Construction of a simple representation for the Green's function of a crystalline film*

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For a one-dimensional Hamiltonian, $H = -(\hbar^2/2m)(d^2/dz^2) + V(z)$, it is well known that the Green's function $G(z,z';E)$ may be written in the simple form $G(z,z';E) = \psi^+(z_>;E)\psi^-(z_<;E)/W(E)$, where $\psi^\pm(z;E)$ are the solutions to the Schrödinger equation, $(E-H)\psi(z;E)=0$, which satisfy outgoing boundary conditions, respectively, at $z \to \pm\infty$, and where $W(E)$ is the Wronskian. Here, an analogous expression is derived for the Green's function of a crystalline film, i.e., of a solid whose one-electron potential $V(\vec{\rho},z)$ has the translational periodicity of a lattice in $\vec{\rho} \equiv (x,y)$, and vanishes as $z \to \pm\infty$.

INTRODUCTION

Although the spectal representation of a Green's function is frequently useful in proving formal results, in practical numerical calculations it is not for a number of reasons. First, since it expresses the Green's function at energy E in terms of a sum over a complete set of wave functions, including those which are far from E in energy, the use of the spectral representation seemingly necessitates the development of approximate schemes for calculating wave functions far from the energy range of interest. Second, even assuming that one knows how to compute all of the complete set of wave functions, in order to use the spectral representation one must still perform a singular integral over products of these functions, which in general is a far from trivial computational problem. Finally, one frequently wishes to find a Green's function for a non-Hermitian "optical potential." In this case the ordinary spectral representation does not exist.

For one-dimensional problems, as is well known, a Green's function may easily be evaluated without the use of the spectral representation. That is, for example, the outgoing Green's function $G^+(z,z';E)$, which is defined by the equation of motion

$$\left(E+\frac{\hbar^2}{2m}\frac{d^2}{dz^2}-V(z)\right)G^+(z,z';E)=\delta(z-z'), \quad (1)$$

by symmetry under the coordinate interchange, $z \rightleftarrows z'$, and by the condition that it be an outgoing function of z as $z\to\pm\infty$, may be written explicitly in the form[1]

$$G^+(z,z';E)=[1/W(E)][\psi^+(z;E)\psi^-(z';E)\Theta(z-z') + \psi^+(z';E)\psi^-(z;E)\Theta(z'-z)]. \quad (2)$$

In Eq. (2), $\psi^\pm(z;E)$ are the two linearly independent solutions of the Schrödinger equation

$$\left(E+\frac{\hbar^2}{2m}\frac{d^2}{dz}-V(z)\right)\psi(z;E)=0 \quad (3)$$

which satisfy outgoing boundary conditions, respectively, as $z\to\pm\infty$, the Wronskian $W(E)$ is defined by

$$W(E)=\frac{\hbar^2}{2m}\left(\frac{d\psi^+(z;E)}{dz}\psi^-(z;E)-\psi^+(z;E)\frac{d\psi^-(z;E)}{dz}\right), \quad (4)$$

and $\Theta(x)$ is the usual step function. [That $W(E)$ is z independent is, of course, a direct consequence of Eq. (3).] Comparing Eq. (2) for $G^+(z,z';E)$ to the spectral representation

$$G^+(z,z';E)=\sum_s\frac{\psi_s(z)\psi_s^*(z')}{E+i\delta-E_s}, \quad (5)$$

where the summation runs over any complete set of solutions to

$$\left(E_s+\frac{\hbar^2}{2m}\frac{d^2}{dz^2}-V(z)\right)\psi_s(z)=0, \quad (6)$$

one sees that the former equation is far simpler to use in practical calculations. First, Eq. (2) only requires knowledge of the two wave functions $\psi^\pm(z;E)$ instead of the complete set $\{\psi_s(z)\}$, and besides, Eq. (2) requires no summation to be performed. [Also, Eq. (2) is trivially generalizable to the case of a non-Hermitian potential.]

In general, in three dimensions there is no representation of the Green's function analogous to Eq. (2). However, in certain special cases there is. The most obvious case is that of a jellium film, i.e., a solid whose one-electron potential $V(\vec{\rho},z)$ is independent of $\vec{\rho}\equiv(x,y)$. In this case the Schrödinger equation separates in x, y, and z, and one finds that

$$G^+(\vec\rho,z;\vec\rho\,'z';E) = \int \frac{d^2k}{(2\pi)^2} e^{i\vec k\cdot(\vec\rho-\vec\rho\,')} G^+\left(z,z';E-\frac{\hbar^2k^2}{2m}\right), \quad (7)$$

in which the Fourier-transformed Green's function $G^+(z,z';E-\hbar^2k^2/2m)$ is given precisely by Eq. (2) (with E replaced by $E-\hbar^2k^2/2m$). In what follows an expression similar to Eq. (2) is derived for the Fourier-transformed Green's function of a crystalline film, i.e., a solid whose one-electron potential $V(\vec\rho,z)$ has the translational periodicity of a lattice in $\vec\rho$, and which vanishes as $z\to\pm\infty$. This formula [Eq. (30)] should prove useful in future calculations concerning the structure of crystal surfaces. One obvious such calculation is that of local field effects at the surface of a crystal irradiated by an electromagnetic wave. In the jellium version of this problem,[2] Eqs. (2) and (7) were of great value, in reducing the amount of numerical computation necessary.

CONSTRUCTION OF THE GREEN'S FUNCTION FOR A CRYSTALLINE FILM

Consider a solid whose one-electron potential $V(\vec\rho,z)$ can be written in the form

$$V(\vec\rho,z)=\sum_{\vec g} e^{i\vec g\cdot\vec\rho}\,V_{\vec g}(z), \quad (8)$$

where $\{\vec g\}$ is a set of two-dimensional reciprocal-lattice vectors, and suppose that the solid is a film which lies roughly between $z=0$ and $z=D$, i.e., that for z sufficiently negative, or for $z>>D$, $V_{\vec g}(z)\approx 0$. One seeks the outgoing Green's function $G^+(\vec\rho,z;\vec\rho\,',z';E)$ which satisfies the inhomogeneous partial differential equation

$$\left(E+\frac{\hbar^2}{2m}\nabla^2-V(\vec\rho,z)\right)G^+(\vec\rho,z;\vec\rho\,',z';E) = \delta^{(2)}(\vec\rho-\vec\rho\,')\delta(z-z'), \quad (9)$$

and which is symmetric under the coordinate interchange $(\vec\rho,z)\rightleftharpoons(\vec\rho\,',z')$.

The first step in the formal solution of Eq. (9) is to make use of two-dimensional crystalline periodicity [Eq. (8)], which immediately implies that $G^+(\vec\rho,z;\vec\rho\,',z';E)$ is of the form

$$G^+(\vec\rho,z;\vec\rho\,',z';E)\int_{2\text{D}-\text{BZ}}\frac{d^2k}{(2\pi)^2} \times\sum_{\vec g,\vec g\,'} e^{i(\vec k+\vec g)\cdot\vec\rho-i(\vec k+\vec g\,')\cdot\vec\rho\,'} \times G^{+}_{\vec k,E;\vec g,\vec g\,'}(z,z'), \quad (10)$$

where the $\vec k$ integral runs over the first two-dimensional Brillouin zone (2D-BZ). Equation (10) is the crystal film analog of Eq. (7). Substituting Eq. (10) into Eq. (9) one obtains a matrix of one-dimensional equations for the $G^+_{\vec k,E;\vec g,\vec g\,'}(z,z')$, namely,

$$\left(E-\frac{\hbar^2}{2m}(\vec k+\vec g)^2+\frac{\hbar^2}{2m}\frac{d^2}{dz^2}\right)G^+_{\vec k,E;\vec g,\vec g\,'}(z,z') - \sum_{\vec g\,''} V_{\vec g-\vec g\,''}(z)G^+_{\vec k,E;\vec g\,'',\vec g\,'}(z,z')=\delta(z-z')\delta_{\vec g,\vec g\,'}, \quad (11)$$

where $\delta_{\vec g,\vec g\,'}$ is a Kronecker δ function. At the same time, since by symmetry under the interchange $(\vec\rho,z)\rightleftharpoons(\vec\rho\,',z')$, $G^+(\vec\rho,z;\rho',z';E)$ must also satisfy the equation

$$\left(E+\frac{\hbar^2}{2m}\nabla'^2-V(\vec\rho\,',z')\right)G^+(\vec\rho,z;\vec\rho\,',z';E) = \delta^{(2)}(\vec\rho-\vec\rho\,')\delta(z-z'), \quad (12)$$

the $G^+_{\vec k,E;\vec g,\vec g\,'}(z,z')$ must satisfy in addition to Eq. (11) the equation

$$\left(E-\frac{\hbar^2}{2m}(\vec k+\vec g)^2+\frac{\hbar^2}{2m}\frac{d^2}{dz^2}\right)G^+_{\vec k,E;\vec g,\vec g\,'}(z,z') - \sum_{\vec g\,''} G^+_{\vec k,E;\vec g,\vec g\,''}(z,z')V_{\vec g\,''-\vec g\,'}(z')=\delta(z-z')\delta_{\vec g,\vec g\,'}. \quad (13)$$

In the special case of a reflection symmetric surface, for which

$$V_{\vec g}(z)=V_{-\vec g}(z), \quad (14)$$

Eqs. (11) and (13) are identical. But in the general case they are not.

The idea to be pursued, in analogy to the one-dimensional case, is to attempt to find solutions to Eq. (11) and (13) in terms of solutions to the corresponding Schrödinger equations,

$$\left(E-\frac{\hbar^2}{2m}(\vec k+\vec g)^2+\frac{\hbar^2}{2m}\frac{d^2}{dz^2}\right)u^{\pm}_{\vec b,\vec g}(z;\vec k,E) - \sum_{\vec g\,''} V_{\vec g-\vec g\,''}(z)u^{\pm}_{\vec b,\vec g\,''}(z;\vec k,E)=0, \quad (15a)$$

$$\left(E-\frac{\hbar^2}{2m}(\vec k+\vec g)^2+\frac{\hbar^2}{2m}\frac{d^2}{dz^2}\right)v^{\pm}_{\vec b,\vec g}(z;\vec k,E) - \sum_{\vec g\,''} v^{\pm}_{\vec b,\vec g\,''}(z';\vec k,E)V_{\vec g\,''-\vec g}(z)=0. \quad (15b)$$

[These equations are identical to one another if Eq. (14) is true. However, for what follows there is no need to restrict to this case.] In general, for a fixed value of E, each of Eqs. (15a) and (15b) will have two linearly independent solutions per reciprocal-lattice vector. This fact accounts for the $\pm$ and b labels of the u's and v's. The superscripts plus and minus are given a precise meaning below.

All that one needs to know about the band index $\vec{b}$ at this point is that there is one value of $\vec{b}$ for each value of $\vec{g}$.

The most important property of the u's and v's in the construction of $G^{+}_{\vec{k},E;\vec{g},\vec{g}'}(z,z')$ is that they satisfy Wronskian relations.[8] In particular, using Eqs. (15) it is easy to show that the quantities $W^{\pm,\pm}_{\vec{b},\vec{b}'}(\vec{k},E)$, defined by

$$W^{\pm,\pm}_{\vec{b},\vec{b}'}(\vec{k},E) \equiv \frac{\hbar^2}{2m}\sum_{\vec{g}}\left(\frac{du^{\pm}_{\vec{b},\vec{g}}(z;\vec{k},E)}{dz}v^{\pm}_{\vec{b}',\vec{g}}(z;\vec{k},E) - u^{\pm}_{\vec{b},\vec{g}}(z;\vec{k},E)\frac{dv^{\pm}_{\vec{b}',\vec{g}}(z;\vec{k},E)}{dz}\right), \tag{16}$$

satisfy

$$\frac{d}{dz}W^{\pm,\pm}_{\vec{b},\vec{b}'}(\vec{k},E)=0. \tag{17}$$

Thus the $W^{\pm,\pm}_{\vec{b},\vec{b}'}(\vec{k},E)$ are constant in z, and represent a matrix of Wronskians for Eqs. (15).

One now proceeds to specify the precise boundary conditions satisfied by the $u^{\pm}_{\vec{b},\vec{g}}(z;\vec{k},E)$ and $v^{\pm}_{\vec{b},\vec{g}}(z;\vec{k},E)$. One will then be able to evaluate the Wronskian matrix formally, and to construct a trial expression for $G^{+}_{\vec{k},E;\vec{g},\vec{g}'}(z,z')$.

In order to impose boundary conditions on the u's and v's, one examines Eqs. (15) in the regions $z\to\pm\infty$. In these regions, because of the assumption of film geometry, Eqs. (15) assume the form

$$0=\left(E-\frac{\hbar^2}{2m}(\vec{k}+\vec{g})^2+\frac{\hbar^2}{2m}\frac{d^2}{dz^2}\right)\times\begin{cases}u^{\pm}_{\vec{b},\vec{g}}(z;\vec{k},E)\\ v^{\pm}_{\vec{b},\vec{g}}(z;\vec{k},E)\end{cases} \tag{18}$$

Therefore asymptotically the u's and v's are linear combinations of plane waves, of the general forms

$$u^{\pm}_{\vec{b},\vec{g}}(z;\vec{k},E)\xrightarrow[z\to\infty]{}\mathcal{A}^{u\pm}_{\vec{b},\vec{g}}(\vec{k},E)e^{i(z-D)K(\vec{k}+\vec{g},E)}+\mathcal{B}^{u\pm}_{\vec{b},\vec{g}}(\vec{k},E)e^{-i(z-D)K(\vec{k}+\vec{g},E)}, \tag{19}$$

$$v^{\pm}_{\vec{b},\vec{g}}(z;\vec{k},E)\xrightarrow[z\to\infty]{}\mathcal{A}^{v\pm}_{\vec{b},\vec{g}}(\vec{k},E)e^{i(z-D)K(\vec{k}+\vec{g},E)}+\mathcal{B}^{v\pm}_{\vec{b},\vec{g}}(\vec{k},E)e^{-i(z-D)K(\vec{k}+\vec{g},E)}$$

and

$$u^{\pm}_{\vec{b},\vec{g}}(z;\vec{k},E)\xrightarrow[z\to-\infty]{}\mathcal{C}^{u\pm}_{\vec{b},\vec{g}}(\vec{k},E)\;e^{izK(\vec{k}+\vec{g},E)}+\mathcal{D}^{u\pm}_{\vec{b},\vec{g}}(\vec{k},E)\;e^{-izK(\vec{k}+\vec{g},E)}, \tag{20}$$

$$v^{\pm}_{\vec{b},\vec{g}}(z;\vec{k},E)\xrightarrow[z\to-\infty]{}\mathcal{C}^{v\pm}_{\vec{b},\vec{g}}(\vec{k},E)\;e^{izK(\vec{k}+\vec{g},E)}+\mathcal{D}^{v\pm}_{\vec{b},\vec{g}}(\vec{k},E)\;e^{-izK(\vec{k}+\vec{g},E)},$$

where $K(\vec{k}+\vec{g},E)$ is defined by

$$K(\vec{k}+\vec{g},E)\equiv\begin{cases}[2mE/\hbar^2-(\vec{k}+\vec{g})^2]^{1/2}, & E>\hbar^2(\vec{k}+\vec{g})^2/2m\\ i[(\vec{k}+\vec{g})^2-2mE/\hbar^2]^{1/2}, & E<\hbar^2(\vec{k}+\vec{g})^2/2m,\end{cases} \tag{21}$$

and where the $\mathcal{A}$'s, $\mathcal{B}$'s, $\mathcal{C}$'s, and $\mathcal{D}$'s are constants are specified by imposing boundary conditions on the u's and v's. In particular, since each of Eqs. (15a) and (15b) is a matrix of second-order differential equations with one matrix row and column per reciprocal-lattice vector, in order to specify each of the $u^{\pm}_{\vec{b},\vec{g}}(z;\vec{k},E)$ and $v^{\pm}_{\vec{b},\vec{g}}(z;\vec{k},E)$ for a given band index $\vec{b}$, one must impose two boundary conditions per $\vec{g}$.

A particularly convenient set of (manifestly linearly independent) u's and a similar set of v's is obtained when one imposes boundary conditions as follows: One requires that

$$\mathcal{A}^{u+}_{\vec{b},\vec{g}}(\vec{k},E)=\mathcal{A}^{v+}_{\vec{b},\vec{g}}(\vec{k},E)=\mathcal{D}^{u-}_{\vec{b},\vec{g}}(\vec{k},E)=\mathcal{D}^{v-}_{\vec{b},\vec{g}}(\vec{k},E)=\delta_{\vec{b},\vec{g}}/iK(\vec{k}+\vec{g},E) \tag{22}$$

and that

$$\mathcal{B}^{u+}_{\vec{b},\vec{g}}(\vec{k},E)=\mathcal{B}^{v+}_{\vec{b},\vec{g}}(\vec{k},E)=\mathcal{C}^{u-}_{\vec{b},\vec{g}}(\vec{k},E)=\mathcal{C}^{v-}_{\vec{b},\vec{g}}(\vec{k},E)=0. \tag{23}$$

Note that Eqs. (22) and (23) correctly correspond to two conditions per reciprocal-lattice vector for each $\vec{b}$.

According to Eqs. (22) and (23) one has the asymptotic formulas

$$u^{+}_{\vec{b},\vec{g}}(z\to\infty;\vec{k},E)=v^{+}_{\vec{b},\vec{g}}(z\to\infty;\vec{k},E)\to\delta_{\vec{b},\vec{g}}e^{i(z-D)K(\vec{k}+\vec{g},E)}/iK(\vec{k}+\vec{g},E) \tag{24}$$

and

$$u^{-}_{\vec{b},\vec{g}}(z\to-\infty;\vec{k},E)=v^{-}_{\vec{b},\vec{g}}(z\to-\infty;\vec{k},E)\to\delta_{\vec{b},\vec{g}}e^{-izK(\vec{k}+\vec{g},E)}/iK(\vec{k}+\vec{g},E). \tag{25}$$

Thus the superscript plus now corresponds to functions which are outgoing on the right ($z\to+\infty$) and the subscript minus corresponds to those which are outgoing on the left ($z\to-\infty$).

Now that one knows the asymptotic properties of the u's and v's, one can calculate the Wronskian matrix (which is guaranteed to be z independent and therefore may as well be calculated in the regions $z\to\pm\infty$, where the u's and v's are known). Using Eqs. (19) and (20), and (22)–(25), one finds from Eqs. (16) and (17) the following results:

$$W^{++}_{\vec{b},\vec{b}'}(\vec{k},E)=W^{--}_{\vec{b},\vec{b}'}(\vec{k},E)=0, \quad (26)$$

$$W^{+-}_{\vec{b},\vec{b}'}(\vec{k},E)=(\hbar^2/m)\mathcal{B}^{v^-}_{\vec{b}',\vec{b}}=(\hbar^2/m)\mathcal{C}^{u^+}_{\vec{b},\vec{b}'}, \quad (27)$$

and

$$W^{-+}_{\vec{b},\vec{b}'}(\vec{k},E)=-(\hbar^2/m)\mathcal{C}^{v^+}_{\vec{b}',\vec{b}}=-(\hbar^2/m)\mathcal{B}^{u^-}_{\vec{b},\vec{b}'}. \quad (28)$$

Note that in addition to having calculated the Wronskian matrix completely, in Eqs. (27) and (28) one has also found (via the z independence of the Wronskian) relations between the $\mathcal{B}$'s and $\mathcal{C}$'s.

At this point one has sufficient knowledge of the u's and v's to propose a trial solution to Eqs. (11) and (13) for $G^{+}_{\vec{k},E;\vec{g},\vec{g}'}(z,z')$, namely,

$$G^{+}_{\vec{k},E;\vec{g},\vec{g}'}(z,z')=\sum_{\vec{b},\vec{b}'}[u^{+}_{\vec{b},\vec{g}}(z;\vec{k},E)M_{\vec{b},\vec{b}'}(\vec{k},E)\times v^{-}_{\vec{b}',\vec{g}'}(z';\vec{k},E)\theta(z-z')+u^{-}_{\vec{b},\vec{g}}(z;\vec{k},E)N_{\vec{b},\vec{b}'}(\vec{k},E)\times v^{+}_{\vec{b}',\vec{g}'}(z';\vec{k},E)\theta(z'-z)], \quad (29)$$

wherein $M_{\vec{b},\vec{b}'}(\vec{k},E)$ and $N_{\vec{b},\vec{b}'}(\vec{k},E)$ are z- and z'-independent matrices, to be determined. (The fact that these matrices are z and z' independent, of course, instantly suggests that they will have to be related to the Wronskian matrix which, as is shown below, is quite true.)

Note that by virtue of Eqs. (24) and (25), the trial function of Eq. (29) automatically satisfies outgoing boundary condition as $z\to\pm\infty$ or $z'\to\pm\infty$. In order that Eq. (29) satisfy Eq. (11), it is necessary and sufficient that the following equations be satisfied *for all* $\vec{g}$, $\vec{g}'$, $\vec{k}$, E, and z:

$$\sum_{\vec{b},\vec{b}'}[u^{+}_{\vec{b},\vec{g}}(z;\vec{k},E)M_{\vec{b},\vec{b}'}(\vec{k},E)v^{-}_{\vec{b}',\vec{g}'}(z;\vec{k},E)-u^{-}_{\vec{b},\vec{g}}(z;\vec{k},E)N_{\vec{b},\vec{b}'}(\vec{k},E)v^{+}_{\vec{b}',\vec{g}'}(z;\vec{k},E)]=0 \quad (30)$$

and

$$\sum_{\vec{b},\vec{b}'}\left(\frac{du^{+}_{\vec{b},\vec{g}}(z;\vec{k},E)}{dz}M_{\vec{b},\vec{b}'}(\vec{k},E)v^{-}_{\vec{b}',\vec{g}'}(z;\vec{k},E)-\frac{du^{-}_{\vec{b},\vec{g}}(z;\vec{k},E)}{dz}N_{\vec{b},\vec{b}'}(\vec{k},E)v^{+}_{\vec{b}',\vec{g}'}(z,\vec{k},E)\right)=\frac{2m}{\hbar^2}\delta_{\vec{g},\vec{g}'}. \quad (31)$$

Equation (30), if satisfied, guarantees that $dG^{+}_{\vec{k},E;\vec{g},\vec{g}'}(z,z')/dz$ contains no term proportional to $\delta(z-z')$ {which is clearly necessary if $dG^{+}_{\vec{k},E;\vec{g},\vec{g}'}(z,z')/dz^2$ is not to contain a term proportional to $d[\delta(z-z')]/dz$}. Equation (31), if satisfied, guarantees that the application of the operator on the left-hand side of Eq. (11) to the trial function of Eq. (29) yields precisely $\delta_{\vec{g},\vec{g}'}\delta(z-z')$.

In addition to Eqs. (30) and (31), in order that the ansatz of Eq. (29) satisfy Eq. (13), it is also necessary that the equation

$$\sum_{\vec{b},\vec{b}'}\left(u^{+}_{\vec{b},\vec{g}}(z;\vec{k},E)M_{\vec{b},\vec{b}'}(\vec{k},E)\frac{dv^{-}_{\vec{b}',\vec{g}'}(z;\vec{k},E)}{dz}-u^{-}_{\vec{b},\vec{g}}(z;\vec{k},E)N_{\vec{b},\vec{b}'}(\vec{k},E)\frac{dv^{+}_{\vec{b}',\vec{g}'}(z;\vec{k},E)}{dz}\right)=-\frac{2m}{\hbar^2}\delta_{\vec{g},\vec{g}'} \quad (32)$$

be satisfied. This equation is the analog of Eq. (31) for the z' and g' variables in $G^{+}_{\vec{k},E;\vec{g},\vec{g}'}(z,z')$. [Equation (30) serves the same function in satisfying Eq. (13) as it did for Eq. (11); i.e., it guarantees that $dG^{+}_{\vec{k},E;\vec{g},\vec{g}'}(z,z')/dz'$ contains no term proportional to $\delta(z-z')$.]

One now seeks to determine whether any matrices $M_{\vec{b},\vec{b}'}(\vec{k},E)$ and $N_{\vec{b},\vec{b}'}(\vec{k},E)$ exist such that Eqs. (30)–(32) are satisfied. To begin, one subtracts the z derivative of Eq. (30) from Eq. (31). This exercise immediately shows that if Eqs. (30) and (31) are true, then Eq. (32) is automatically satisfied. Thus Eq. (32) need not be considered further.

To solve Eqs. (30) and (31), one first multiplies Eq. (30) by $dv^{-}_{\vec{b}'',\vec{g}}(z;\vec{k},E)/dz$ and Eq. (31) by $v^{-}_{\vec{b}'',\vec{g}}(z;\vec{k},E)$. Summing the resulting equations on $\vec{g}$, subtracting one from the other, and using the definitions of Eqs. (16), one then obtains the relation

$$\sum_{\vec{b},\vec{b}'}[W^{+-}_{\vec{b},\vec{b}''}(\vec{k},E)M_{\vec{b},\vec{b}'}(\vec{k},E)v^{-}_{\vec{b}',\vec{g}'}(z;\vec{k},E)-W^{--}_{\vec{b},\vec{b}''}N_{\vec{b},\vec{b}'}(\vec{k},E)v^{+}_{\vec{b},\vec{g}'}(z;\vec{k},E)]=v^{-}_{\vec{b}'',\vec{g}'}(z;\vec{k},E) \quad (33)$$

or, using Eq. (26), the equation for $M_{\vec{b},\vec{b}'}(\vec{k},E)$,

$$\sum_{\vec{b},\vec{b}'}W^{+-}_{\vec{b},\vec{b}''}(\vec{k},E)M_{\vec{b},\vec{b}'}(\vec{k},e)v^{-}_{\vec{b}',\vec{g}'}(z;\vec{k},E)=v^{-}_{\vec{b}'',\vec{g}'}(z;\vec{k},E). \quad (34)$$

A similar equation is obtained for $N_{\vec{b},\vec{b}'}(\vec{k},E)$ by multiplying Eq. (30) by $dv^{+}_{\vec{b}'',\vec{g}}(z;\vec{k},E)/dz$ and Eq. (31) by $v^{+}_{\vec{b}'',\vec{g}}(z;\vec{k},E)$. Again subtracting one of the resulting equations from the other, summing on $\vec{g}$, and using Eqs. (16) and (26), one finds that $N_{\vec{b},\vec{b}'}(\vec{k},E)$ must satisfy

$$-\sum_{\vec b,\vec b'} W^{-+}_{\vec b,\vec b''}(\vec k,E)N_{\vec b,\vec b'}(\vec k,E)v^{+}_{\vec b',\vec g'}(z;\vec k,E) = v^{+}_{\vec b'',\vec g'}(z;\vec k,E). \quad (35)$$

Equations (34) and (35) must be true for all values of z, $\vec b''$, and $\vec g'$. By virtue of the linear independence of the v's these equations are therefore equivalent to the relations

$$\sum_{\vec b} W^{+-}_{\vec b,\vec b''}(\vec k,E)M_{\vec b,\vec b'}(\vec k,E)=\delta_{\vec b'',\vec b'}, \quad (36)$$

$$\sum_{\vec b} (-W^{-+}_{\vec b,\vec b''})N_{\vec b,\vec b'}(\vec k,E)=\delta_{\vec b'',\vec b'}, \quad (37)$$

which state that M and N must be the transposed matrix inverses of W^{+-} and $-W^{-+}$, respectively.

Equations (37) and (38) are necessary conditions for the satisfaction of Eqs. (30) and (31). It remains to show that they also represent sufficient conditions. Thus suppose that Eqs. (36) and (37) are true. Then using Eqs. (16) and (26) it follows that the equations

$$\sum_{\vec g}\left(v^{+}_{\vec b,\vec g}(z;\vec k,E)S_{\vec g,\vec g'}(z;\vec k,E) - \frac{dv^{+}_{\vec b,\vec g}(z;\vec k,E)}{dz}T_{\vec g,\vec g'}(z;\vec k,E)\right)=0, \quad (38)$$

$$\sum_{\vec g}\left(v^{-}_{\vec b,\vec g}(z;\vec k,E)S_{\vec g,\vec g'}(z;\vec k,E) - \frac{dv^{-}_{\vec b,\vec g}(z;\vec k,E)}{dz}T_{\vec g,\vec g'}(z;\vec k,E)\right)=0 \quad (39)$$

are satisfied for all $\vec b$ and $\vec g'$, where $S_{\vec g,\vec g'}(z,\vec k,E)$ and $T_{\vec g,\vec g'}(z;\vec k,E)$ are defined by

$$S_{\vec g,\vec g'}(z;\vec k,E) \equiv \sum_{\vec b,\vec b'}\left(\frac{du^{+}_{\vec b,\vec g}(z;\vec k,E)}{dz}M_{\vec b,\vec b'}(\vec k,E)v^{-}_{\vec b',\vec g}(z;\vec k,E) - \frac{du^{-}_{\vec b,\vec g}(z;\vec k,E)}{dz}N_{\vec b,\vec b'}(\vec k,E)v^{+}_{\vec b',\vec g'}(z;\vec k,E) - \frac{2m}{\hbar^2}\delta_{\vec g,\vec g'}\right) \quad (40)$$

and

$$T_{\vec g,\vec g'}(z;\vec k,E) \equiv \sum_{\vec b,\vec b'}[u^{+}_{\vec b,\vec g}(z;\vec k,E)M_{\vec b,\vec b'}(\vec k,E)v^{-}_{\vec b',\vec g'}(z;\vec k,E) - u^{-}_{\vec b,\vec g}(z,\vec k,E)N_{\vec b,\vec b'}(\vec k,E)v^{+}_{\vec b',\vec g'}(z;\vec k,E)]. \quad (41)$$

But by the linear independence of the functions $v^{\pm}_{\vec b,\vec g}(z;\vec k,E)$ [and the fact that these functions satisfy the *second-order* differential equation, Eq. (15b)], one knows that the matrix

$$\begin{pmatrix} (v^{+}_{\vec b,\vec g}(z;\vec k,E)) & \left(-\frac{dv^{+}_{\vec b,\vec g}(z;\vec k,E)}{dz}\right) \\ (v^{-}_{\vec b,\vec g}(z;\vec k,E)) & \left(-\frac{dv^{-}_{\vec b,\vec g}(z;\vec k,E)}{dz}\right)\end{pmatrix} \quad (42)$$

is nonsingular. Thus Eqs. (38) and (39) imply that

$$S_{\vec g,\vec g'}(z;\vec k,E)=T_{\vec g,\vec g'}(z;\vec k,E)=0 \quad (43)$$

or, equivalently [cf. the definitions of S and T, Eqs. (40) and (41)], that Eqs. (30) and (31) are true.

Thus it has been shown that if the matrices $M_{\vec b,\vec b'}(\vec k,E)$ and $N_{\vec b,\vec b'}(\vec k,E)$ are the transposed inverses of the Wronskian matrices $W^{\pm}_{\vec b,\vec b'}{}^{\mp}(\vec k,E)$ and $-W^{\mp}_{\vec b,\vec b'}{}^{\pm}(\vec k,E)$, respectively, then the ansatz of Eq. (29) satisfies all the conditions to be the Green's function for a crystalline film.

The final formula for the two-dimensional Fourier transform of the Green's function of a crystalline film is given here, for convenience, as follows:

$$G^{+}_{\vec k,E;\vec g,\vec g'}(z,z') = \sum_{\vec b,\vec b'}\{u^{+}_{\vec b,\vec g}(z;\vec k,E)[W^{+-}(\vec k,E)]^{-1T}_{\vec b,\vec b'} \times v^{-}_{\vec b',\vec g'}(z';\vec k,E)\theta(z-z') + u^{-}_{\vec b,\vec g}(z;\vec k,E)[-W^{-+}(\vec k,E)]^{-1T}_{\vec b,\vec b'} \times v^{+}_{\vec b',\vec g'}(z';\vec k,E)\theta(z'-z)\}.$$

The Wronskian matrices $W^{\pm}$ and their transposed inverses are defined in Eqs. (16), (36), and (37). The wave functions u and v are defined by Eqs. (15), (24), and (25). The superscript T means "transpose."

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