Green's-function method for crystal films and surfaces*

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The Green's-function method is adapted to the problem of an electron moving in a crystal film. The potential is taken as spherical in the atomic spheres and as dependent only on the coordinate normal to the film in the regions just outside the bounding atom planes. The appropriate new structure constants are defined. With the aid of the necessary logarithmic derivatives a rather small set of simultaneous linear equations is obtained from which eigenvalues and eigenfunctions can be calculated. In conjunction with the density functional formalism this procedure provides a convenient method for self-consistently calculating the electronic structure of films and surfaces. Comparison with earlier work by Pharisean, Scherer, Cooper, and Beeby is made.

In solid-state physics Green's-function methods were originally used for the solution of the one-particle Schrödinger equation in periodic lattices.[1,2] More recently, similar methods have been developed, under the name of "scattered-wave method" for calculating one-particle orbitals for molecules of moderate size and clusters of up to about 20 atoms.[3,4] Such calculations can also be made self-consistently by using the density-functional theory in which the effective one-particle potential is a functional of the electron density.[5,6,3]

There have also been a substantial number of papers dealing with the application of the Green's-function method to the geometries of crystal films and surfaces.[7-12] In the present paper we present a direct adaptation of the Kohn-Rostoker approach[2] to films and surfaces (thick films) which is conceptually very simple, has variational accuracy, and avoids shortcomings in earlier work which we shall discuss briefly at the end of this paper. We believe that the present approach offers a useful alternative to other methods which have been used to deal with such systems.[13,14]

In a film geometry, periodicity parallel to the surfaces is preserved; a twofold symmetry is present; and the wave functions are accurately describable in terms of bulk wave functions, except in the outermost 2 or 3 layers. Therefore we shall find in this formulation that film and surface problems of simple crystals are comparable in complexity to an infinite-lattice problem with up to about 3 or 4 atoms per unit cell.[15]

Consider a film of a simple monatomic lattice with $2N$ layers parallel to the x-y plane (see Fig. 1). The potential energy has two-dimensional translational symmetry

$$V(\vec{r}+\vec{\sigma}_m)=V(\vec{r})\,,\quad m=1,2 \tag{1}$$

where the translation vectors $\vec{\sigma}_m'$ have the form

$$\vec{\sigma}_m=(\sigma_{mx},\sigma_{my},0)\,. \tag{2}$$

We address here the problem of finding the solutions of the Schrödinger equation

$$[-\nabla^2+V(\vec{r})-E]\psi(\vec{r})=0\,, \tag{3}$$

subject to the boundary conditions

$$\lim_{z\to\pm\infty}\psi(\vec{u}\,z)=0\,, \tag{4}$$

$$\vec{u}\equiv(x,y,0)\,, \tag{5}$$

and to the periodicity conditions

$$\psi(\vec{r}+\vec{\sigma}_m)=e^{i\vec{q}\cdot\vec{\sigma}_m}\psi(\vec{r})\,, \tag{6}$$

where $\vec{q}$ is a two-dimensional wave vector

$$\vec{q}=(q_x,q_y,0)\,. \tag{7}$$

We also define (nonuniquely) a unit cell τ which contains the origin and one atom from each layer, and which extends to $\pm\infty$ in the z direction (see Fig. 1). This unit cell and its translated counterparts fill the entire space. We denote the origin and the corresponding points in the other unit cells by $\vec{u}_s\equiv(x_s,y_s,0)$ and the cross-sectional area in the x-y plane of the unit cell by a. The periodicity condition (6) may now be replaced by boundary conditions on the surface of the unit cell τ. Let $\vec{r}$ and $\vec{r}_c$ be conjugate points on this surface, such that

$$\vec{r}_c=\vec{r}+\vec{\sigma}_m\,. \tag{8}$$

Then

$$\psi(\vec{r}_c)=e^{i\vec{q}\cdot\vec{\sigma}_m}\psi(\vec{r})\,,$$

$$\frac{\partial\psi(\vec{r}^{\,c})}{\partial n^c}=-e^{i\vec{q}\cdot\vec{\sigma}_m}\frac{\partial\psi(\vec{r})}{\partial n}\,, \tag{9}$$

where n and n^c denote outward normals at $\vec{r}$ and $\vec{r}_c$.

We now follow a Green's-function procedure similar to that of Kohn and Rostoker.[2] However, whereas in that paper the Green's function satisfied all boundary conditions on the surface of the unit cell, it will here satisfy only the periodicity condition (6), with the condition (4) at $z=\pm\infty$ being imposed on all approximate solutions $\psi(\vec{r})$ which are considered. This results in a useful simplification

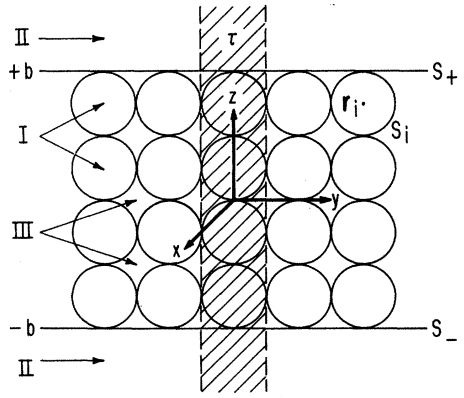

FIG. 1. Crystal film. τ is the unit cell, extending from $z=-\infty$ to $+\infty$ and having cross-sectional area a. Regions I (atomic spheres), II ($|z|>b$), and III (interstices) are shown. S_i, S_+, and S_- are the bounding surfaces. $\vec{r}_i$ is a nuclear position vector.

of the formalism.

For our Green's function we choose the function

$$G(\vec{r},\vec{r}')\equiv-\frac{1}{4\pi}\sum_s\frac{\exp[i\kappa|\vec{r}-\vec{r}'-\vec{u}_s|]}{|\vec{r}-\vec{r}'-u_s|}e^{i\vec{q}\cdot\vec{u}_s}, \tag{10}$$

where

$$\kappa=+E^{1/2}, \quad E>0$$
$$=+i(-E)^{1/2}, \quad E<0. \tag{11}$$

Evidently G has the following properties in the unit cell τ and on its boundary:

$$(-\nabla^2-E)G(\vec{r},\vec{r}')=-\delta(\vec{r}-\vec{r}'),$$
$$G(\vec{r}^{\,c},\vec{r}')=e^{i\vec{q}\cdot\vec{\sigma}_m}G(\vec{r},\vec{r}'), \tag{12}$$

$$\frac{\partial G(\vec{r}^{\,c},\vec{r}')}{\partial n^c}=-e^{i\vec{q}\cdot\vec{\sigma}_m}\frac{\partial G(\vec{r},\vec{r}')}{\partial n}, \tag{13}$$

and

$$G(\vec{r}',\vec{r})=G^*(\vec{r},\vec{r}'). \tag{14}$$

In view of these properties the Schrödinger equation (3) and boundary conditions (9) can be replaced by the integral equation

$$\psi(\vec{r})=\int_\tau G(\vec{r},\vec{r}')\,V(\vec{r}')\,\psi(\vec{r}')\,d\vec{r}' \tag{15}$$

with the boundary condition (4) remaining imposed on $\psi(\vec{r})$.

We now divide the unit cell τ into three regions in which we assume suitable forms for the potential $V(\vec{r})$ (see Fig. 1).

Region I: Nonoverlapping spheres of radius ρ surrounding each nuclear site $\vec{r}_i$, in which $V(\vec{r})$ is taken to be spherically symmetric.

Region II: Two surface strips (not overlapping these spheres) in which $V(\vec{r})$ depends only on z, i.e., $V(\vec{r})=v(z)$, $|z|\geq b$.

Region III: The remaining space, in which $V(\vec{r})$ is taken to be a constant, V_0, which is set equal to zero.

The new feature is region II, which is the analog of the "exterior sphere" in the work of Johnson.[4] This region, and the assumed behavior of $V(\vec{r})$ in it, appear to be the appropriate choices for dealing with the geometry of a film.

Within each sphere of region I, say the one surrounding $\vec{r}_j$, we expand $\psi(\vec{r})$ in terms of the angular-momentum solutions of the Schrödinger equation (3),

$$\psi(\vec{r})=\sum_L C_L^i R_i^i Y_L(\Theta), \tag{16}$$

where L stands for the usual quantum numbers l and m, Y_L is a normalized spherical harmonic of the argument $\Theta\equiv(\theta,\varphi)$, and R_i is the regular radial solution which is taken to be unity on the surface of the sphere.

We now turn to region II and denote the two strips $z>b$ and $z<-b$ by $\xi=\pm$, respectively. Then, in each strip ξ we again expand $\psi(\vec{r})$ in terms of eigenfunctions of the Schrödinger equation the following form:

$$\psi(\vec{r})=\sum_h C_h^i f_h^i(z)\,e^{i(\vec{q}+\vec{Q}_h)\cdot\vec{u}}. \tag{17}$$

Here $\vec{u}\equiv(x,y,0)$; the $\vec{Q}_h$ are the two-dimensional reciprocal-lattice vectors

$$\vec{Q}_h=(Q_{hx},Q_{hy},0),$$
$$\vec{Q}_h\cdot\vec{\sigma}_m=2\pi\times(\text{integer}); \tag{18}$$

and the function $f^+(z)$, satisfies the following equations:

$$\left(-\frac{d^2}{dz^2}+v(z)-[E-(\vec{q}+\vec{Q}_h)^2]\right)f^+(z)=0, \quad z>b \tag{19}$$

$$f^+(+\infty)=0. \tag{20}$$

$$f^+(b)=1. \tag{21}$$

with exactly analogous equations for $f^-(z)$.

Let $\vec{r}$ be a point in regions I+II. Then since in regions I+II $\psi(\vec{r})$ satisfies the Schrödinger equation (3) and $G(\vec{r},\vec{r}')$ the inhomogeneous equation (12), the integral equation (15) can, by an integration by parts, be transformed as follows:

$$0=\psi(\vec{r})-\int_{\text{I+II}}G(\vec{r},\vec{r}')(\nabla'^2+E)\,\psi(\vec{r}')\,d\vec{r}'$$
$$=\int_{S_\text{I}+S_\text{II}}\{G(\vec{r},\vec{r}')\nabla'\psi(\vec{r}')-[\nabla'G(\vec{r},\vec{r}')]\,\psi(\vec{r}')\}\,d\vec{s}'. \tag{22}$$

where $d\vec{s}'$ is the outward surface element vector and S_I and S_II are the surfaces bounding regions I

TABLE I. Green's function expansions. The Green's function $G(\vec{r},\vec{r}\,')$ is defined in Eq. (10). $\vec{r}$ is located just inside regions I+II, near the surfaces indicated; $\vec{r}\,'$ just on or outside regions I+II, near the surfaces indicated. ρ_i, Θ_i denote radial and angular coordinates relative to the nucleus $\vec{r}_i$. $\vec{u}\equiv(x,y,0)$. $\kappa=E^{1/2}$ [see Eq. (11)]. $\vec{Q}_h$ are two-dimensional reciprocal-lattice vectors [see Eq. (18)]. $\kappa_h=[E-(\vec{Q}_h+\vec{q})^2]^{1/2}$. The structure constants A are given in the Appendix.

r \ r'	S_i	S_+	S_-
S_i	$\sum_{L,L'}[A_{LL'}j_l(\kappa\rho_i)j_{l'}(\kappa\rho_i')$ $+\kappa\delta_{LL'}j_l(\kappa\rho_i)n_l(\kappa\rho_i')]Y_L(\Theta_i)Y^*_{L'}(\Theta_i')$	$\sum_{L,h'}A^{i,+}_{Lh'}j_l(\kappa\rho_i)Y_L(\Theta_i)$ $\times\exp[-i(\vec{q}+\vec{Q}_{h'})\vec{u}'+i\kappa_{h'}(z'-b)]$	$\sum_{L,h'}A^{i,-}_{Lh'}j_l(\kappa\rho_i)Y_L(\Theta_i)$ $\times\exp[-i(\vec{q}+\vec{Q}_{h'})\vec{u}'-i\kappa_h(z'+b)]$
S_j $j\neq i$	$\sum_{L,L'}A^{ij}_{LL'}j_l(\kappa\rho_j)j_{l'}(\kappa\rho_i')$ $\times Y_L(\Theta_j)Y^*_{L'}(\Theta_i')$	Same as above with $i\to j$	Same as above with $i\to j$
S_+	$\sum_{h,L'}A^{+,i}_{hL'}\exp[i(\vec{q}+\vec{Q}_h)\vec{u}$ $+i\kappa_h(z-b)]j_{l'}(\kappa\rho_i')Y^*_{L'}(\Theta_i')$	$\sum_h A^{+,+}_h\exp[i(\vec{q}+\vec{Q}_h)(\vec{u}-\vec{u}')$ $+i\kappa_h(z-z')]$	$\sum_h A^{+,-}_h\exp[i(\vec{q}+\vec{Q}_h)(\vec{u}-\vec{u}')$ $+i\kappa_h(z-z'-2b)]$
S_-	$\sum_{h,L'}A^{-,i}_{hL'}\exp[i(\vec{q}+\vec{Q}_h)\vec{u}$ $-i\kappa_h(z+b)]j_{l'}(\kappa\rho_i')Y^*_{L'}(\Theta_i')$	$\sum_h A^{-,+}_h\exp[i(\vec{q}+\vec{Q}_h)(\vec{u}-\vec{u}')$ $+i\kappa_h(z'-z-2b)]$	$\sum_h A^{-,-}_h\exp[i(\vec{q}+\vec{Q}_h)(\vec{u}-\vec{u}')$ $+i\kappa_h(z'-z)]$

and II, respectively.

From this equation we want to extract a set of homogeneous linear equations for the expansion coefficients C_L and C_h, Eqs. (16) and (17). This requires expansions of the Green's function $G(\vec{r},\vec{r}\,')$ for $\vec{r}$ just inside and $\vec{r}\,'$ on or just outside any one of the bounding surfaces of region I and II: S_i, spheres surrounding nucleus i; and $S_\pm$, the planes $z=\pm b$. We give the result in Table I.

We now choose $\vec{r}$ to lie just inside the ith atomic sphere, multiply (22) by $Y^*(\Theta_i)$, use the Green's-function expansions of Table I and integrate $\vec{r}$ over S_i and $\vec{r}\,'$ over the entire surface $S_{\rm I}+S_{\rm II}$. This results in the set of equations

$$\rho^2 j_l\Big(\sum_{L'}\rho^2[A_{LL'}(j_l\cdot L^i_{l'}-j'_{l'})]C^i_{L'}+\sum_{L',j\neq i}\rho^2[A^{ij}_{LL'}(j_l\cdot L^j_{l'}-j'_{l'})]C^j_{L'}+\sum_{h'}a[A^{i,+}_{Lh'}(-L^+_{h'}+i\kappa_{h'})C^+_{h'}+A^{i,-}_{Lh'}(L^-_{h'}+i\kappa_{h'})C^-_{h'}]\Big)=0,\quad i=1,2,\ldots 2N \tag{23}$$

where

$$j_l\equiv j_l(\kappa\rho),\quad j'_l\equiv\left(\frac{d}{d\rho'}j_l(\kappa\rho')\right)_{\rho'=\rho},$$

$$n_l\equiv n_l(\kappa\rho),\quad n'_l\equiv\left(\frac{d}{d\rho'}n_l(\kappa\rho)\right)_{\rho'=\rho}, \tag{24}$$

$$L^i_l\equiv\left(\frac{dR^i_l(r)}{dr}\Big/R^i_l(r)\right)_{r=\rho}=\left(\frac{dR^i_l(r)}{dr}\right)_{r=\rho}, \tag{25}$$

$$L^+_h=\left(\frac{df^+(z)}{dz}\Big/f^+(z)\right)_{z=b}=\left(\frac{df^+(z)}{dz}\right)_{z=b}, \tag{26}$$

$$L^-_h=\left(\frac{df^-(z)}{dz}\Big/f^-(z)\right)_{z=-b}=\left(\frac{df^-(z)}{dz}\right)_{z=-b}. \tag{27}$$

Next we choose $\vec{r}$ to lie just above the plane surface S_+ $(z\equiv b)$, multiply (22) by $\exp[-i(\vec{q}+\vec{Q}_h)\cdot\vec{u}]$, use the Green's-function expansions of Table I, and integrate $\vec{r}$ over the unit cell boundary on the plane $z=b$ (of area a) and $\vec{r}\,'$ over the entire surface $S_{\rm I}+S_{\rm II}$. This results in the following equation:

$$a\Big(\rho^2\sum_{j,L'}A^{+,j}_{hL'}(j_l\cdot L^j_{l'}-j'_{l'})C^j_{L'}+aA^{+,-}_h(+L^-_h+i\kappa_h)C^-_h+aA^{+,+}_h(-L^+_h-i\kappa_h)C^+_h\Big)=0. \tag{28}$$

Similarly, taking $\vec{r}$ just below the planar surface S_- $(z\equiv -b)$, gives

$$a\Big(\rho^2\sum_{j,L'}A^{-,j}_{hL'}(j_l\cdot L^j_{l'}-j'_{l'})C^j_{L'}+aA^{-,-}_h(L^-_h+i\kappa_h)C^-_h+aA^{-,+}_h(-L^+_h+i\kappa_h)C^+_h\Big)=0. \tag{29}$$

Equations (23), (28), and (29) represent a set of homogeneous linear equations for the coefficients C^i_L, C^+_h, C^-_h. By introducing a total of M such coefficients, one is led to an $M\times M$ determinantal consistency equation. This gives a relationship between the energy E and the two-dimensional wave vector $\vec{q}$, which allows the determination of the eigenvalues:

$$F(E,\vec{q})=0\to E_\alpha(\vec{q}). \tag{30}$$

Substitution of these into Eqs. (23), (28), and (29) yields the expansion coefficients C_L^i, C_h^+, C_h^- of the solutions to within a constant factor.

Of course, one should take advantage of the twofold symmetry of the film, which assures in advance that certain pairs of the above coefficients are equal or otherwise simply related to each other. In practice, since surface effects extend appreciably only two or three layers into the interior, it is sufficient to study films of four to six layers. For four layers one has the following independent coefficients: $C_L^{(1)}$, $C_L^{(2)}$, C_h^+. The problem is therefore comparable to a bulk problem with three atoms per unit cell, although of course somewhat more complex.

We believe that this formalism, combined with a self-consistency scheme based on the density-functional theory, will be useful for solving problems of the electronic structure of films and surfaces.

We conclude with a few remarks of comparison with earlier Green's-function theories of films and surfaces. Reference 7 is limited to one-dimensional "slabs." References 8 and 9 make the incorrect assumption that inside the crystal the eigenfunctions have a simple Bloch form whereas, in reality, they are linear combinations of at least two Bloch functions with wave vectors $\vec{k}=(k_x, k_y, \pm k_z)$, and of exponentially decaying (or growing) waves. Further, outside the crystal, the potential is taken as constant, which is a rather crude representation of real surfaces. In Ref. 10 the inside solution is taken to be the sum of two Bloch waves, still an incorrect form. In Ref. 11, the potential outside the surface is constant up to an infinite barrier. Reference 12, which does allow a z-dependent potential in the surface region, approaches the problem from the T-matrix standpoint. It requires first the calculation of the T-matrix for each layer $\tau_\nu(\vec{k}+\kappa, \vec{k}+\kappa')$ and then the solution of an infinite set of equations coupling these planes. This paper does not fully take advantage of the exact description of the wave propagation in the region of constant potential, offered by the Green's-function method. Also, it does not have the variational accuracy of the present approach.

APPENDIX: STRUCTURE CONSTANTS

In Table I we listed the various forms of expansion of the Green's function (10) involving certain structure constants, such as $A_{LL'}$, $A_{Lh}^{i,+}$, etc. The constants enter the linear equations (23), (28), and (29) whose solutions yield the eigenvalues and eigenfunctions of the original problem. In this Appendix we give expressions for these coefficients.

The Green's function $G(\vec{r}, \vec{r}')$ is given by Eq. (10) or, alternatively by the momentum sum

$$G(\vec{r}, \vec{r}')=\frac{1}{a}\sum_h \exp[i(\vec{q}+\vec{Q}_h)(\vec{u}-\vec{u}')] \times\frac{1}{2i\kappa_h}\exp[i\kappa_h(z_>-z_<)]\,, \tag{A1}$$

where $\vec{Q}_h$, $\vec{u}$ and κ_h are defined under Table I and $z_<$ and $z_>$ denote, respectively, the smaller or greater of quantities z and z'; a is the cross-sectional area of the unit cell.

Using the coordinate sum (10) for $G(\vec{r}, \vec{r}')$ and following Ref. 2, we find for $\vec{r}$ just inside and $\vec{r}'$ just outside the sphere S_i of center $\vec{r}_i$ and radius ρ,

$$G(\vec{r}, \vec{r}')=\sum_{L,L'}[\kappa\delta_{LL'}j_l(\kappa\rho_i)h_l(\kappa\zeta_i') +A_{LL'}j_l(\kappa\rho_i)j_l'(\kappa\rho_i')]Y_L(\Theta_i)Y_L^*(\Theta_i'), \tag{A2}$$

where

$$\kappa\equiv E^{1/2}, \qquad L\equiv(l, m),$$
$$\rho_i\equiv|\vec{r}-\vec{r}_i|, \quad \rho_i'=|\vec{r}'-\vec{r}_i|,$$
$$\Theta_i\equiv(\theta_i, \varphi_i), \quad \Theta_i'\equiv(\theta_i', \varphi_i'),$$

and $A_{LL'}$ is given in terms of the coefficients D_L, and $C_{\bar{l}, m-m'; lm; l'm'}$ by the following relation [see Eqs. (A14) and (A13) of Ref. 2]:

$$A_{lm;l'm'}=4\pi i^{(l-l')}\sum_{\bar{l}} i^{-\bar{l}}D_{\bar{l}, m-m'}C_{\bar{l}, m-m'; lm; l'm'}\,, \tag{A3}$$

where

$$C_{i\bar{m};lm;l'm'}\equiv\int Y_{\bar{l}m}(\Theta)Y_{lm}^*(\Theta)Y_{l'm'}(\Theta)\,d\Omega \tag{A4}$$

and

$$D_{\bar{l},\bar{m}}\equiv\kappa\sum_{s\neq0}e^{i\vec{q}\cdot\vec{u}_s}[n_{\bar{l}}(\kappa u_s)-ij_{\bar{l}}(\kappa u_s)]Y_{\bar{l}\bar{m}}^*(\Theta_s) -\frac{i\kappa}{(4\pi)^{1/2}}\delta_{\bar{l}0}\,\delta_{\bar{m}0}; \tag{A5}$$

here $u_s\equiv|\vec{u}_s|$ [cf. Eq. (A2.22) of Ref. 2].

Similarly, for $\vec{r}$ just inside S_j and $\vec{r}'$ just outside $S_i (i\neq j)$, $G(\vec{r}, \vec{r}')$ has the form

$$G(\vec{r}, \vec{r}')=\sum_{L,L'}A_{LL'}^{ji}j_l(\kappa\rho_j)j_l(\kappa\rho_i')Y_L(\Theta_j)Y_{L'}^*(\Theta_i), \tag{A6}$$

where, in analogy with (A3), $A_{LL'}^{ji}$ is given by

$$A_{lm;l'm'}^{ji}=4\pi i^{(l-l')}\sum_{\bar{l}}D_{\bar{l},m-m'}^{ji}C_{\bar{l},m-m';lm;l'm'}\,; \tag{A7}$$

here C is the same as in (A4) and

$$D_{\bar{l},\bar{m}}^{ji}\equiv\kappa\exp[i\vec{q}\cdot(\vec{r}_j-\vec{r}_i)]\sum_s e^{i\vec{q}\cdot\vec{r}_{jis}} \times[n_{\bar{l}}(\kappa r_{jis})-ij_{\bar{l}}(\kappa r_{jis})]Y_{\bar{l}\bar{m}}(\Theta_{jis})\,, \tag{A8}$$

where

$$\vec{r}_{jis} = \vec{u}_s - \vec{r}_j + \vec{r}_i \tag{A9}$$

and Θ_{jis} corresponds to the direction of this vector [cf. Ref. 9, Eq. (A13)].

Next we take $\vec{r}$ just above S_+ and $\vec{r}'$ just outside S_i. Then, using (A1), $G(\vec{r}, \vec{r}')$ can be written as

$$G(\vec{r}, \vec{r}') = \sum_{h,L'} A^{+,i}_{hL'} \exp[i(\vec{q}+\vec{Q}_h)\cdot\vec{u} + i\kappa_h(z-b)] \times j_{l'}(\kappa\rho_i')Y^*_{L'}(\Theta_i'), \tag{A10}$$

where

$$A_{hL'} = \frac{(4\pi)(-i)^l}{2i\kappa_h}\frac{e^{i\kappa_h b}}{a}\exp[i\vec{P}^+_h\cdot\vec{r}_i]Y_{L'}(\Theta^+_h), \tag{A11}$$

with

$$\vec{P}^+_h \equiv (q_x+Q_{hx},\ q_y+Q_{hy},\ \kappa_h),$$
$$\Theta^+_h \equiv (\theta^+_h,\ \varphi^+_h) \equiv \text{polar angles of } \vec{P}^+_h. \tag{A12}$$

Similarly, if $\vec{r}$ is just below S_- and $\vec{r}'$ just outside S_i, we find

$$G(\vec{r}, \vec{r}') = \sum_{h,L'} A^{-,i}_{hL'} \exp[i(\vec{q}+\vec{Q}_h)\cdot\vec{u} - i\kappa_h(z+b)] \times j_{l'}(\kappa\rho_i')Y^*_{L'}(\Theta_i'), \tag{A13}$$

where

$$A^{-,i}_{hL'} = \frac{(4\pi)(-i)^l}{2i\kappa_h}\frac{e^{i\kappa_h b}}{a}\exp[i\vec{P}^-_h\cdot\vec{r}_i]Y_{L'}(\Theta^-_h) \tag{A14}$$

with

$$\vec{P}^-_h \equiv (q_x+Q_{hx},\ q_y+Q_{hy},\ -\kappa_h), \tag{A15}$$
$$\Theta^-_h \equiv (\theta^-_h,\ \varphi^-_h) \equiv \text{polar angles of } P^-_h. \tag{A16}$$

Next we take $\vec{r}$ just inside S_i and $\vec{r}'$ just above S_+. This gives

$$G(\vec{r}, \vec{r}') = \sum_{L,h'} A^{i,+}_{Lh'} j_l(\kappa\rho_i)Y_L(\Theta_i) \times \exp[-i(\vec{q}+\vec{Q}_{h'})\cdot\vec{u}' + i\kappa_{h'}(z'-b)], \tag{A17}$$

where

$$A^{i,+}_{Lh'} = \frac{(4\pi)(i)^l}{2i\kappa_h}\frac{\exp(i\kappa_{h'}b)}{a}\exp[i\vec{P}^-_{h'}\cdot\vec{r}_i]Y^*_L(\Theta^-_{h'}). \tag{A18}$$

Similarly, if $\vec{r}$ is just inside S_i and $\vec{r}'$ just below S_-, we find

$$G(\vec{r}, \vec{r}') = \sum_{L,h'} A^{i,-}_{Lh'} j_l(\kappa\rho_i)Y_L(\Theta_i) \times \exp[-i(\vec{q}+\vec{Q}_{h'})\cdot\vec{u}' - i\kappa_{h'}(z'+b)], \tag{A19}$$

where

$$A^{i,-}_{Lh'} = \frac{(4\pi)i^l}{2i\kappa_{h'}}\frac{\exp(i\kappa_{h'}b)}{a}\exp(i\vec{P}^+_{h'}\cdot\vec{r}_i)Y^*_L(\Theta^+_{h'}). \tag{A20}$$

Next we take $\vec{r}$ just above S_+ and $\vec{r}'$ just below S_+, which gives, by (A1),

$$G(\vec{r}, \vec{r}') = \sum_h A^{+,+}_h \exp[i(\vec{q}+\vec{Q}_h)\cdot(\vec{u}-\vec{u}') + i\kappa_h(z-z')], \tag{A21}$$

with

$$A^{+,+}_h = 1/2i\kappa_h a. \tag{A22}$$

Similarly, with $\vec{r}$ just above S_+ and $\vec{r}'$ just above S_-, we find

$$G(\vec{r}, \vec{r}') = \sum_h A^{+,-}_h \exp[i(\vec{q}+\vec{Q}_h)\cdot(\vec{u}-\vec{u}') + i\kappa_h(z-z'-2b)], \tag{A23}$$

where

$$A^{+,-}_h = \exp(2i\kappa_h b)/2i\kappa_h a. \tag{A24}$$

When $\vec{r}$ is just below S_- and $\vec{r}'$ just below S_+, we find

$$G(\vec{r}, \vec{r}') = \sum_h A^{-,+}_h \exp[i(\vec{q}+\vec{Q}_h)\cdot(\vec{u}-\vec{u}') + i\kappa_h(z'-z-2b)], \tag{A25}$$

with

$$A^{-,+}_h = \exp(2i\kappa_h b)/2i\kappa_h a; \tag{A26}$$

and when $\vec{r}$ is just below S_- and $\vec{r}'$ just above S_-,

$$G(\vec{r}, \vec{r}') = \sum_h A^{-,-}_h \exp[i(\vec{q}+\vec{Q}_h)\cdot(\vec{u}-\vec{u}') + i\kappa_h(z'-z)], \tag{A27}$$

with

$$A^{-,-}_h = 1/2i\kappa_h a. \tag{A28}$$

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