} H_{01}^{-1}H_{12}^{-1}(E-H_{11})+H_{01}^{-1}(E-H_{00})H_{12}^{-1} & -H_{01}^{-1}H_{12}^{-1}H_{01}^{+} \\ H_{12}^{+} & 0 \end{pmatrix}. \tag{54}$$

Therefore

$$\lambda_R^{-1}\frac{\partial\lambda_I}{\partial E}=\frac{1}{\lambda_R(E)}\,\mathrm{Im}\left(\vec{e}(\lambda)\cdot\frac{\partial T}{\partial E}\,\vec{e}(\lambda)\right). \tag{55}$$

Equation (55) is easily evaluated since it only requires knowledge of the transfer matrix $T(\vec{k}_{\parallel},E)$ and its eigensolutions at real E. The sign of (55) then identifies with λ's with $|\lambda(\vec{k}_{\parallel},E)|=1$ should be used in (12), (17), and (18) with $E^{+}=E$ real. The effective fields $\Phi_1(\vec{k}_{\parallel},E)$ and $\Phi_2(\vec{k}_{\parallel},E)$ are therefore now evaluated, exactly, at real energies. One should, however, retain a very small imaginary part δ in the E^{+} [shown explicitly in (19) and (20)] for the surface Green's function, in order to account for possible states (described by poles) existing outside the branch cuts of the bulk continuum.

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