

**Green's functions for surface physics**

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The following theorem is proved for a partial differential eigenvalue equation in a periodic system:  $-2\pi i \int_{\text{cell}} \vec{P}_0[\Psi^\dagger(\vec{k}n), \psi(\vec{k}'n')] \cdot d\vec{S} = v_j(\vec{k}n) \delta_{ijk} \delta_{nn'}$ , if  $\epsilon(\vec{k}'n') = \epsilon(\vec{k}n)$  and  $k'_i = k_i$  for  $i \neq j$ . Here  $\epsilon(\vec{k}n)$  is an eigenvalue,  $\psi(\vec{k}n)$  is an eigenfunction, and  $\vec{\Psi}(\vec{k}n)$  is a solution to the adjoint eigenvalue problem satisfying  $\int_{\text{cell}} d\vec{x} \Psi^\dagger(\vec{x}; \vec{k}n) \cdot \psi(\vec{x}; \vec{k}'n') = \delta_{nn'}$ . Also,  $v_j(\vec{k}n) \equiv \partial \epsilon(\vec{k}n) / \partial k_j$ ,  $s_j$  is a cross section of the unit cell, and  $\vec{P}_0$  is the bilinear concomitant. The above theorem is used to evaluate the bulk Green's function in closed form:  $G_0(\vec{x}\vec{x}'; \vec{k}\epsilon) = -2\pi i \{ \sum_{n_l} [\psi(\vec{x}; \vec{k}k_{n_l}^+) \Psi^\dagger(\vec{x}'; \vec{k}k_{n_l}^+) / v_3(\vec{k}k_{n_l}^+) ] \theta(x_3 - x'_3) - \sum_{n_l} [\psi(\vec{x}; \vec{k}k_{n_l}^-) \Psi^\dagger(\vec{x}'; \vec{k}k_{n_l}^-) / v_3(\vec{k}k_{n_l}^-) ] \theta(x'_3 - x_3) \}$ , where  $\vec{k} \equiv (k_1, k_2)$ . The  $k_{n_l}$  are those values of  $k_3$  for which  $\epsilon(\vec{k}k_{n_l}) = \epsilon$ , partitioned into the two sets  $k_{n_l}^+$  and  $k_{n_l}^-$  according to the boundary conditions on  $G_0$ . A Green's function  $G(\vec{x}\vec{x}'; \vec{k}\epsilon)$  in the presence of an interface is given by the above expression if  $\psi$  is replaced by  $\Psi$ , an eigenfunction that grows out of  $\psi$  as the interface is approached. This expression also gives the exact many-body Green's function  $\mathcal{G}_0$  (or  $\mathcal{G}$ ) if  $\epsilon(\vec{k}n)$  and  $\psi$  (or  $\Psi$ ) are interpreted as solutions to an eigenvalue problem involving the self-energy. Finally, the expression holds for nondifferential equations—e.g., the matrix eigenvalue equation for phonons or electrons in a localized representation; in this case, the derivation is based on the analytic properties of  $\epsilon(\vec{k}n)$  and  $\psi(\vec{k}n)$  at complex  $\vec{k}$ .

**I. INTRODUCTION**

There are Green's-function techniques for equilibrium problems involving interfaces—such as the calculation of electronic structure—and for nonequilibrium processes—such as tunneling, photoemission, field emission, and low-energy-electron diffraction. In this paper I derive a very general result that should simplify the evaluation, understanding, and employment of Green's functions in surface physics.

As an example, my result for the “retarded” bulk Green's function in the case of an arbitrary eigenvalue equation involving a (formally) self-adjoint operator or matrix is

$$G_0^*(\vec{x}\vec{x}'; \vec{k}\epsilon) = -2\pi i \sum_{n_l} \psi(\vec{x}; \vec{k}k_{n_l}n) \psi^\dagger(\vec{x}'; \vec{k}k_{n_l}^*n) \times [v_3(\vec{k}k_{n_l}n)]^{-1} \text{sgn}(x_3 - x'_3), \quad (1.1)$$

where

$$\vec{k} = (k_1, k_2), \quad \vec{k} = (\vec{k}, k_3) \quad (1.2)$$

and the  $\psi(\vec{x}; \vec{k}n)$  are Bloch functions for complex  $\vec{k}$  with the normalization

$$\int_{\text{cell}} d\vec{x} \psi^\dagger(\vec{x}; \vec{k}^*n) \cdot \psi(\vec{x}; \vec{k}n) = \delta_{nn'}. \quad (1.3)$$

In our notation,

$$v^\dagger \equiv (v^T)^*, \quad (1.4)$$

where  $v^T$  is the transpose of the vector  $v$ ; if  $v$  is a scalar,  $v^\dagger = v^*$ . The  $k_{n_l}$  are those values of  $k_3$  which satisfy two requirements: First,

$$\epsilon(\vec{k}k_{n_l}n) = \epsilon, \quad (1.5)$$

where  $\epsilon(\vec{k}n)$  is the eigenvalue for the  $n$ th branch and the wave vector  $\vec{k}$ . Second,

$$\text{Im}k_{n_l} \text{sgn}(x_3 - x'_3) > 0 \quad (1.6a)$$

if  $k_{n_l}$  is complex, or

$$v_3(\vec{k}k_{n_l}n) \text{sgn}(x_3 - x'_3) > 0 \quad (1.6b)$$

if  $k_{n_l}$  is real, where

$$v_j(\vec{k}n) \equiv \frac{\partial \epsilon(\vec{k}n)}{\partial k_j}. \quad (1.7)$$

As mentioned in a previous paper,<sup>1</sup> the solutions to (1.5) come in pairs, and (1.6) selects the appropriate member of the pair—a wave “propagating away from” the plane  $x_3 = x'_3$ , if  $k_{n_l}$  is real, or decaying away from this plane if  $k_{n_l}$  is complex.

Equation (1.1) is complementary to the expression that we obtained earlier in a mixed Wannier-Bloch representation<sup>1</sup>:

$$G_0^*(X_3 - X'_3; \vec{k}n\epsilon) = -2\pi i \sum_l \frac{e^{ik_{n_l}(X_3 - X'_3)}}{v_3(\vec{k}k_{n_l}n)} \text{sgn}(X_3 - X'_3) + G_{\text{BC}}. \quad (1.8)$$

An advantage of this earlier result is that it involves only the eigenvalues  $\epsilon(k_3)$  at complex  $k_3$ , and not the eigenfunctions  $\psi(\vec{x}; k_3)$ . Equation (1.1), however, has two advantages that should usually be more important: there is no branch-cut contribution  $G_{\text{BC}}$ , and the Green's function is in the coordinate representation or an arbitrary localized representation, rather than specifically the Wannier-Bloch representation.

If the values of  $\vec{x}$  are discrete, as they are in the lattice-dynamics problem for phonons and the matrix eigenvalue problem for electrons in a localized representation, then  $\int d\vec{x}$  in (1.3) is to be interpreted as  $\sum_{\vec{x}}$ , and  $\delta(\vec{x} - \vec{x}')$  in the following is to be interpreted as  $\delta_{\vec{x}\vec{x}'}$ . Also, for phonons  $\psi(\vec{x})$  is a three-dimensional vector, and for electrons in a localized representation it is an  $s$ -dimensional vector, where  $s$  is the number of basis functions employed for the atom (or unit cell) labeled by  $\vec{x}$ . For electrons in the coordinate representation,  $\psi(\vec{x})$  is a scalar, spinor, or four-component wave function, depending on the differential equation being used. In the case of the Schrödinger equation,  $\vec{x}$  may include a spin coordinate and  $n$  a spin quantum number.

The "advanced" Green's function  $G_0^-(\epsilon)$  is given by (1.1) if (1.6b) is replaced by

$$v_3(\vec{k}k_n n) \operatorname{sgn}(x_3 - x'_3) < 0. \quad (1.6b')$$

That is,  $G_0^-$  involves waves "propagating toward" the plane  $x_3 = x'_3$ , if  $k_n$  is real, or decaying away from this plane if  $k_n$  is complex. The "time-ordered" (zero-temperature, noninteracting fermion) Green's function is given by (1.1), with (1.6b) holding for  $\epsilon > \epsilon_F$ , and (1.6b') for  $\epsilon < \epsilon_F$ , where  $\epsilon_F$  is the Fermi energy.

The phrases "propagating away from" and "retarded" are used figuratively in this paper, and are defined by (1.6b). Similarly, "propagating toward" and "advanced" are defined by (1.6b'), and "time-ordered" is defined by either (1.6b) or (1.6b'), as described above. Whether this usage is literally correct depends on how the eigenvalue  $\epsilon$  arises from the frequency  $\omega$  through some time-dependent equation which is not considered here. For example, in the case of phonons the original equation is second order in the time, so

$$\epsilon = \omega^2, \quad (1.9)$$

where  $\omega$  is the phonon frequency. Then my labeling of the Green's functions is literally correct only for  $\omega > 0$ ; for  $\omega < 0$ ,  $G^+$  is really the advanced Green's function and  $G^-$  the retarded Green's function. Also, for phonons  $v_j = 2\omega V_j$ , where  $V_j$  is the actual group velocity.

The paper is organized as follows: In Sec. II the basic mathematical ideas are introduced. Perhaps the most important of these is the "bilinear concomitant," an object which is very useful in constructing Green's functions.<sup>2-4</sup> The mathematical abstractions are illustrated with physical examples in Sec. III, and the bilinear concomitant  $\bar{P}$  is connected to a current  $\vec{j}$ . In Sec. IV, I specialize to a periodic solid and consider the eigenvalue problem for complex  $\vec{k}$ . I then set out to evaluate the bulk Green's function  $G_0$  in Sec. V. In Sec. VI,

I prove a central theorem that relates  $\bar{P}$  to  $\vec{v} \equiv \vec{\nabla}_{\vec{k}} \epsilon(\vec{k})$ . This is a generalization of the well-known theorem<sup>5</sup> that the expectation value of the velocity is equal to the derivative of the energy eigenvalue with respect to  $\vec{k}$  for an electron in a periodic solid. In Sec. VII, the results of the preceding two sections are combined to give the final expression for  $G_0$ . This same expression is shown, in Secs. VIII-X, to give the Green's function in the presence of an interface, if  $\psi$  is replaced by  $\Psi$ , an eigenfunction that grows out of  $\psi$  as the interface is approached. Furthermore, it is shown in Sec. XI that this expression holds for the exact many-body Green's function  $\mathcal{G}_0(\epsilon)$  [or  $\mathcal{G}(\epsilon)$ ] if  $\epsilon(\vec{k}n)$  and  $\psi(\vec{k}n)$  [or  $\Psi(\vec{k}n)$ ] are the solutions to an eigenvalue problem involving the self-energy  $\Sigma(\epsilon)$ .

Up to this point, the treatment is concerned with partial differential (or integro-differential) equations. For equations containing no derivatives—such as the matrix eigenvalue equations for phonons, for magnons, and for electrons in a localized representation—the bilinear concomitant can be taken to be identically zero and the treatment of Secs. V-VII and IX-X is not applicable. In Sec. XII, therefore, I turn to a different approach, one that involves the properties of  $\epsilon(\vec{k}n)$  and  $\psi(\vec{k}n)$  [or  $\Psi(\vec{k}n)$ ] at complex  $\vec{k}$ . In Sec. XIII, I show that  $\epsilon(\vec{k}n)$  and  $\psi(\vec{k}n)$  usually have the required properties if  $H_0(\vec{k})$ , defined in (4.5), is an analytic function of  $\vec{k}$  [and the  $\psi(\vec{k}n)$  for  $\vec{k}$  real comprise a complete set]. When  $G_0$  [or one of the other Green's functions  $G$ ,  $\mathcal{G}_0$ , or  $\mathcal{G}$ ] is evaluated in Sec. XIV, by means of a contour integration, the result is identical to that obtained in the earlier part of the paper. A concluding summary is given in Sec. XV.

## II. MATHEMATICAL PRELIMINARIES

Let  $L(\vec{x}, \vec{x}')$  be some time-independent operator. The generalization of Green's theorem is<sup>2</sup>

$$\begin{aligned} & \int_V d\vec{x} \int_V d\vec{x}' w^\dagger(\vec{x}) \cdot [L(\vec{x}, \vec{x}') \cdot v(\vec{x}')] \\ &= \int_V d\vec{x} \int_V d\vec{x}' [\bar{L}(\vec{x}', \vec{x}) \cdot w(\vec{x})]^\dagger \cdot v(\vec{x}') \\ & \quad + \int_S \bar{P}[w^\dagger, v] \cdot d\vec{S}, \end{aligned} \quad (2.1a)$$

where  $w$  and  $v$  are any two functions.  $\bar{P}[w^\dagger, v]$  is a function of  $w^\dagger$  and  $v$  and their derivatives, called the "bilinear concomitant"<sup>2,4</sup> (or "conjoint"<sup>3</sup>), and  $S$  is the surface bounding the volume  $V$ .  $\bar{L}$  is called the "formal adjoint" of  $L$ , and  $w$  and  $v$  are said to satisfy "adjoint boundary conditions" if

$$\int_S \bar{P}[w^\dagger, v] \cdot d\vec{S} = 0. \quad (2.2)$$

Equation (2.1a) can be written more simply as

$$\int_V d\vec{x} w^\dagger(Lv) = \int_V d\vec{x} (\bar{L}w)^\dagger v + \int_S \bar{P}[w^\dagger, v] \cdot d\vec{S}. \quad (2.1b)$$

[In our notation, the first function in an expression like  $w^\dagger(Lv)$  is regarded as a function of  $\vec{x}$ , and the second as a function of  $\vec{x}'$ . Integration with respect to  $\vec{x}'$ , over the volume  $V$ , is always implied if not explicitly shown. Integration with respect to  $\vec{x}$ , which may be over any volume, is always explicitly shown and never implied. An inner product is always implied in expressions like  $w^\dagger v$  and  $Lv$  if  $v$  is a vector and  $L$  a matrix. In  $(\bar{L}w)^\dagger v$ ,  $v$  is regarded as a function of  $\vec{x}$  and  $w$  as a function of  $\vec{x}'$ . Finally,  $\bar{P}$  is always a function of  $\vec{x}$ , and  $\bar{\nabla}$  means  $\bar{\nabla}_{\vec{x}}$ .]

In this paper, we consider operators of the form

$$L = \epsilon - H, \quad (2.3a)$$

where  $\epsilon$  is a complex number. Then

$$\bar{L} = \epsilon^* - \bar{H}. \quad (2.3b)$$

Let

$$H = T + V, \quad (2.4a)$$

where  $T$  consists of all those terms containing derivatives and  $V$  is the remainder of  $H$ . It will be assumed that

$$T(\vec{x}, \vec{x}') = T(\vec{x}')\delta(\vec{x} - \vec{x}'). \quad (2.4b)$$

Since  $\bar{P}$  arises from the derivatives in  $L$  when one performs integrations by parts to get from the expression involving  $L$  in (2.1) to the expression involving  $\bar{L}$ ,  $L$ ,  $-H$ , and  $-T$  all have the same bilinear concomitant  $\bar{P}$ . If there are no derivatives in  $L$ , the boundary term in (2.1) vanishes; we can therefore take

$$\bar{P}[w^\dagger, v] = 0, \quad \text{for all } w \text{ and } v, \quad \text{if } T = 0. \quad (2.5)$$

Consider the homogeneous equation

$$\int_V d\vec{x}' L(\vec{x}, \vec{x}') \cdot v(\vec{x}') = 0 \quad (2.6a)$$

or, in the simpler notation

$$Lv = 0. \quad (2.6b)$$

The "adjoint problem" is

$$\bar{L}\bar{v} = 0. \quad (2.7)$$

According to (2.1),  $v$  and  $\bar{v}$  will automatically satisfy adjoint boundary conditions. With  $L$  given by (2.3),

$$Hv = \epsilon v, \quad (2.8a)$$

$$\bar{H}\bar{v} = \epsilon^* \bar{v}. \quad (2.8b)$$

For a given set of boundary conditions on  $v$ , we

will have some set of solutions corresponding to different (eigen)values of  $\epsilon$ :

$$Hv_n = \epsilon_n v_n \quad (2.9a)$$

$$\bar{H}\bar{v}_n = \epsilon_n^* \bar{v}_n. \quad (2.9b)$$

Suppose there is a set of  $v_n$  and  $\bar{v}_n$  such that

$$\int_S \bar{P}[\bar{v}_n^\dagger, v_n] \cdot d\vec{S} = 0. \quad (2.10)$$

Then (2.1), with  $L \rightarrow -H$ , gives

$$-\int_V d\vec{x} \bar{v}_n^\dagger (Hv_n) + \int_V d\vec{x} (\bar{H}\bar{v}_n)^\dagger v_n = 0, \quad (2.11)$$

so by (2.9)

$$\int_V d\vec{x} \bar{v}_n^\dagger v_n = 0 \quad \epsilon_n \neq \epsilon_n. \quad (2.12)$$

That is, the  $v_n$  and  $\bar{v}_n$  satisfying adjoint boundary conditions are biorthogonal.

Equation (2.1) follows from

$$w^\dagger(Tv) - (\bar{T}w)^\dagger v = -\bar{\nabla} \cdot \bar{P}[w^\dagger, v] \quad (2.13)$$

(provided that  $\bar{P}[w^\dagger, v]$  is sufficiently well-behaved for Gauss's divergence theorem to hold). Also, (2.2) follows from

$$\bar{\nabla} \cdot \bar{P}[w^\dagger, v] = 0. \quad (2.14)$$

If  $v_n$  and  $\bar{v}_n$  are solutions to (2.6) and (2.7), then (2.1) gives

$$\int_S \bar{P}[\bar{v}_n^\dagger, v_n] \cdot d\vec{S} = 0, \quad \epsilon_n \neq \epsilon_n. \quad (2.15a)$$

This will be satisfied if

$$\bar{\nabla} \cdot \bar{P}[\bar{v}_n^\dagger, v_n] = 0, \quad \epsilon_n \neq \epsilon_n. \quad (2.15b)$$

In one dimension, this becomes  $dP/dx = 0$ , or

$$P[\bar{v}_n^\dagger, v_n] = \text{const}, \quad \epsilon_n \neq \epsilon_n. \quad (2.16)$$

When

$$\bar{H} = H, \quad (2.17)$$

$H$  is said to be "formally self-adjoint." The solutions  $v_n$ ,  $\epsilon_n$  to (2.9a) and  $\bar{v}_n$ ,  $\epsilon_n^*$  to (2.9b) are then distinguished only by the boundary conditions. If  $\bar{v}_n$  and  $v_n$  satisfy the same boundary conditions,  $H$  is said to be "self-adjoint" or "Hermitian"; then we have the familiar result

$$\bar{v}_n = v_n, \quad \epsilon_n^* = \epsilon_n. \quad (2.18)$$

### III. EXAMPLES

Consider the one-particle Schrödinger equation with a possibly nonlocal potential  $V(\vec{x}, \vec{x}')$ , for which

$$H = -(\hbar^2/2m) \nabla^2 \delta(\vec{x} - \vec{x}') + V(\vec{x}, \vec{x}'), \quad (3.1a)$$

$$V^*(\vec{x}', \vec{x}) = V(\vec{x}, \vec{x}'), \quad (3.1b)$$

$$\epsilon = E, \quad (3.1c)$$

where  $E$  is the energy of the particle. After integrating by parts twice, one obtains (2.1) with

$$\bar{H} = H, \quad (3.2a)$$

$$\bar{P}[w^*, v] = +(\hbar^2/2m)(w^* \vec{\nabla} v - v \vec{\nabla} w^*). \quad (3.2b)$$

In fact, (2.1) reduces to the classic version of Green's theorem:

$$\int_V d\vec{x} (w^* \nabla^2 v - v \nabla^2 w^*) = \int_S (w^* \vec{\nabla} v - v \vec{\nabla} w^*) \cdot d\vec{S}. \quad (3.3)$$

According to (3.2a),  $H$  is formally self-adjoint. Then it will be truly self-adjoint, or Hermitian, for those functions  $w$  and  $v$  that satisfy the same adjoint boundary conditions—for example, if  $w$  and  $v$  both satisfy the usual periodic boundary conditions, or if  $w$  and  $v$  both vanish on some boundary, or at infinity.

For the one-dimensional Schrödinger equation,  $P$  is essentially the Wronskian:

$$P[w^*, v] = \frac{\hbar^2}{2m} \left( w^* \frac{dv}{dx} - v \frac{dw^*}{dx} \right). \quad (3.4)$$

In this case, (2.16) expresses the familiar fact that the Wronskian is a constant for two eigenfunctions with the same eigenvalue.

For a charged particle of spin zero moving relativistically in a time-independent electromagnetic field, we can choose

$$H = [(-i\hbar \vec{\nabla} - (e/c)\vec{A})^2 c^2 + m^2 c^4] \delta(\vec{x} - \vec{x}'), \quad (3.5a)$$

$$\epsilon = (E - eA_0)^2, \quad (3.5b)$$

where  $\vec{A}$  is the vector potential and  $A_0$  is the scalar potential. The one finds that

$$\bar{H} = H, \quad (3.6a)$$

$$\bar{P}[w^*, v] = \hbar^2 c^2 (w^* \vec{\nabla} v - v \vec{\nabla} w^*) - i \cdot 2\hbar c e \vec{A} w^* v. \quad (3.6b)$$

For the Dirac equation with no fields,

$$H = -[i\hbar c \vec{\alpha} \cdot \vec{\nabla} - mc^2 \beta] \delta(\vec{x} - \vec{x}'), \quad (3.7a)$$

$$\epsilon = E, \quad (3.7b)$$

where the  $\alpha_j$  and  $\beta$  are  $4 \times 4$  matrices and

$$\alpha_j^\dagger = \alpha_j, \quad \beta_j^\dagger = \beta_j. \quad (3.7c)$$

One obtains

$$\bar{H} = H, \quad (3.8a)$$

$$\bar{P}[w^\dagger, v] = -i\hbar c w^\dagger \vec{\alpha} v, \quad (3.8b)$$

where  $w$  and  $v$  each have four components, and inner products are implied as usual.

For the lattice-dynamics eigenvalue problem associated with phonons,

$$H(\vec{x}, \vec{x}') = M_{\vec{x}}^{-1/2} \Phi(\vec{x}, \vec{x}') M_{\vec{x}'}^{-1/2}, \quad (3.9a)$$

$$\Phi^\dagger(\vec{x}', \vec{x}) = \Phi(\vec{x}, \vec{x}'), \quad (3.9b)$$

$$\epsilon = \omega^2, \quad (3.9c)$$

where  $\Phi(\vec{x}, \vec{x}')$  is the real  $3 \times 3$  force-constant matrix coupling the vibrations of atoms at  $\vec{x}$  and  $\vec{x}'$ ,  $M_{\vec{x}}$  is the mass of the atom at  $\vec{x}$ , and  $\omega$  is the vibrational frequency. We can think of (2.8a) in this case as being an "integral equation" with discrete values for  $\vec{x}$ . Equation (2.1) holds with

$$\bar{H} = H, \quad (3.10a)$$

$$\bar{P}[w^\dagger, v] \equiv 0. \quad (3.10b)$$

Equation (3.10b) can also be taken to hold for other integral equations.<sup>2</sup>

It is no coincidence that  $\bar{P}$  in (3.2), (3.6), and (3.8) is related to the probability current  $\vec{j}$  by

$$\vec{j} = C \bar{P}[\vec{v}^\dagger, v], \quad (3.11)$$

where  $v$  is a wave function and  $C$  is a constant: If  $L(\vec{x}t)$  is a time-dependent operator [with  $V$  of (2.4a) taken to be local for simplicity], then the analog of (2.13) is

$$w^\dagger (Lv) - (\bar{L}w)^\dagger v = \vec{\nabla} \cdot \bar{P}[w^\dagger, v] + \partial P_0[w^\dagger, v] / \partial t, \quad (3.12)$$

where  $P$  now has a fourth component. Suppose that  $v$  is a solution to (2.6b) and that  $w = \bar{v}$ ; then (3.12) becomes

$$\vec{\nabla} \cdot \bar{P}[\bar{v}^\dagger, v] + \partial P_0[\bar{v}^\dagger, v] / \partial t = 0. \quad (3.13)$$

This is an equation of continuity, or conservation law. If  $j_0 \equiv CP_0[\bar{v}^\dagger, v]$  and  $\vec{j} \equiv C\bar{P}[\bar{v}^\dagger, v]$ ,  $C$  being an appropriate normalization constant, and if  $v$  is a quantum-mechanical wave function, then  $j_0$  is the probability density and  $\vec{j}$  the probability current density.

#### IV. PERIODIC SYSTEM

In a periodic solid, a general lattice vector is given by

$$\vec{X} = l_1 \vec{a}_1 + l_2 \vec{a}_2 + l_3 \vec{a}_3 \quad (4.1a)$$

and a general position vector by

$$\vec{x} = x_1 \vec{a}_1 + x_2 \vec{a}_2 + x_3 \vec{a}_3, \quad (4.1b)$$

where  $\bar{a}_j$  is a primitive lattice vector. Also, a general reciprocal-lattice vector is given by

$$\bar{K} = m_1 \bar{b}_1 + m_2 \bar{b}_2 + m_3 \bar{b}_3, \quad (4.1c)$$

and a general wave vector by

$$\bar{k} = k_1 \bar{b}_1 + k_2 \bar{b}_2 + k_3 \bar{b}_3, \quad (4.1d)$$

where  $\bar{b}_j$  is a primitive reciprocal-lattice vector:

$$\bar{a}_i \cdot \bar{b}_j = 2\pi \delta_{ij}. \quad (4.1e)$$

Let  $H_0$  be a translationally invariant operator:

$$H_0(\bar{x} + \bar{X}, \bar{x}' + \bar{X}) = H_0(\bar{x}, \bar{x}'). \quad (4.2)$$

The results of Sec. II can be taken over with  $L \rightarrow L_0$ ,  $H \rightarrow H_0$ ,  $T \rightarrow T_0$ , etc., and (2.9a) becomes

$$H_0 \psi(\bar{k}n) = \epsilon(\bar{k}n) \psi(\bar{k}n) \quad (4.3a)$$

or, in more explicit notation,

$$\int_V d\bar{x}' H_0(\bar{x}, \bar{x}') \cdot \psi(\bar{x}'; \bar{k}n) = \epsilon(\bar{k}n) \psi(\bar{x}; \bar{k}n). \quad (4.3b)$$

According to Bloch's theorem,

$$\psi(\bar{x}; \bar{k}n) = e^{i\bar{k} \cdot \bar{x}} u(\bar{x}; \bar{k}n), \quad (4.4a)$$

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$$\begin{aligned} & \int_V d\bar{x} \int_V d\bar{x}' w^\dagger(\bar{x}) \cdot [e^{-i\bar{k} \cdot \bar{x}} H_0(\bar{x}, \bar{x}') e^{i\bar{k} \cdot \bar{x}'} \cdot v(\bar{x}')] \\ &= \int_V d\bar{x} \int_V d\bar{x}' [e^{-i\bar{k} \cdot \bar{x}'} \bar{H}_0(\bar{x}', \bar{x}) e^{i\bar{k} \cdot \bar{x}} \cdot w(\bar{x})]^\dagger \cdot v(\bar{x}') - \int_S \bar{P}_0 [e^{-i\bar{k} \cdot \bar{x}} w^\dagger(\bar{x}), e^{i\bar{k} \cdot \bar{x}} v(\bar{x})] \cdot d\bar{S}. \end{aligned} \quad (4.9)$$

We conclude that

$$\bar{H}_0(\bar{x}\bar{x}'; \bar{k}) = e^{-i\bar{k} \cdot \bar{x}} \bar{H}_0(\bar{x}, \bar{x}') e^{i\bar{k} \cdot \bar{x}'}, \quad (4.10a)$$

$$\bar{P}_k^\dagger [w^\dagger(\bar{x}), v(\bar{x})] = \bar{P}_0 [e^{-i\bar{k} \cdot \bar{x}} w^\dagger(\bar{x}), e^{i\bar{k} \cdot \bar{x}} v(\bar{x})], \quad (4.10b)$$

where  $\bar{P}_0$  and  $\bar{P}_k$  are the respective bilinear concomitants of  $-H_0$  and  $-H_0(\bar{k})$ . If (4.10a) is substituted into (4.8), we see that (4.7) will be satisfied if we choose

$$\bar{\psi}(\bar{x}; \bar{k}n) = e^{i\bar{k} \cdot \bar{x}} \bar{u}(\bar{x}; \bar{k}n) \quad (4.11a)$$

or

$$\bar{\psi}^\dagger(\bar{x}; \bar{k}n) = e^{-i\bar{k} \cdot \bar{x}} \bar{u}^\dagger(\bar{x}; \bar{k}n). \quad (4.11a')$$

Bloch's theorem, when applied to (4.7), says that

$$\bar{u}(\bar{x} + \bar{X}; \bar{k}n) = \bar{u}(\bar{x}; \bar{k}n). \quad (4.11b)$$

If  $H_0$  is formally self-adjoint,

$$\bar{H}_0(\bar{x}, \bar{x}') = H_0(\bar{x}, \bar{x}'), \quad (4.12)$$

then (4.10) gives

$$u(\bar{x} + \bar{X}; \bar{k}n) = u(\bar{x}; \bar{k}n), \quad (4.4b)$$

where  $\bar{k}$  is possibly complex. Here  $n$  distinguishes different solutions for the same  $\bar{k}$ --i.e., different branches. If we let

$$H_0(\bar{x}\bar{x}'; \bar{k}) \equiv e^{-i\bar{k} \cdot \bar{x}} H_0(\bar{x}, \bar{x}') e^{i\bar{k} \cdot \bar{x}'}, \quad (4.5)$$

then (4.3) becomes

$$H_0(\bar{k}) \mu(\bar{k}n) = \epsilon(\bar{k}n) \mu(\bar{k}n) \quad (4.6a)$$

or

$$\int_V d\bar{x}' H_0(\bar{x}\bar{x}'; \bar{k}) \cdot u(\bar{x}'; \bar{k}n) = \epsilon(\bar{k}n) \mu(\bar{x}; \bar{k}n). \quad (4.6b)$$

The adjoint problems to (4.3) and (4.6) are

$$\bar{H}_0 \bar{\psi}(\bar{k}n) = \epsilon^*(\bar{k}n) \bar{\psi}(\bar{k}n), \quad (4.7)$$

$$\bar{H}_0(\bar{k}) \bar{\mu}(\bar{k}n) = \epsilon^*(\bar{k}n) \bar{\mu}(\bar{k}n). \quad (4.8)$$

Letting  $w^\dagger(\bar{x}) \rightarrow e^{-i\bar{k} \cdot \bar{x}} w^\dagger(\bar{x})$  and  $v(\bar{x}) \rightarrow e^{i\bar{k} \cdot \bar{x}} v(\bar{x})$  in (2.1), with  $L \rightarrow -H_0$  we get

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$$\bar{H}_0(\bar{x}\bar{x}'; \bar{k}) = H_0(\bar{x}\bar{x}'; \bar{k}^*), \quad (4.13)$$

so (4.8) can be rewritten

$$H_0(\bar{k}^*) \bar{\mu}(\bar{k}n) = \epsilon^*(\bar{k}n) \bar{\mu}(\bar{k}n). \quad (4.14)$$

We can then take

$$\epsilon^*(\bar{k}n) = \epsilon(\bar{k}^*n), \quad (4.15a)$$

$$\bar{u}(\bar{k}n) = u(\bar{k}^*n), \quad (4.15b)$$

$$\bar{\psi}(\bar{k}n) = \psi(\bar{k}^*n), \quad (4.15c)$$

the last equation following from (4.11a).

We now return to the general case and specify that  $V$  is a parallelepiped defined by

$$x_j^A < x_j \leq x_j^B, \quad j=1, 2, 3, \quad (4.16a)$$

$$x_j^B - x_j^A = L_j, \quad (4.16b)$$

where  $L_j$  is an integer and  $L_j \rightarrow \infty$  is understood.

In the remainder of this section, it will be more appealing to work within a single unit cell, which we choose to be a parallelepiped defined by

$$x_j^a < x_j \leq x_j^b, \quad j=1, 2, 3, \quad (4.17a)$$

$$x_j^b - x_j^a = 1. \quad (4.17b)$$

Call the volume of the unit cell  $v$  and the surface enclosing it  $s$ . Then

$$V = Nv, \quad N \equiv L_1 L_2 L_3.$$

We rewrite (4.6b) as

$$\int_v d\vec{x}' h_0(\vec{x}\vec{x}'; \vec{k}) \cdot u(\vec{x}'; \vec{k}n) = \epsilon(\vec{k}n) u(\vec{x}; \vec{k}n), \quad (4.18)$$

where

$$h_0(\vec{x}\vec{x}'; \vec{k}) \equiv e^{-i\vec{k} \cdot \vec{x}} \sum_{\vec{x}'} H_0(\vec{x}, \vec{x}' + \vec{x}') e^{i\vec{k} \cdot (\vec{x}' + \vec{x}')}. \quad (4.19)$$

[If  $V_0$  is a local operator,  $h_0(\vec{k}) = H_0(\vec{k})$ .] The adjoint problem is

$$\int_v d\vec{x}' \bar{h}_0(\vec{x}\vec{x}'; \vec{k}) \cdot \bar{u}(\vec{x}'; \vec{k}n) = \epsilon^*(\vec{k}n) \bar{u}(\vec{x}; \vec{k}n). \quad (4.20)$$

If we limit our attention to functions  $w(\vec{x})$  and  $v(\vec{x})$  which are periodic,

$$w(\vec{x} + \vec{X}) = w(\vec{x}), \quad v(\vec{x} + \vec{X}) = v(\vec{x}), \quad (4.21)$$

(4.9) becomes

$$\begin{aligned} & \int_v d\vec{x} \int_v d\vec{x}' w^\dagger(\vec{x}) \cdot \left[ \sum_{\vec{x}\vec{x}'} e^{-i\vec{k} \cdot (\vec{x} + \vec{x}')} H_0(\vec{x} + \vec{X}, \vec{x}' + \vec{X}') e^{i\vec{k} \cdot (\vec{x}' + \vec{X}')} \cdot v(\vec{x}') \right] \\ &= \int_v d\vec{x} \int_v d\vec{x}' \left[ \sum_{\vec{x}\vec{x}'} e^{-i\vec{k} \cdot (\vec{x}' + \vec{x}')} \bar{H}_0(\vec{x}' + \vec{X}', \vec{x} + \vec{X}) e^{i\vec{k} \cdot (\vec{x} + \vec{X})} \cdot w(\vec{x}) \right]^\dagger \cdot v(\vec{x}') \\ & \quad - \int_s \sum_{\vec{x}} \bar{P}_0[e^{-i\vec{k} \cdot (\vec{x} + \vec{X})} w^\dagger(\vec{x}), e^{i\vec{k} \cdot (\vec{x} + \vec{X})} v(\vec{x})] \cdot d\vec{S}. \end{aligned} \quad (4.22)$$

On the right-hand side, we have used the fact that  $\int_s$  is the same as the sum of  $\int_s$  over all the  $N$  unit cells within  $S$ . (The integrals over the interior surfaces cancel: each interior surface is shared by two unit cells. The magnitude of the integrand is the same when the integral is performed for the first and second cells. But the outward normals point in opposite directions. Therefore the sum of the integrals is zero.) Now make use of the translational invariance expressed by (4.2)

$$\begin{aligned} & \sum_{\vec{x}} \sum_{\vec{x}'} e^{-i\vec{k} \cdot (\vec{x} + \vec{x}')} H_0(\vec{x} + \vec{X}, \vec{x}' + \vec{X}') e^{i\vec{k} \cdot (\vec{x}' + \vec{X}')} \\ &= \sum_{\vec{x}} \sum_{\vec{x}''} e^{-i\vec{k} \cdot \vec{x}} H_0(\vec{x}, \vec{x}' + \vec{X}'') e^{i\vec{k} \cdot (\vec{x}' + \vec{X}'')}, \end{aligned} \quad (4.23)$$

where  $\vec{x}'' \equiv \vec{x}' - \vec{X}$ . The values of  $\vec{x}'$  lie within  $V$ , so the values of  $\vec{x}''$  are such that  $\vec{x}'' + \vec{X}$  lies within  $V$ . In the following, we will change the limits of summation on  $\vec{x}''$ , taking it to have the same range of values as  $\vec{x}'$ . If  $\vec{X}$  is far from the boundary of  $V$  this will introduce negligible error, provided that we now require

$$H_0(\vec{x}, \vec{x}') \rightarrow 0 \quad \text{as } |\vec{x} - \vec{x}'| \rightarrow \infty. \quad (4.24)$$

There can be appreciable error if  $\vec{X}$  is near the

boundary, but the fraction of lattice points near the boundary decreases to zero as  $L_1, L_2, L_3 \rightarrow \infty$ , so the fractional error in the summation of (4.23) will also go to zero in this limit. We can consequently rewrite (4.23) as

$$\begin{aligned} & \sum_{\vec{x}} \sum_{\vec{x}'} e^{-i\vec{k} \cdot (\vec{x} + \vec{x}')} H_0(\vec{x} + \vec{X}, \vec{x}' + \vec{X}') e^{i\vec{k} \cdot (\vec{x}' + \vec{X}')} \\ &= N e^{-i\vec{k} \cdot \vec{x}} \sum_{\vec{x}'} H_0(\vec{x}, \vec{x}' + \vec{X}') e^{i\vec{k} \cdot (\vec{x}' + \vec{X}')}. \end{aligned} \quad (4.25a)$$

Similarly, the translational invariance of  $\bar{H}_0$  implies that

$$\begin{aligned} & \sum_{\vec{x}'} \sum_{\vec{x}} e^{-i\vec{k} \cdot (\vec{x}' + \vec{x}')} \bar{H}_0(\vec{x}' + \vec{X}', \vec{x} + \vec{X}) e^{i\vec{k} \cdot (\vec{x} + \vec{X})} \\ &= N e^{-i\vec{k} \cdot \vec{x}'} \sum_{\vec{x}} \bar{H}_0(\vec{x}', \vec{x} + \vec{X}) e^{i\vec{k} \cdot (\vec{x} + \vec{X})}. \end{aligned} \quad (4.25b)$$

Since  $\bar{P}_0[w^\dagger, v]$  involves only  $w^\dagger$  and  $v$  and their derivatives bilinearly,<sup>2</sup>

$$\begin{aligned} & \bar{P}_0[e^{-i\vec{k} \cdot (\vec{x} + \vec{X})} w^\dagger(\vec{x}), e^{i\vec{k} \cdot (\vec{x} + \vec{X})} v(\vec{x})] \\ &= \bar{P}_0[e^{-i\vec{k} \cdot \vec{x}} w^\dagger(\vec{x}), e^{i\vec{k} \cdot \vec{x}} v(\vec{x})]. \end{aligned} \quad (4.25c)$$

Putting these results into (4.22) and dividing by  $N$ , we obtain

$$\begin{aligned} & \int_{\nu} d\bar{x} \int_{\nu} d\bar{x}' w^{\dagger}(\bar{x}) \cdot \left[ e^{-i\bar{k} \cdot \bar{x}} \sum_{\bar{x}'} H_0(\bar{x}, \bar{x}' + \bar{X}') e^{i\bar{k} \cdot (\bar{x}' + \bar{X}')} \cdot v(\bar{x}') \right] \\ &= \int_{\nu} d\bar{x} \int_{\nu} d\bar{x}' \left[ e^{-i\bar{k} \cdot \bar{x}} \sum_{\bar{x}} \bar{H}_0(\bar{x}', \bar{x} + \bar{X}) e^{i\bar{k} \cdot (\bar{x} + \bar{X})} \cdot w(\bar{x}) \right]^{\dagger} \cdot v(\bar{x}') - \int_s \bar{P}_0 [e^{-i\bar{k} \cdot \bar{x}} w^{\dagger}(\bar{x}), e^{i\bar{k} \cdot \bar{x}} v(\bar{x})] \cdot d\bar{S}. \end{aligned} \quad (4.26)$$

We conclude that

$$\bar{h}_0(\bar{x}\bar{x}'; \bar{k}) = e^{-i\bar{k} \cdot \bar{x}} \sum_{\bar{x}'} \bar{H}_0(\bar{x}, \bar{x}' + \bar{X}') e^{i\bar{k} \cdot (\bar{x}' + \bar{X}')}, \quad (4.27a)$$

$$\bar{p}_{\bar{k}}[w^{\dagger}(\bar{x}), v(\bar{x})] = \bar{P}_0 [e^{-i\bar{k} \cdot \bar{x}} w^{\dagger}(\bar{x}), e^{i\bar{k} \cdot \bar{x}} v(\bar{x})] \quad (4.27b)$$

$$= \bar{P}_{\bar{k}} [w^{\dagger}(\bar{x}), v(\bar{x})], \quad (4.27b')$$

where  $\bar{p}_{\bar{k}}$  is the bilinear concomitant of  $-h_0(\bar{k})$ .

Equations (4.21), (4.25c), and (4.27b) imply that

$$\bar{p}_{\bar{k}}[w^{\dagger}(\bar{x} + \bar{X}), v(\bar{x} + \bar{X})] = \bar{p}_{\bar{k}}[w^{\dagger}(\bar{x}), v(\bar{x})]. \quad (4.28)$$

Now, for every point on  $s$  at  $\bar{x}$  there is another point at either  $\bar{x} + \bar{a}_j$  or  $\bar{x} - \bar{a}_j$ , where  $\bar{a}_j$  is one of the primitive lattice vectors. Since the outward normals at the two points are in opposite directions, (4.28) implies that

$$\int_s \bar{p}_{\bar{k}}[w^{\dagger}, v] \cdot d\bar{S} = 0. \quad (4.29)$$

That is, periodic functions automatically satisfy adjoint boundary conditions when the general volume  $V$  of (2.1) is taken to be a unit cell and  $H \rightarrow h_0(\bar{k})$ . In particular,

$$\int_s \bar{p}_{\bar{k}}[\bar{u}^{\dagger}(\bar{k}n), u(\bar{k}n')] \cdot d\bar{S} = 0. \quad (4.30)$$

Thus the  $u(\bar{k}n)$  and  $\bar{u}(\bar{k}n)$  form a set of the kind defined by (2.9) and (2.10), and we have (2.12) in the form

$$\int_{\nu} d\bar{x} \bar{u}^{\dagger}(\bar{k}n) u(\bar{k}n') = 0, \quad \epsilon(\bar{k}n') \neq \epsilon(\bar{k}n). \quad (4.31)$$

In this paper I ignore the complication of degeneracy at fixed  $\bar{k}$  and choose the normalization

$$\int_{\nu} d\bar{x} \bar{u}^{\dagger}(\bar{k}n) u(\bar{k}n') = \delta_{nn'} \quad (4.32a)$$

or, in view of (4.11a'),

$$\int_{\nu} d\bar{x} \bar{\psi}^{\dagger}(\bar{k}n) \psi(\bar{k}n') = \delta_{nn'}. \quad (4.32b)$$

## V. METHOD FOR EVALUATING $G_0$

The Green's function  $G_0(\bar{x}\bar{x}'; \epsilon)$  is defined to be a solution to

$$\int_{\nu} d\bar{x}'' L_0(\bar{x}\bar{x}''; \epsilon) \cdot G_0(\bar{x}''\bar{x}'; \epsilon) = \delta(\bar{x} - \bar{x}'), \quad (5.1)$$

$$L_0(\bar{x}\bar{x}'; \epsilon) = \epsilon - H_0(\bar{x}, \bar{x}'). \quad (5.2)$$

We look for a solution in the form

$$\begin{aligned} G_0(\bar{x}\bar{x}'; \epsilon) = & \sum_{\bar{k}n} [\alpha^+(\bar{x}'; \bar{k}n) \psi(\bar{x}; \bar{k}n) \theta(x_3 - x'_3) \\ & + \alpha^-(\bar{x}'; \bar{k}n) \psi(\bar{x}; \bar{k}n) \theta(x'_3 - x_3)], \end{aligned} \quad (5.3)$$

where

$$k_i = m_i / L_i, \quad i = 1 \text{ or } 2. \quad (5.4)$$

In view of (5.1), the  $\bar{k}$  values in the sum of (5.3) are those for which

$$\epsilon(\bar{k}n) = \epsilon. \quad (5.5)$$

Also, (13.11) and (13.14) imply that we can take

$$-\frac{1}{2} < k_i \leq \frac{1}{2}, \quad i = 1 \text{ or } 2, \quad (5.6a)$$

$$-\frac{1}{2} < \text{Re} k_3 \leq \frac{1}{2}. \quad (5.6b)$$

In writing results like (7.9), we will actually replace the  $\bar{k}$  values of (5.6a) by the equivalent  $\bar{k}$  values lying in the first two-dimensional Brillouin zone (BZ). The values of the coefficients  $\alpha^{\pm}$  are determined by the boundary conditions on  $G_0(\bar{x}\bar{x}'; \epsilon)$  at fixed  $\bar{x}'$  and  $\epsilon$ . For each  $\bar{k}$  and  $n$ , either let

$$\alpha^+(\bar{x}'; \bar{k}n) \equiv \alpha^+(\bar{x}'; \bar{k}n) - \alpha^-(\bar{x}'; \bar{k}n), \quad (5.7a)$$

$$\alpha^-(\bar{x}'; \bar{k}n) \equiv 0, \quad (5.7b)$$

$$\alpha(\bar{x}'; \bar{k}n) \equiv \alpha^-(\bar{x}'; \bar{k}n), \quad (5.7c)$$

or else let

$$\alpha^+(\bar{x}'; \bar{k}n) \equiv 0, \quad (5.8a)$$

$$\alpha^-(\bar{x}'; \bar{k}n) \equiv \alpha^-(\bar{x}'; \bar{k}n) - \alpha^+(\bar{x}'; \bar{k}n), \quad (5.8b)$$

$$\alpha(\bar{x}'; \bar{k}n) \equiv \alpha^+(\bar{x}'; \bar{k}n). \quad (5.8c)$$

After this arbitrary choice is made, let the  $k_3$  for which (5.7) holds (at fixed  $\bar{k}$  and  $n$ ) be called  $k_{nl}^+$ , and let the  $k_3$  for which (5.8) holds be called  $k_{nl}^-$ .

Then (5.3) can be written

$$G_0(\bar{x}\bar{x}'; \epsilon) = G_0^S(\bar{x}\bar{x}'; \epsilon) + G_0^{\text{NS}}(\bar{x}\bar{x}'; \epsilon), \quad (5.9a)$$

$$G_0^S(\vec{x}\vec{x}'; \epsilon) \equiv \sum_{\vec{k}'} \sum_{n'l'} a^+(\vec{x}'; \vec{k}'n'l') \psi(\vec{x}; \vec{k}'k_{n'l}^+, n') \Theta(x_3 - x_3') + \sum_{\vec{k}'} \sum_{n'l'} a^-(\vec{x}'; \vec{k}'n'l') \psi(\vec{x}; \vec{k}'k_{n'l}^-, n') \Theta(x_3' - x_3), \quad (5.9b)$$

$$G_0^{NS} \equiv \sum_{\vec{k}n} \alpha(\vec{x}'; \vec{k}n) \psi(\vec{x}; \vec{k}n), \quad (5.9c)$$

with a slight change of notation. We have separated  $G_0$  into a "singular" part  $G_0^S$  and a "nonsingular" part  $G_0^{NS}$ :

$$\int_V d\vec{x}'' L_0(\vec{x}\vec{x}''; \epsilon) \cdot G_0^S(\vec{x}''\vec{x}'; \epsilon) = \delta(\vec{x} - \vec{x}'), \quad (5.10a)$$

$$\int_V d\vec{x}'' L_0(\vec{x}\vec{x}''; \epsilon) \cdot G_0^{NS}(\vec{x}''\vec{x}'; \epsilon) = 0. \quad (5.10b)$$

( $G_0^S$  is "a particular solution to the inhomogeneous equation" and  $G_0^{NS}$  is "the general solution to the homogeneous equation.") Although  $L_0 G_0^S$  has a  $\delta$ -function singularity, we require that  $G_0^S$  itself be a function with no singularities at  $x_3 = x_3'$ ; this restricts the treatment below to the case

$$T_0 \neq 0. \quad (5.11)$$

(More precisely,  $H_0$  must contain a derivative with respect to  $x_3$ .) We also assume that  $\bar{T}_0 \bar{\psi}(\vec{x}; \vec{k}n)$ ,  $\bar{T}_0 \bar{\psi}(\vec{x}; \vec{k}n)$ , and

$$\int_V d\vec{x}'' V_0(\vec{x}\vec{x}''; \epsilon) \cdot G_0^S(\vec{x}''\vec{x}'; \epsilon)$$

are not singular at  $x_3 = x_3'$ .

From (2.13), we have

$$\begin{aligned} \bar{\psi}^\dagger(\vec{x}; \vec{k}n) \cdot [T_0 \cdot G_0^S(\vec{x}\vec{x}'; \epsilon)] - [\bar{T}_0 \cdot \bar{\psi}(\vec{x}; \vec{k}n)]^\dagger \cdot G_0^S(\vec{x}\vec{x}'; \epsilon) \\ = -\vec{\nabla} \cdot \bar{P}_0[\bar{\psi}^\dagger(\vec{x}; \vec{k}n), G_0^S(\vec{x}\vec{x}'; \epsilon)] \end{aligned} \quad (5.12)$$

or, since  $L_0 = \epsilon - H_0 = \epsilon - (T_0 + V_0)$ ,

$$\bar{\psi}^\dagger(\vec{x}; \vec{k}n) = \int_{x_1^A}^{x_1^B} dx_1 \int_{x_2^A}^{x_2^B} dx_2 P_{03}[\bar{\psi}^\dagger(\vec{k}n), G_0^S(\vec{x}'; \epsilon)] \Big|_{x_3=x_3'-\delta x_3}^{x_3=x_3'+\delta x_3}. \quad (5.17)$$

Now substitute (5.9b) into (5.17), with

$$\bar{\psi}^\dagger(\vec{x}; \vec{k}n) - \bar{\psi}^\dagger(\vec{x}'; \vec{k}k_{n1}^+ n);$$

the result is

$$\begin{aligned} \sum_{\vec{k}'} \sum_{n'l'} a^+(\vec{x}'; \vec{k}'n'l') \int_{S_3} \bar{P}_0[\bar{\psi}^\dagger(\vec{k}k_{n1}^+ n), \psi(\vec{k}'k_{n'l}^+, n')] \cdot d\vec{S} \\ - \sum_{\vec{k}'} \sum_{n'l'} a^-(\vec{x}'; \vec{k}'n'l') \int_{S_3} \bar{P}_0[\bar{\psi}^\dagger(\vec{k}k_{n1}^+ n), \psi(\vec{k}'k_{n'l}^-, n')] \cdot d\vec{S} = \bar{\psi}^\dagger(\vec{x}'; \vec{k}k_{n1}^+ n) \end{aligned} \quad (5.18)$$

$$\begin{aligned} \bar{\psi}^\dagger(\vec{k}n)[L_0 G_0^S(\vec{x}'; \epsilon)] + \bar{\psi}^\dagger(\vec{k}n)[(V_0 - \epsilon)G_0^S(\vec{x}'; \epsilon)] \\ + [\bar{T}_0 \bar{\psi}(\vec{k}n)]^\dagger G_0^S(\vec{x}'; \epsilon) \\ = \vec{\nabla} \cdot \bar{P}_0[\bar{\psi}^\dagger(\vec{k}n), G_0^S(\vec{x}'; \epsilon)]. \end{aligned} \quad (5.13)$$

If this equation is integrated over the volume  $\delta V$  defined by

$$x_1^A \leq x_1 \leq x_1^B, \quad (5.14a)$$

$$x_2^A \leq x_2 \leq x_2^B, \quad (5.14b)$$

$$x_3' - \delta x_3 \leq x_3 \leq x_3' + \delta x_3, \quad (5.14c)$$

in terms of the  $x_i^A$  and  $x_i^B$  of (4.16), the second and third terms will give no contribution as  $\delta x_3 \rightarrow 0$ , because these terms involve no singularities.

However, (5.10a) implies that the first term gives a contribution of  $\bar{\psi}^\dagger(\vec{x}'; \vec{k}n)$ . Therefore

$$\bar{\psi}^\dagger(\vec{x}'; \vec{k}n) = \int_{S(\delta V)} \bar{P}_0[\bar{\psi}^\dagger(\vec{k}n), G_0^S(\vec{x}'; \epsilon)] \cdot d\vec{S}, \quad (5.15)$$

where  $S(\delta V)$  is the surface of  $\delta V$  and we have assumed that  $\bar{P}_0[\bar{\psi}^\dagger(\vec{k}n), G_0^S(\vec{x}'; \epsilon)]$  is sufficiently well behaved for Gauss's theorem to hold. As  $\delta x_3 \rightarrow 0$ , the sides of  $S(\delta V)$  become vanishingly thin and give no contribution to the surface integral of (5.15). On the "top surface," where  $x_3 = x_3' + \delta x_3$ , the normal is parallel to  $\vec{b}_3$  and  $\bar{P}_0 \cdot d\vec{S} = P_{03} dx_1 dx_2$ , where  $P_{0j}$  is defined by

$$\bar{P}_0 = (P_{01} \vec{a}_1 + P_{02} \vec{a}_2 + P_{03} \vec{a}_3) / \vec{a}_3 \cdot \vec{a}_1 \times \vec{a}_2. \quad (5.16)$$

Similarly, on the bottom surface, where  $x_3 = x_3' - \delta x_3$ , the normal is parallel to  $-\vec{b}_3$  and  $\bar{P}_0 \cdot d\vec{S} = -P_{03} dx_1 dx_2$ . We can therefore write



as  $\delta x_3 \rightarrow 0$ , where  $S_3$  is the surface defined by

$$x_i^A \leq x_i \leq x_i^B, \quad i=1 \text{ or } 2, \quad (5.19a)$$

$$x_3 = x_3', \quad (5.19b)$$

having its normal parallel to  $\vec{b}_3$ .

VI. THEOREM

In this section I prove the following theorem:

$$-2\pi i \int_{s_j} \vec{P}_0[\vec{\psi}^\dagger(\vec{k}n), \psi(\vec{k}'n')] \cdot d\vec{S} = v_j(\vec{k}n) \delta_{k_j k_j'} \delta_{n n'}, \quad (6.1a)$$

if

$$\epsilon(\vec{k}'n') = \epsilon(\vec{k}n), \quad (6.1b)$$

$$k_i' = k_i, \quad i \neq j, \quad (6.1c)$$

$$-\frac{1}{2} < \text{Re} k_j \leq \frac{1}{2}, \quad -\frac{1}{2} < \text{Re} k_j' \leq \frac{1}{2}. \quad (6.1d)$$

[A slight generalization of this result is given as (6.23).] Here  $s_j$  is any surface defined by

$$x_i^{(0)} - 1 \leq x_i \leq x_i^{(0)}, \quad i \neq j, \quad (6.2a)$$

$$x_j = x_j^{(0)}, \quad (6.2b)$$

having its normal parallel to  $\vec{b}_j$ , with  $x_1^{(0)}, x_2^{(0)}$ , and  $x_3^{(0)}$  being arbitrary real constants. It is assumed that  $\epsilon(\vec{k}n)$  is differentiable with respect to  $k_j$  at the point  $\vec{k}$ , that  $\vec{P}_0[\vec{\psi}^\dagger(\vec{k}n), \psi(\vec{k}'n')]$  is integrable over  $s_j$  [and over the rest of the surface  $s$  of (6.16)], and that  $\psi(\vec{k}'n')$  is a continuous function of  $k_j$  at the point  $\vec{k} = \vec{k}'$ . It is also assumed that  $T_0 \neq 0$ —or, more precisely, that  $H_0$  contains at least one derivative with respect to  $x_j$ .

According to (6.2),  $s_j$  can be any cross section of any parallelepiped unit cell having its normal parallel to  $\vec{b}_j$ . For example, if  $\mathcal{P}_3$  is an arbitrary plane parallel to  $\vec{a}_1$  and  $\vec{a}_2$ , then  $s_3$  is that part of  $\mathcal{P}_3$  lying within some unit cell intersected by  $\mathcal{P}_3$ , and the normal to  $s_3$  is parallel to  $\vec{a}_1 \times \vec{a}_2$ . Similarly,  $s_1$  is parallel to  $\vec{a}_2$  and  $\vec{a}_3$ , and  $s_2$  to  $\vec{a}_3$  and  $\vec{a}_1$ .

We begin the proof by applying (2.1):

$$\begin{aligned} & \int_V d\vec{x} \vec{\psi}^\dagger(\vec{k}n) [H_0 \psi(\vec{k} + \Delta \vec{k}, n')] \\ &= \int_V d\vec{x} [\vec{H}_0 \vec{\psi}(\vec{k}n)]^\dagger \psi(\vec{k} + \Delta \vec{k}, n') \\ & - \int_S \vec{P}_0[\vec{\psi}^\dagger(\vec{k}n), \psi(\vec{k} + \Delta \vec{k}, n')] \cdot d\vec{S}, \end{aligned} \quad (6.3)$$

or

$$\begin{aligned} & [\epsilon(\vec{k} + \Delta \vec{k}, n') - \epsilon(\vec{k}n)] \int_V d\vec{x} \vec{\psi}^\dagger(\vec{k}n) \psi(\vec{k} + \Delta \vec{k}, n') \\ &= - \int_S \vec{P}_0[\vec{\psi}^\dagger(\vec{k}n), \psi(\vec{k} + \Delta \vec{k}, n')] \cdot d\vec{S}, \end{aligned} \quad (6.4)$$

where  $\vec{k}$  and  $\vec{k} + \Delta \vec{k}$  are arbitrary complex wave vectors. According to (4.4) and (4.11a'),

$$\begin{aligned} & \int_V d\vec{x} \vec{\psi}^\dagger(\vec{k}n) \psi(\vec{k} + \Delta \vec{k}, n') \\ &= \int_V d\vec{x} \vec{\psi}^\dagger(\vec{k}n) \psi(\vec{k} + \Delta \vec{k}, n') \sum_{\vec{X}} e^{i\Delta \vec{k} \cdot \vec{X}}. \end{aligned} \quad (6.5)$$

Now, the argument just below (4.22) implies that

$$\begin{aligned} & \int_S \vec{P}_0[e^{-i\vec{k} \cdot \vec{X}} w^\dagger(\vec{X}), e^{i(\vec{k} + \Delta \vec{k}) \cdot \vec{X}} v(\vec{X})] \cdot d\vec{S} \\ &= \int_S \sum_{\vec{X}} \vec{P}_0[e^{-i\vec{k} \cdot (\vec{X} + \vec{X})} w^\dagger(\vec{X}), \\ & \quad e^{i(\vec{k} + \Delta \vec{k}) \cdot (\vec{X} + \vec{X})} v(\vec{X})] \cdot d\vec{S} \end{aligned} \quad (6.6)$$

if  $w$  and  $v$  are periodic, and the argument just above (4.25c) leads to the generalization

$$\begin{aligned} & \vec{P}_0[e^{-i\vec{k} \cdot (\vec{X} + \vec{X})} w^\dagger(\vec{X}), e^{i(\vec{k} + \Delta \vec{k}) \cdot (\vec{X} + \vec{X})} v(\vec{X})] \\ &= \vec{P}_0[e^{-i\vec{k} \cdot \vec{X}} w^\dagger(\vec{X}), e^{i(\vec{k} + \Delta \vec{k}) \cdot \vec{X}} v(\vec{X})] e^{i\Delta \vec{k} \cdot \vec{X}}. \end{aligned} \quad (6.7)$$

When the above results are combined, with  $w \rightarrow \bar{u}(\vec{k}n)$  and  $v \rightarrow u(\vec{k} + \Delta \vec{k}, n')$ , we obtain

$$\begin{aligned} & [\epsilon(\vec{k} + \Delta \vec{k}, n') - \epsilon(\vec{k}n)] \int_V d\vec{x} \vec{\psi}^\dagger(\vec{k}n) \psi(\vec{k} + \Delta \vec{k}, n') \\ & \quad \times \sum_{\vec{X}} e^{i\Delta \vec{k} \cdot \vec{X}} \\ &= - \int_S \vec{P}_0[\vec{\psi}^\dagger(\vec{k}n), \psi(\vec{k} + \Delta \vec{k}, n')] \cdot d\vec{S} \\ & \quad \times \sum_{\vec{X}} e^{i\Delta \vec{k} \cdot \vec{X}}. \end{aligned} \quad (6.8)$$

At this point we choose

$$\Delta k_i = k_i' - k_i = m_i, \quad i=1 \text{ or } 2, \quad (6.9)$$

so that

$$\Delta \vec{k} \cdot \vec{X} = 2\pi l_1 m_1 + 2\pi l_2 m_2 + 2\pi l_3 \Delta k_3 \quad (6.10)$$

by (4.1). According to (4.16),  $\vec{X}$  has a range of values given by putting

$$l_i = l_i^{(0)}, l_i^{(0)} + 1, \dots, l_i^{(0)} + (L_i - 1) \quad (6.11)$$

into (4.1a). Therefore

$$\sum_{\vec{X}} e^{i\Delta \vec{k} \cdot \vec{X}} = L_1 L_2 \sum_{l_3=1}^{l_3^{(0)} + (L_3 - 1)} (e^{i2\pi \Delta k_3})^{l_3} \quad (6.12)$$

$$\begin{aligned} &= L_1 L_2 e^{i2\pi \Delta k_3 l_3^{(0)}} \\ & \quad \times (1 - e^{i2\pi \Delta k_3 L_3}) / (1 - e^{i2\pi \Delta k_3}). \end{aligned} \quad (6.13)$$

We write

$$\Delta k_3 = k_3' - k_3 + \delta k_3, \quad (6.14)$$

where  $\delta k_3$  is chosen so that

$$\Delta k_3 \neq \text{integer} / L_3. \quad (6.15)$$

Then (6.8) can be divided by (6.13), and

$$\begin{aligned} & [\epsilon(\vec{k} + \Delta\vec{k}, n') - \epsilon(\vec{k}n)] \int_v d\vec{x} \bar{\psi}^\dagger(\vec{k}n) \psi(\vec{k} + \Delta\vec{k}, n') \\ &= - \int_s \bar{P}_0[\bar{\psi}^\dagger(\vec{k}n), \psi(\vec{k} + \Delta\vec{k}, n')] \cdot d\vec{S}. \end{aligned} \quad (6.16)$$

After the  $x_j^{(0)}$  have been specified, let  $x_j^b = x_j^{(0)}$ , so that the unit cell  $v$  as defined by (4.17) has the  $s_j$  defined by (6.2) as its "front surfaces." Also, let  $t_j$  be the "back surface" defined by (6.2a) and

$$x_j = x_j^{(0)} - 1, \quad (6.2b')$$

having its (outward) normal in the direction of  $-\vec{b}_j$ . Since  $t_j$  is displaced by  $-\vec{a}_j$  from  $s_j$ , and the normals are in opposite directions for the two surfaces, (6.7) implies that

$$\begin{aligned} & \int_{t_j} \bar{P}_0[\bar{\psi}^\dagger(\vec{k}n), \psi(\vec{k} + \Delta\vec{k}, n')] \cdot d\vec{S} \\ &= -e^{-2\pi i \Delta k_j} \int_{s_j} \bar{P}_0[\bar{\psi}^\dagger(\vec{k}n), \psi(\vec{k} + \Delta\vec{k}, n')] \cdot d\vec{S}. \end{aligned} \quad (6.17)$$

This result, in conjunction with (6.9), allows us to simplify (6.16):

$$\begin{aligned} & [\epsilon(\vec{k} + \Delta\vec{k}, n') - \epsilon(\vec{k}n)] \int_v d\vec{x} \bar{\psi}^\dagger(\vec{k}n) \psi(\vec{k} + \Delta\vec{k}, n') \\ &= -(1 - e^{-2\pi i \Delta k_3}) \int_{s_3} \bar{P}_0[\bar{\psi}^\dagger(\vec{k}n), \psi(\vec{k} + \Delta\vec{k}, n')] \cdot d\vec{S}. \end{aligned} \quad (6.18)$$

First consider the case  $k_3' - k_3 = \text{integer} \equiv m_3$ . Using (6.1b) and (6.14), and keeping only the first-order term in  $(1 - e^{-2\pi i \delta k_3})$ , we obtain

$$\begin{aligned} & [\epsilon(\vec{k}', k_3' + \delta k_3; n') - \epsilon(\vec{k}', k_3'; n')] \\ & \times \int_v d\vec{x} \bar{\psi}^\dagger(\vec{k}n) \psi(\vec{k} + \Delta\vec{k}, n') \\ &= -2\pi i \delta k_3 \int_{s_3} \bar{P}_0[\bar{\psi}^\dagger(\vec{k}n), \psi(\vec{k} + \Delta\vec{k}, n')] \cdot d\vec{S}, \end{aligned} \quad \delta k_3 \rightarrow 0, \quad (6.19)$$

or

$$\begin{aligned} & \frac{\partial \epsilon(\vec{k} + \vec{K}, n')}{\partial k_3} \int_v d\vec{x} \bar{\psi}^\dagger(\vec{k}n) \psi(\vec{k} + \vec{K}, n') \\ &= -2\pi i \int_{s_3} \bar{P}_0[\bar{\psi}^\dagger(\vec{k}n), \psi(\vec{k}'n')] \cdot d\vec{S}, \end{aligned} \quad (6.20)$$

where  $\vec{K}$  is the reciprocal-lattice vector defined by  $m_1, m_2$ , and  $m_3$  according to (4.1c). In view of (13.11) and (13.14),  $\epsilon(\vec{k} + \vec{K}, n')$  and  $\psi(\vec{k} + \vec{K}, n')$  can

be replaced by  $\epsilon(\vec{k}'n')$  and  $A_{\vec{K}}(\vec{k}'n')\psi(\vec{k}'n')$  in (6.20). Then (4.32b) gives

$$\begin{aligned} & -2\pi i \int_{s_3} \bar{P}_0[\bar{\psi}^\dagger(\vec{k}n), \psi(\vec{k}'n')] \cdot d\vec{S} \\ &= A_{\vec{K}}(\vec{k}n) \frac{\partial \epsilon(\vec{k}n)}{\partial k_3} \delta_{nn'}. \end{aligned} \quad (6.21)$$

Next consider the case  $k_3' - k_3 \neq \text{integer}$ . Then as  $\delta k_3 \rightarrow 0$  in (6.18),  $(1 - e^{-2\pi i \Delta k_3})$  remains non-zero and (6.1b) requires that

$$\int_{s_3} \bar{P}_0[\bar{\psi}^\dagger(\vec{k}n), \psi(\vec{k}'n')] \cdot d\vec{S} = 0. \quad (6.22)$$

When (6.21) and (6.22) are combined, and the derivation is repeated for  $j=1$  and  $2$ , we obtain

$$\begin{aligned} & -2\pi i \int_{s_j} \bar{P}_0[\bar{\psi}^\dagger(\vec{k}n), \psi(\vec{k}'n')] \cdot d\vec{S} \\ &= A_{\vec{K}}(\vec{k}n) v_j(\vec{k}n) \delta_{k_j+m_j, k_j'} \delta_{nn'}, \end{aligned} \quad (6.23a)$$

where  $\delta_{k_j+m_j, k_j'} = 1$  if  $k_j' - k_j = \text{integer} \equiv m_j$  and 0 otherwise. We recall that (6.23a) holds if

$$\epsilon(\vec{k}'n') = \epsilon(\vec{k}n), \quad (6.23b)$$

$$k_i' = k_i + m_i, \quad i \neq j, \quad (6.23c)$$

where  $m_i$  is any integer, and that  $\vec{K}$  is related to  $m_1, m_2$ , and  $m_3$  through (4.1c). If

$$A_{\vec{K}}(\vec{k}n) = 1 \quad (6.24)$$

then (6.23a) reduces to (6.1a) (with  $\delta_{k_j, k_j'} - \delta_{k_j+m_j, k_j'}$ ). Equation (6.24) will obviously hold if we set  $m_i = 0, i \neq j$ , and force  $m_j = 0$  by restricting  $\text{Re}k_j$  and  $\text{Re}k_j'$  to the interval  $(-\frac{1}{2}, \frac{1}{2}]$ , i.e., if we replace (6.23c) by (6.1c) and (6.1d).

When  $\vec{k}' = \vec{k}$  and  $n' = n$ , (6.1a) is the generalization of a well-known theorem of solid-state physics,<sup>5(b)</sup> that the average value of the probability current density is equal to the derivative of the energy eigenvalue with respect to  $\vec{k}$  for an electron in a periodic solid. [A weaker version of (6.1a) is

$$-2\pi i \int_v d\vec{x} \bar{P}_0 = \vec{v} \equiv v_1 \vec{a}_1 + v_2 \vec{a}_2 + v_3 \vec{a}_3.]$$

Another expression for  $v_j(\vec{k}n) \equiv \partial \epsilon(\vec{k}n) / \partial k_j$  can also be generalized: According to the Hellmann-Feynman theorem<sup>5(a)</sup> (otherwise known as first-order perturbation theory) and (13.4),

$$\begin{aligned} & \frac{\partial \epsilon(\vec{k}n)}{\partial k_j} = \int_v d\vec{x} \int_{v'} d\vec{x}' \bar{u}^\dagger(\vec{x}; \vec{k}n) \\ & \times \left( \frac{\partial}{\partial k_j} H_0(\vec{x}\vec{x}'; \vec{k}) \right) u(\vec{x}'; \vec{k}n), \end{aligned} \quad (6.25)$$

so

$$v_j(\vec{k}n) = 2\pi i \int_{v'} d\vec{x} \bar{\psi}^\dagger(\vec{x}; \vec{k}n) [T_{0j}, x_j] \psi(\vec{x}; \vec{k}n) + 2\pi i \int_{v'} d\vec{x} \int_{v'} d\vec{x}' \bar{\psi}^\dagger(\vec{x}; \vec{k}n) (x'_j - x_j) \times V_0(\vec{x}, \vec{x}') \psi(\vec{x}'; \vec{k}n). \quad (6.26)$$

VII. FINAL RESULT FOR  $G_0$

The two-dimensional analog of (6.6) is

$$\int_{s_3} \bar{P}_0 [e^{-i\vec{k} \cdot \vec{x}} w^\dagger(\vec{x}), e^{i\vec{k}' \cdot \vec{x}} v(\vec{x})] \cdot d\vec{S} = \int_{s_3} \sum_{\vec{x}} \bar{P}_0 [e^{-i\vec{k} \cdot (\vec{x} + \vec{x}')} w^\dagger(\vec{x}) e^{i\vec{k}' \cdot (\vec{x} + \vec{x}')} v(\vec{x}')] \cdot d\vec{S}, \quad (7.1)$$

$$\vec{X} \equiv l_1 \vec{a}_1 + l_2 \vec{a}_2, \quad (7.2)$$

if  $w$  and  $v$  are periodic. In this section we choose

$$x_3^{(0)} = x_3', \quad (7.3)$$

so that the little surface  $s_3$  defined by (6.2) lies within the big surface  $S_3$  defined by (5.19). Combining (6.7) and (7.1), and letting  $\vec{k} + \Delta\vec{k} \rightarrow \vec{k}'$ ,  $w - \bar{u}(\vec{k}n)$ ,  $v - u(\vec{k}'n')$ , gives

$$\int_{s_3} \bar{P}_0 [\bar{\psi}^\dagger(\vec{k}n), \psi(\vec{k}'n')] \cdot d\vec{S} = \int_{s_3} \bar{P}_0 [\bar{\psi}^\dagger(\vec{k}n), \psi(\vec{k}'n')] \cdot d\vec{S} \sum_{\vec{x}} e^{i(\vec{k}' - \vec{k}) \cdot \vec{x}}. \quad (7.4)$$

The same (well-known) argument that produced (6.13) leads to the result

$$\sum_{\vec{x}} e^{i(\vec{k}' - \vec{k}) \cdot \vec{x}} = \prod_{i=1}^2 e^{i2\pi(k'_i - k_i)x_i^{(0)}} \frac{1 - e^{i2\pi(k'_i - k_i)L_i}}{1 - e^{i2\pi(k'_i - k_i)}} \quad (7.5a)$$

$$= L_1 L_2 \delta_{\vec{k}\vec{k}'}, \quad (7.5b)$$

if  $\vec{k}$  and  $\vec{k}'$  satisfy (5.4) and (5.6a). Then (6.1) and (7.4) give

$$-2\pi i \int_{s_3} \bar{P}_0 [\bar{\psi}^\dagger(\vec{k}n), \psi(\vec{k}'n')] \cdot d\vec{S} = L_1 L_2 v_3(\vec{k}n) \delta_{\vec{k}\vec{k}'} \delta_{nn'}, \quad (7.6)$$

if  $k_3$  and  $k'_3$  satisfy (5.6b). We therefore have

$$\int_{s_3} \bar{P}_0 [\bar{\psi}^\dagger(\vec{k}k_{n1}^\dagger n), \psi(\vec{k}'k_{n1}^\dagger n')] \cdot d\vec{S} = 0, \quad (7.7a)$$

$$\int_{s_3} \bar{P}_0 [\bar{\psi}^\dagger(\vec{k}k_{n1}^\dagger n), \psi(\vec{k}'k_{n1}^\dagger n')] \cdot d\vec{S} = L_1 L_2 v_3(\vec{k}k_{n1}^\dagger n) \delta_{\vec{k}\vec{k}'} \delta_{nn'} \delta_{11'} / (-2\pi i), \quad (7.7b)$$

which reduces (5.18) to

$$a^\dagger(\vec{x}'; \vec{k}n) = \mp 2\pi i \bar{\psi}^\dagger(\vec{x}'; \vec{k}k_{n1}^\dagger n) / v_3(\vec{k}k_{n1}^\dagger n) L_1 L_2. \quad (7.8)$$

Then (5.9) gives, with  $(L_1 L_2)^{-1} \sum_{\vec{k}} \rightarrow \int_{BZ} d\vec{k}$ ,

$$G_0(\vec{x}\vec{x}'; \epsilon) = \int_{BZ} d\vec{k} G_0(\vec{x}\vec{x}'; \vec{k}\epsilon), \quad (7.9a)$$

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$$G_0(\vec{x}\vec{x}'; \vec{k}\epsilon) = -2\pi i \left( \sum_{n1} \frac{\psi(\vec{x}; \vec{k}k_{n1}^\dagger n) \bar{\psi}^\dagger(\vec{x}'; \vec{k}k_{n1}^\dagger n)}{v_3(\vec{k}k_{n1}^\dagger n)} \theta(x_3 - x_3') - \sum_{n1} \frac{\psi(\vec{x}; \vec{k}k_{n1}^- n) \bar{\psi}^\dagger(\vec{x}'; \vec{k}k_{n1}^- n)}{v_3(\vec{k}k_{n1}^- n)} \theta(x_3' - x_3) \right) + G_0^{NS}(\vec{x}\vec{x}'; \vec{k}\epsilon), \quad (7.9b)$$

$$G_0^{NS}(\vec{x}\vec{x}'; \vec{k}\epsilon) = \sum_{nk_3} \alpha(\vec{x}'; \vec{k}k_3 n) \psi(\vec{x}; \vec{k}k_3 n). \quad (7.9c)$$

Recall that the coefficients  $\alpha$  are determined by the boundary conditions on  $G_0$ , and that the  $\vec{k}$  values in the sums of (7.9) are those satisfying (5.5) and (5.6b). We write (7.9) in the shorter form

$$G_0(\vec{x}\vec{x}'; \vec{k}\epsilon) = -2\pi i \sum_{n1} \frac{\psi(\vec{x}; \vec{k}k_{n1}^\dagger n) \bar{\psi}^\dagger(\vec{x}'; \vec{k}k_{n1}^\dagger n)}{v_3(\vec{k}k_{n1}^\dagger n)} \times \text{sgn}(x_3 - x_3') + G_0^{NS}(\vec{x}\vec{x}'; \vec{k}\epsilon), \quad (7.10)$$

where it is understood that  $k_{n1} = k_{n1}^\dagger$  for  $\text{sgn}(x_3 - x_3') = +1$  and  $k_{n1} = k_{n1}^-$  for  $\text{sgn}(x_3 - x_3') = -1$ . We recall (4.15c):

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$$\bar{\psi}(\vec{k}k_3 n) = \psi(\vec{k}k_3^* n) \quad (7.11)$$

if the operator  $H_0$  is formally self-adjoint.

VIII. SYSTEM WITH AN INTERFACE

When an interface is present,  $H_0$  is changed to  $H$ , an operator with only two-dimensional translational invariance:

$$H(\vec{x} + \vec{X}, x_3; \vec{x}' + \vec{X}, x_3') = H(\vec{x}, \vec{x}'). \quad (8.1)$$

For reference, we write down the analog of (4.1):

$$\vec{X} = l_1 \vec{a}_1 + l_2 \vec{a}_2 \quad (\vec{X} = \vec{X} + l_3 \vec{a}_3), \quad (8.2a)$$

$$\vec{x} = x_1 \vec{a}_1 + x_2 \vec{a}_2 \quad (\vec{x} = \vec{x} + x_3 \vec{a}_3), \quad (8.2b)$$

$$\vec{K} = m_1 \vec{b}_1 + m_2 \vec{b}_2 \quad (\vec{K} = \vec{K} + m_3 \vec{b}_3), \quad (8.2c)$$

$$\bar{k} = k_1 \bar{b}_1 + k_2 \bar{b}_2 \quad (\bar{k} = \bar{k} + k_3 \bar{b}_3). \quad (8.2d)$$

Let the interface be at  $x_3 = 0$  and let the medium in the region  $x_3 \geq 0$  be called  $M_{\geq}$ . (Either  $M_{>}$  or  $M_{\leq}$  may be vacuum.) We assume that

$$H(\bar{x}, \bar{x}') - H_0^>(\bar{x}, \bar{x}') \text{ as } x_3 \rightarrow -\infty \text{ and } x_3' \rightarrow \infty, \quad (8.3a)$$

$$-H_0^<(\bar{x}, \bar{x}') \text{ as } x_3 \rightarrow -\infty \text{ and } x_3' \rightarrow -\infty, \quad (8.3b)$$

$$-0 \text{ as } |x_3 - x_3'| \rightarrow \infty, \quad (8.3c)$$

where  $H_0^>$  is the bulk operator for  $M_{\geq}$ .

Let  $\psi_{\geq}(\bar{k}n)$  be an eigenfunction of  $H_0^>$  with wave vector  $\bar{k}$  and eigenvalue  $\epsilon_{\geq}(\bar{k}n)$ , and let  $\Psi_{\geq}$  be any solution to

$$[\epsilon_{\geq}(\bar{k}n) - H] \Psi_{\geq}(\bar{k}n) = 0, \quad (8.4a)$$

for which

$$\Psi_{\geq}(\bar{x}; \bar{k}n) - \psi_{\geq}(\bar{x}; \bar{k}n) \text{ as } x_3 \rightarrow \pm\infty. \quad (8.4b)$$

That is,  $\Psi$  grows out of  $\psi$  as the interface is approached. Also, let  $\bar{\Psi}_{\geq}$  be a solution to

$$[\epsilon_{\geq}^*(\bar{k}n) - \bar{H}] \bar{\Psi}_{\geq}(\bar{k}n) = 0, \quad (8.5a)$$

for which

$$\bar{\Psi}_{\geq}(\bar{x}; \bar{k}n) - \bar{\psi}_{\geq}(\bar{x}; \bar{k}n) \text{ as } x_3 \rightarrow \pm\infty. \quad (8.5b)$$

Equation (8.4) does not uniquely specify  $\Psi$ , since (8.4b) will still be satisfied if an arbitrary set of rapidly decaying solutions to (8.4a) is added to  $\Psi$ . Similarly, (8.5) does not uniquely specify  $\bar{\Psi}$ .

In the following, I focus on the medium  $M_{\leq}$  for concreteness, and temporarily drop the subscript:

$$H_0 = H_0^<, \quad \epsilon = \epsilon_{\leq}, \quad \psi = \psi_{\leq}, \quad \Psi = \Psi_{\leq}. \quad (8.6)$$

$\Psi$  is a two-dimensional Bloch function:

$$\Psi(\bar{x}; \bar{k}n) = e^{i\bar{k} \cdot \bar{x}} U(\bar{x}; \bar{k}n), \quad (8.7a)$$

$$U(\bar{x} + \bar{X}, x_3; \bar{k}n) = U(\bar{x}; \bar{k}n). \quad (8.7b)$$

So is  $\bar{\Psi}$ , and (4.11a') requires that

$$\bar{\Psi}^{\dagger}(\bar{x}; \bar{k}n) = e^{-i\bar{k} \cdot \bar{x}} \bar{U}^{\dagger}(\bar{x}; \bar{k}n), \quad (8.8a)$$

$$\bar{U}^{\dagger}(\bar{x} + \bar{X}, x_3; \bar{k}n) = \bar{U}^{\dagger}(\bar{x}; \bar{k}n). \quad (8.8b)$$

### IX. A COROLLARY

In this section, I prove a corollary to the theorem of Sec. VI:

$$-2\pi i \int_{\sigma_3} \bar{\Psi}^{\dagger}(\bar{k}n), \Psi(\bar{k}'n') \cdot d\bar{S} = v_3(\bar{k}n) \delta_{k_3 k_3'} \delta_{nm'} \quad (9.1a)$$

if

$$\epsilon(\bar{k}'n') = \epsilon(\bar{k}n), \quad (9.1b)$$

$$k_i' = k_i, \quad i = 1 \text{ or } 2, \quad (9.1c)$$

$$-\frac{1}{2} < \text{Re } k_3 \leq \frac{1}{2}, \quad -\frac{1}{2} < \text{Re } k_3' \leq \frac{1}{2}. \quad (9.1d)$$

Here  $\bar{P}$  is the bilinear concomitant of  $-H$ , and  $\sigma_3$  is a surface defined exactly as  $s_3$  was [in (6.2), with  $j=3$ ] but which may be near the interface, or arbitrarily far beyond it, rather than in the bulk.

We begin by letting  $\Omega$  be the volume defined by

$$x_i^{(0)} - 1 \leq x_i \leq x_i^{(0)}, \quad i = 1 \text{ or } 2, \quad (9.2a)$$

$$x_3^{(0)} \leq x_3 \leq x_3^{(1)}, \quad (9.2b)$$

with  $x_3^{(1)} - x_3^{(0)} = \text{integer}$ . In order to obtain (9.6b), we will let

$$x_3^{(0)} \rightarrow -\infty. \quad (9.2c)$$

The volume  $\Omega$  is a "long parallelepiped" stretching from the plane  $x_3 = x_3^{(0)}$ , deep within the bulk of  $M_{\leq}$ , to another plane  $x_3 = x_3^{(1)}$  which may be near the interface (or may lie beyond the interface, within  $M_{>}$ ). We let  $\sigma$  be the surface of  $\Omega$ , and break  $\sigma$  up into three "front surfaces"  $\sigma_j$  and three "back surfaces"  $\tau_j$ , with the normals to  $\sigma_j$  and  $\tau_j$  being parallel to  $\bar{b}_j$  and  $-\bar{b}_j$ , respectively.

The two dimensional analog of (6.7) is

$$\begin{aligned} \bar{P}[e^{-i\bar{k} \cdot (\bar{x} + \bar{x}')} w^{\dagger}(\bar{x}), e^{i\bar{k}' \cdot (\bar{x} + \bar{x}')} v(\bar{x})] \\ = \bar{P}[e^{-i\bar{k} \cdot \bar{x}} w^{\dagger}(\bar{x}), e^{i\bar{k}' \cdot \bar{x}} v(\bar{x})] e^{i(\bar{k}' - \bar{k}) \cdot \bar{X}}, \end{aligned} \quad (9.3)$$

with  $w(\bar{x})$  and  $v(\bar{x})$  having two-dimensional periodicity. In view of (8.7) and (8.8), we then have

$$\begin{aligned} \int_{\tau_i} \bar{P}[\bar{\Psi}^{\dagger}(\bar{x}; \bar{k}n), \Psi(\bar{x}; \bar{k}'n')] \cdot d\bar{S} \\ = -e^{-2\pi i \theta_i - k_i} \int_{\sigma_i} \bar{P}[\bar{\Psi}^{\dagger}(\bar{x}; \bar{k}n), \Psi(\bar{x}; \bar{k}'n')] \cdot d\bar{S}, \end{aligned} \quad (9.4)$$

$i = 1 \text{ or } 2,$

since  $\tau_i$  is displaced from  $\sigma_i$  by  $\bar{X} = -\bar{a}_i$ , and since the normals to  $\tau_i$  and  $\sigma_i$  point in opposite directions. If (9.1c) is now invoked, (9.4) will cause the contributions from the "long sides" of  $\sigma$  to cancel, leaving

$$\begin{aligned} \int_{\sigma} \bar{P}[\bar{\Psi}^{\dagger}(\bar{k}n), \Psi(\bar{k}'n')] \cdot d\bar{S} \\ = \int_{\sigma_3 + \tau_3} \bar{P}[\bar{\Psi}^{\dagger}(\bar{k}n), \Psi(\bar{k}'n')] \cdot d\bar{S}. \end{aligned} \quad (9.5)$$

That is, the surface integral reduces to an integral over the "end caps" at the top and bottom of  $\sigma$ .

But since  $\Psi$  and  $\bar{\Psi}$  satisfy adjoint boundary conditions, according to (9.1b) and the comment following (2.7) [which still holds if  $V \rightarrow \Omega$  and  $S \rightarrow \sigma$  in (2.1b) and (2.2)], the left-hand side of (9.5) vanishes, and  $\int_{\sigma_3} = -\int_{\tau_3}$ . Equations (6.2) and (9.2) show that  $\tau_3$  and  $s_3$  consist of the same points; however, their normals point in opposite direc-

tions, so  $\int_{\tau_3} = -\int_{s_3}$ . We thus have

$$\int_{\sigma_3} \bar{P}[\bar{\Psi}^\dagger(\bar{k}n), \Psi(\bar{k}'n')] \cdot d\bar{S}$$

$$= \int_{s_3} \bar{P}[\bar{\Psi}^\dagger(\bar{k}n), \Psi(\bar{k}'n')] \cdot d\bar{S} \quad (9.6a)$$

$$= \int_{s_3} \bar{P}_0[\bar{\Psi}^\dagger(\bar{k}n), \psi(\bar{k}'n')] \cdot d\bar{S} \quad (9.6b)$$

in view of (9.2c), so (9.1) is the same as (6.1) for  $j=3$ .

### X. EVALUATION OF $G$

$G(\bar{x}\bar{x}'; \epsilon)$  is defined to be a solution to

$$\int_V d\bar{x}'' L(\bar{x}\bar{x}'', \epsilon) \cdot G(\bar{x}''\bar{x}'; \epsilon) = \delta(\bar{x} - \bar{x}'), \quad (10.1)$$

$$L = \epsilon - H. \quad (10.2)$$

(The boundaries of  $V$  parallel to  $\bar{a}_1$  and  $\bar{a}_2$  are far from the interface on both sides.) As in Sec. V, we look for a solution in the form

$$G(\bar{x}\bar{x}'; \epsilon) = \sum_{\bar{k}m} [\beta^+(\bar{x}'; \bar{k}m) \Phi(\bar{x}; \bar{k}m) \theta(x_3 - x_3') + \beta^-(\bar{x}'; \bar{k}m) \Phi(\bar{x}; \bar{k}m) \theta(x_3' - x_3)], \quad (10.3)$$

with the  $\bar{k}$  satisfying (5.4). The  $\Phi(\bar{k}m)$  are the solutions to

$$H\Phi(\bar{k}m) = \epsilon(\bar{k}m)\Phi(\bar{k}m), \quad (10.4a)$$

$$\epsilon(\bar{k}m) = \epsilon, \quad (10.4b)$$

satisfying some specified boundary conditions.

It will be assumed that

$$\Phi(\bar{k}m) = \sum_{\bar{k}_3 n} c(\bar{k}n) \Psi(\bar{k}n), \quad (10.5a)$$

where the  $\Psi(\bar{k}n)$  satisfy (8.4) with  $\epsilon(\bar{k}n) = \epsilon$ . This is a reasonable assumption in view of (8.3). [If  $\Phi$  decays to zero more rapidly than  $H - H_0$  in the limit  $x_3, x_3' \rightarrow -\infty$ , it is conceivable that (10.5a) may break down; in this exceptional case, the present treatment will have to be modified.] There are two "natural" ways to specify the boundary conditions on  $\Phi$ : The first way is to choose the boundary conditions such that  $\Phi(\bar{k}m) \rightarrow \psi(\bar{k}n)$  as  $x_3 \rightarrow -\infty$ , with  $\text{Im}k_3 \leq 0$ ; i.e., all the  $c(\bar{k}n)$  in (10.5a) except

one are made to equal zero. In this case,  $\Phi(\bar{x}; \bar{k}m)$  will ordinarily grow without bound as  $x_3 \rightarrow +\infty$ . The other way is to choose the boundary conditions so that  $\Phi(\bar{k}m)$  remains bounded as  $x_3 \rightarrow -\infty$  and  $x_3 \rightarrow +\infty$ . In this case, we write the analog of (10.5a) in  $M_3$ ,

$$\Phi(\bar{k}m) = \sum_{\bar{k}_3 n} c_>(\bar{k}n) \Psi_>(\bar{k}n), \quad (10.5b)$$

set  $c_>(\bar{k}n) \equiv c(\bar{k}n) = 0$  for  $\text{Im}k_3 > 0$  and  $c_>(\bar{k}n) = 0$  for  $\text{Im}k_3 < 0$ , and then match the two expressions (10.5) for  $\Phi(\bar{k}m)$  (in the appropriate interfacial boundary conditions) at some plane  $x_3 = x_M$  to determine the possible sets of coefficients  $c_>$ . Notice that the  $\Phi(\bar{k}m)$  can include solutions localized near the interface on one or both sides, i.e., "surface states" as well as "bulk states."

Combining (10.3) and (10.5a), we have

$$G(\bar{x}\bar{x}'; \epsilon) = \sum_{\bar{k}n} [\gamma^+(\bar{x}'; \bar{k}n) \Psi(\bar{x}; \bar{k}n) \theta(x_3 - x_3') + \gamma^-(\bar{x}'; \bar{k}n) \Psi(\bar{x}; \bar{k}n) \theta(x_3' - x_3)], \quad (10.6)$$

which is the analog of (5.3). We can now simply carry over the treatment of Secs. V and VII, with  $G_0 \rightarrow G$ ,  $\alpha \rightarrow \gamma$ ,  $\psi \rightarrow \Psi$ ,  $L_0 \rightarrow L$ ,  $H_0 \rightarrow H$ ,  $T_0 \rightarrow T$ ,  $V_0 \rightarrow V$ ,  $P_0 \rightarrow P$ , and  $s_3 \rightarrow \sigma_3$  [and  $x_3^{(1)} = x_3'$  replacing (7.3)], to obtain

$$G(\bar{x}\bar{x}'; \epsilon) = \int_{\text{BZ}} d\bar{k} G(\bar{x}\bar{x}'; \bar{k}\epsilon), \quad (10.7a)$$

$$G(\bar{x}\bar{x}'; \bar{k}\epsilon) = -2\pi i \sum_{n\bar{l}} \frac{\Psi(\bar{x}; \bar{k}k_{n\bar{l}}) \bar{\Psi}^\dagger(\bar{x}'; \bar{k}k_{n\bar{l}})}{v_3(\bar{k}k_{n\bar{l}})} \times \text{sgn}(x_3 - x_3') + G^{\text{NS}}(\bar{x}\bar{x}'; \bar{k}\epsilon), \quad (10.7b)$$

$$G^{\text{NS}}(\bar{x}\bar{x}'; \bar{k}\epsilon) = \sum_{n\bar{k}_3} \gamma(\bar{x}'; \bar{k}k_3 n) \Psi(\bar{x}; \bar{k}k_3 n). \quad (10.7c)$$

Had we assumed  $G^{\text{NS}} = 0$  and left  $G$  in the form

$$G(\bar{x}\bar{x}'; \bar{k}\epsilon) = \sum_{n\bar{l}} \frac{\Psi(\bar{x}; \bar{k}k_{n\bar{l}}) \bar{\Psi}^\dagger(\bar{x}'; \bar{k}k_{n\bar{l}})}{\int_{s_3} \bar{P}[\bar{\Psi}^\dagger(\bar{k}n), \Psi(\bar{k}n)] \cdot d\bar{S}} \times \text{sgn}(x_3 - x_3'), \quad (10.8)$$

we would have had the generalization and simplification of a result due to Feibelman.<sup>6</sup>

With the subscripts of Sec. VIII restored, (10.7) is

$$G^{\bar{z}}(\bar{x}\bar{x}'; \bar{k}\epsilon) = -2\pi i \left[ \sum_{n\bar{l}} \frac{\Psi_{\bar{z}}(\bar{x}; \bar{k}k_{n\bar{l}}) \bar{\Psi}_{\bar{z}}^\dagger(\bar{x}'; \bar{k}k_{n\bar{l}})}{v_{\bar{z}}(\bar{k}k_{n\bar{l}})} \theta(x_3 - x_3') - \sum_{n\bar{l}} \frac{\Psi_{\bar{z}}(\bar{x}; \bar{k}k_{n\bar{l}}) \bar{\Psi}_{\bar{z}}^\dagger(\bar{x}'; \bar{k}k_{n\bar{l}})}{v_{\bar{z}}(\bar{k}k_{n\bar{l}})} \theta(x_3' - x_3) \right] + \sum_{n\bar{k}_3} \gamma_{\bar{z}}(\bar{x}'; \bar{k}k_3 n) \Psi_{\bar{z}}(\bar{x}; \bar{k}k_3 n), \quad (10.9)$$

$$v_s^>(\vec{k}n) \equiv \frac{\partial \epsilon_s(\vec{k}n)}{\partial k_3}. \quad (10.10)$$

Here  $G^<$  is the Green's function for the medium  $M_<$ , in the region  $x_3 < 0$ , and  $G^>$  is the Green's function for the medium  $M_>$ , in the region  $x_3 > 0$ . The  $k_3$  of (10.9), which are those values satisfying

$$\epsilon_s(\vec{k}k_3n) = \epsilon, \quad (10.11)$$

for fixed  $\vec{k}$  and  $n$ , have been arbitrarily broken up into the two sets  $k_{n1}^+$  and  $k_{n1}^-$ . After one has decided which  $k_3$  will be called  $k_{n1}^+$  and which will be called  $k_{n1}^-$ , the coefficients  $\gamma$  are determined by the boundary conditions imposed on  $G(\vec{x}\vec{x}')$  at fixed  $\vec{x}'$ .

### XI. MANY-BODY GREEN'S FUNCTIONS $\mathcal{G}_0$ AND $\mathcal{G}$

The exact single-particle Green's function  $\mathcal{G}$  satisfies the Dyson-Schwinger equation<sup>7</sup>

$$\int_V d\vec{x}'' \mathcal{L}(\vec{x}\vec{x}'') \cdot \mathcal{G}(\vec{x}''\vec{x}') = \delta(\vec{x} - \vec{x}'), \quad (11.1)$$

where

$$\mathcal{L}(\epsilon) = \epsilon - \mathcal{H}(\epsilon), \quad (11.2a)$$

$$\mathcal{H}(\epsilon) = T + \mathcal{U}(\epsilon), \quad (11.2b)$$

$$\mathcal{U}(\epsilon) = V + \Sigma(\epsilon) - \mu, \quad (11.2c)$$

$\mu$  is the chemical potential, and  $\Sigma(\vec{x}\vec{x}'; \epsilon)$  is the (temperature-dependent) self-energy. [For <sup>4</sup>He atoms and superconducting electrons,  $\mathcal{G}$  and  $\Sigma$  are  $2 \times 2$  matrices.<sup>8</sup> To allow for interaction with a quantized field  $\phi$ , one can add a term  $-g\Gamma\phi$  to the right-hand side of (11.2c), with  $g$  representing the coupling constant and  $\Gamma$  the vertex part.<sup>7</sup>] In view of (11.1), we look for a solution in the form (10.6):

$$\mathcal{G}(\vec{x}\vec{x}'; \epsilon) = \sum_s [\gamma_s^+(\vec{x}') \Psi_s(\vec{x}; \epsilon) \theta(x_3 - x'_3) + \gamma_s^-(\vec{x}') \Psi_s(\vec{x}; \epsilon) \theta(x'_3 - x_3)], \quad (11.3a)$$

where the  $\Psi_s(\vec{x}; \epsilon)$  are the solutions to

$$\mathcal{H}(\epsilon) \Psi_s(\epsilon) = \epsilon \Psi_s(\epsilon) \quad (11.3b)$$

satisfying some set of boundary conditions.

In addition to the representation (11.3), which is of interest in the present section, there are two other representations of  $\mathcal{G}$ . If some set of solutions  $\Psi_s(\epsilon)$  to the equation

$$\mathcal{H}(\epsilon) \Psi_s(\epsilon) = \epsilon_s(\epsilon) \Psi_s(\epsilon) \quad (11.4a)$$

is complete,

$$\frac{1}{N} \sum_s \Psi_s(\vec{x}; \epsilon) \bar{\Psi}_s^\dagger(\vec{x}'; \epsilon) = \delta(x - x'), \quad (11.4b)$$

then  $\mathcal{G}$  has the biorthogonal spectral representation<sup>7,9</sup>

$$\mathcal{G}(\vec{x}\vec{x}'; \epsilon) = \frac{1}{N} \sum_s \frac{\Psi_s(\vec{x}; \epsilon) \bar{\Psi}_s^\dagger(\vec{x}'; \epsilon)}{\epsilon - \epsilon_s(\epsilon)}. \quad (11.4c)$$

[The factor  $1/N$  in (11.4) is inserted to be consistent with (14.1) and (14.2).]  $\Psi$  is a "quasiparticle eigenfunction." The fact that  $\Sigma^\dagger(\vec{x}'\vec{x}) \neq \Sigma(\vec{x}\vec{x}')$  in general means that  $\mathcal{H}(\epsilon)$  is not formally self-adjoint and  $\epsilon_s$  is consequently complex; i.e., the time-dependent function  $\Psi_s e^{-i\omega t}$  is damped.

There is also the Lehmann spectral representation,<sup>8</sup> which has the form

$$\mathcal{G}(\vec{x}\vec{x}'; \epsilon) = \sum_s \frac{\chi_s(\vec{x}) \chi_s^\dagger(\vec{x}')}{\epsilon - \mathcal{E}_s} \quad (11.5a)$$

at zero temperature. This equation and (11.1) imply that  $\chi_s$  is a solution to

$$\mathcal{H}(\mathcal{E}_s) \chi_s = \mathcal{E}_s \chi_s. \quad (11.5b)$$

If the values of  $s$  become continuous in (11.4c),

$$(\epsilon - \epsilon_s)^{-1} \rightarrow a_s(\epsilon) (\epsilon - \epsilon_s + i\delta)^{-1} + b_s(\epsilon) (\epsilon - \epsilon_s - i\delta)^{-1},$$

with  $a_s(\epsilon) + b_s(\epsilon) = 1$ . The same kind of replacement is to be made in (11.5a).

According to (2.1),

$$\bar{\mathcal{L}}(\epsilon) = \epsilon^* - \bar{\mathcal{H}}(\epsilon), \quad (11.6a)$$

$$\bar{\mathcal{H}}(\vec{x}\vec{x}'; \epsilon) = \bar{H}(\vec{x}\vec{x}') + \Sigma^\dagger(\vec{x}'\vec{x}; \epsilon) - \mu, \quad (11.6b)$$

with  $H = T + V$ . As before,  $\bar{\Psi}_s(\epsilon)$  is defined to be a solution to

$$\bar{\mathcal{H}}(\epsilon) \bar{\Psi}_s(\epsilon) = \epsilon_s^*(\epsilon) \bar{\Psi}_s(\epsilon). \quad (11.7)$$

In the bulk, we assume that the self-energy  $\Sigma_0$  has the same periodicity as the lattice, so that Bloch's theorem gives

$$\psi_s(\epsilon) = \psi(\vec{k}n\epsilon), \quad \epsilon_s(\epsilon) = \epsilon(\vec{k}n\epsilon), \quad (11.8)$$

where  $\psi$  is a bulk solution. [We are using  $\epsilon$  to represent the parameter in the Green's function or self-energy and  $\epsilon(\vec{k}n\epsilon)$  to represent the eigenvalue of (11.4a).] Similarly,  $\Sigma$  for the system with an interface is assumed to have the same two-dimensional periodicity as  $H$ , and  $\Psi$  is taken to satisfy the analog of (8.4). The treatment of Secs. V-X can then be repeated with  $G \rightarrow \mathcal{G}$ ,  $L \rightarrow \mathcal{L}$ ,  $H \rightarrow \mathcal{H}$ , and  $V \rightarrow \mathcal{U}$ . (The parameter  $\epsilon$  is regarded as fixed throughout this treatment.) Consequently, the Green's function for a system with an interface is given by

$$\mathcal{G}(\vec{x}\vec{x}'; \epsilon) = \int_{\text{BZ}} d\vec{k} \mathcal{G}(\vec{x}\vec{x}'; \vec{k}\epsilon), \quad (11.9a)$$

$$\mathcal{G}(\vec{x}\vec{x}'; \vec{k}\epsilon) = -2\pi i \sum_{nl} \frac{\Psi(\vec{x}; \vec{k}k_{nl}\epsilon) \bar{\Psi}^\dagger(\vec{x}'; \vec{k}k_{nl}\epsilon)}{v_s(\vec{k}k_{nl}\epsilon)} \times \text{sgn}(x_3 - x'_3), \quad (11.9b)$$

where  $\Psi$  and  $\bar{\Psi}$  in this section are solutions to (11.4a) and (11.7), and

$$v_3(\bar{k}n\epsilon) \equiv \frac{\partial \epsilon(\bar{k}n\epsilon)}{\partial k_3}. \quad (11.10)$$

As before, the  $k_{nl}$  are those  $k_3$  values for which

$$\epsilon(\bar{k}k_{nl}n\epsilon) = \epsilon, \quad (11.11)$$

and are partitioned into two sets, corresponding to  $\text{sgn}(x_3 - x'_3) = +1$  and  $\text{sgn}(x_3 - x'_3) = -1$ . If required by the boundary conditions, a nonsingular part  $g^{\text{NS}}$  is to be added to (11.9), as in (10.7) or (10.9). Equation (11.9) with  $\Psi \rightarrow \psi$  gives the bulk Green's function  $g_0$ .

Correlation functions other than single-particle Green's functions satisfy "effective wave equations" like (11.1),<sup>7</sup> and can consequently be written in forms similar to (11.9).

## XII. NONDIFFERENTIAL EQUATIONS

If  $T_0 = 0$ , the results of Secs. II and IV still hold, but the method of Secs. V and VI for evaluating the Green's function no longer works: since we can take

$$\bar{P}_0[w^\dagger, v] \equiv 0, \quad \text{for all } w \text{ and } v, \quad (12.1a)$$

(5.12) reduces to  $0 = 0$ . Also, (2.1) becomes

$$\int_V d\bar{x} w^\dagger(L_0 v) = \int_V d\bar{x} (\bar{L}_0 w)^\dagger v; \quad (12.1b)$$

i.e., all  $w$  and  $v$  satisfy adjoint boundary conditions. Then (2.10)–(2.12) imply that (6.3) also reduces to  $0 = 0$ . The final result of Sec. V and the theorem of Sec. VI are therefore no longer valid. (As mentioned previously, this will also be the case for  $T_0 \neq 0$  if  $T_0$  contains no derivatives with respect to  $x_3$ , in Sec. V, or with respect to  $x_j$ , in Sec. VI.) We now turn to a method which is more general, in the sense that nondifferential equations can be treated, but also slightly less general, in that there are additional requirements concerning the  $\epsilon(\bar{k}n)$  and the  $\psi(\bar{k}n)$  or  $\Psi(\bar{k}n)$ .

The method involves the analytic properties of  $\epsilon(\bar{k}n)$  and  $\psi(\bar{k}n)$  [or  $\Psi(\bar{k}n)$ ] at complex  $\bar{k}$ .<sup>10-13</sup> In particular, we require the following in evaluating  $G_0$  or  $g_0$ : (i)  $\epsilon(\bar{k}n)$  and  $\psi(\bar{x}; \bar{k}n)\bar{\psi}^\dagger(\bar{x}'; \bar{k}n)$  are analytic functions of  $k_3$  at fixed real  $k_1$  and  $k_2$ , except for branch points off the real axis that they have in common. [Note that  $\psi\bar{\psi}^\dagger$  is independent of the choice of phase for  $\psi$ , in view of the normalization condition (4.32b).] (ii) As  $|\text{Im}k_3| \rightarrow \infty$ , with  $k_1$  and  $k_2$  fixed,

$$|\epsilon(\bar{k}n)| \rightarrow \infty. \quad (12.2a)$$

Also, as  $\text{Im}k_3 \text{sgn}(x_3 - x'_3) \rightarrow \infty$ ,

$$\psi(\bar{x}; \bar{k}n)\bar{\psi}^\dagger(\bar{x}'; \bar{k}n) = u(\bar{x}; \bar{k}n)\bar{u}^\dagger(\bar{x}'; \bar{k}n)e^{i\bar{k} \cdot (\bar{x} - \bar{x}')} e^{ik_3(x_3 - x'_3)}$$

$$< \infty. \quad (12.2b)$$

That is, the expression in (12.2b) either goes to zero or remains bounded. [A slightly less stringent requirement is that this expression divided by  $\epsilon(\bar{k}n)$  goes to zero as  $\text{Im}k_3 \text{sgn}(x_3 - x'_3) \rightarrow \infty$ , with  $\bar{x}$ ,  $\bar{x}'$ ,  $k_1$ ,  $k_2$ , and  $\text{Re}k_3$  fixed, "almost everywhere" in the interval  $-\frac{1}{2} < \text{Re}k_3 \leq \frac{1}{2}$ .] (iii) The product  $\psi\bar{\psi}^\dagger$  is periodic in reciprocal space:

$$\begin{aligned} \psi(\bar{x}; \bar{k}, k_3 + m_3, n)\bar{\psi}^\dagger(\bar{x}'; \bar{k}, k_3 + m_3, n) \\ = \psi(\bar{x}; \bar{k}n)\bar{\psi}^\dagger(\bar{x}'; \bar{k}n). \end{aligned} \quad (12.3)$$

For the evaluation of  $G$  or  $g$ ,  $\psi \rightarrow \Psi$  in the above requirements.

## XIII. PROPERTIES OF $\epsilon(\bar{k}n)$ AND $\psi(\bar{k}n)$

In this section I show that the requirements of Sec. XII are satisfied in the bulk (except in the "pathological" cases defined below) if  $H_0(\bar{k})$  is an analytic function of  $k_3$  for fixed  $k_1$  and  $k_2$ . {We are now regarding  $H_0(\bar{k})$  as a matrix, with elements  $[H_0(\bar{k})]_{ij}$ , evaluated in some representation; the preceding statement means that each matrix element is an analytic function of  $k_3$ .} Exceptional phenomena involving nonanalytic  $H_0(\bar{k})$ —such as the Kohn anomalies in the phonon frequencies of a metal<sup>10</sup>—will have to be treated separately.

I begin by extending the arguments of Krieger<sup>12</sup> to a general operator  $H_0$  which need not be local or formally self-adjoint. In this more general case, Krieger's Eqs. (1), (2), (5)–(7), (10) (after an obvious correction), and (13)–(17) still hold. Repeating the treatment with  $H_0 \rightarrow \bar{H}_0$  yields (19), and (20) is the same as my (4.32a). Then (21)–(24) follow as before, so we have the result that  $\epsilon(\bar{k}n)$  and  $\psi(\bar{x}; \bar{k}n)\bar{\psi}^\dagger(\bar{x}'; \bar{k}n)$  are analytic functions of  $k_3$  except for branch points that they have in common. If  $H_0$  is formally self-adjoint, Krieger's (11) holds; i.e., there can be no branch-point singularities on the real axis. In the case of an operator which is not formally self-adjoint, we regard such singularities as "pathological."

It is easy to see that Krieger's  $\bar{U}$  is the same as our  $\bar{u}^\dagger$  when  $\bar{H}_0 = H_0$ : write

$$u(\bar{k}n) = f(\bar{k}n) + ig(\bar{k}n), \quad (13.1a)$$

with  $f$  and  $g$  real for  $\bar{k}$  real. Then

$$\bar{u}^\dagger(\bar{k}n) = f^\dagger(\bar{k}^*n) - ig^\dagger(\bar{k}^*n) \quad (13.1b)$$

by (4.15). Schwarz's reflection principle implies that

$$f^\dagger(\bar{k}^*n) = f^T(\bar{k}n), \quad (13.2a)$$

$$g^\dagger(\bar{k}^*n) = g^T(\bar{k}n), \quad (13.2b)$$

so

$$\bar{u}^\dagger(\bar{k}n) = f^T(\bar{k}n) - ig^T(\bar{k}n). \quad (13.3)$$

Thus  $\bar{u}^\dagger$  is Krieger's analytic continuation of  $u^\dagger$  into the complex plane, and  $\psi(\bar{x}; \bar{k}n)\bar{\psi}^\dagger(\bar{x}'; \bar{k}n)$  is the analytic continuation of  $\psi(\bar{x}; \bar{k}n)\psi^\dagger(\bar{x}'; \bar{k}n)$ .

Now consider requirement (ii) of Sec. XII. We assume that the  $k_3$  dependence of  $e^{i\bar{k}\cdot(\bar{x}'-\bar{x})}$  dominates the  $k_3$  dependence of  $\bar{u}^\dagger(\bar{x}; \bar{k}n)u(\bar{x}'; \bar{k}n)$  for  $x_3' \neq x_3$ , and that  $\bar{u}^\dagger(\bar{x}; \bar{k}n)u(\bar{x}'; \bar{k}n)$  remains bounded for  $x_3' = x_3$ , as  $|\text{Im}k_3| \rightarrow \infty$ . [As mentioned in Sec. XII, it is actually sufficient that  $\bar{u}^\dagger(\bar{x}; \bar{k}n)u(\bar{x}'; \bar{k}n)/\epsilon(\bar{k}n) \rightarrow 0$  for  $x_3' = x_3$ .] If  $V_0$  is local— $V_0(\bar{x}, \bar{x}') = V_0(\bar{x})\delta(\bar{x} - \bar{x}')$ —we make two further assumptions: (i)  $T_0$  contains at least one derivative with respect to  $x_3$  and (ii) if  $\partial^n/\partial x_3^n$  is the highest derivative with respect to  $x_3$  in  $T_0$ , then  $k_3^n$  dominates the factor multiplying it in

$$\bar{u}^\dagger(\bar{x}; \bar{k}n)e^{-i\bar{k}\cdot\bar{x}}T_0e^{i\bar{k}\cdot\bar{x}'}u(\bar{x}; \bar{k}n)$$

as  $|\text{Im}k_3| \rightarrow \infty$ . We regard cases for which these assumptions are not satisfied, i.e., cases in which the dominant  $k_3$  dependence arises from  $\bar{u}^\dagger(\bar{x}; \bar{k}n)u(\bar{x}'; \bar{k}n)$  rather than  $e^{i\bar{k}\cdot(\bar{x}'-\bar{x})}$ , as "pathological."

Equation (12.2b) follows immediately from the first assumption of the preceding paragraph. To get (12.2a), note that (4.6b) and (4.32a) give

$$\begin{aligned} \epsilon(\bar{k}n) &= \int_{\nu} d\bar{x} \bar{u}^\dagger(\bar{x}; \bar{k}n)e^{-i\bar{k}\cdot\bar{x}}T_0e^{i\bar{k}\cdot\bar{x}'}u(\bar{x}; \bar{k}n) \\ &+ \int_{\nu} d\bar{x} \int_{\nu} d\bar{x}' \bar{u}^\dagger(\bar{x}; \bar{k}n)e^{-i\bar{k}\cdot\bar{x}} \\ &\quad \times V_0(\bar{x}, \bar{x}')e^{i\bar{k}\cdot\bar{x}'}u(\bar{x}'; \bar{k}n). \end{aligned} \quad (13.4)$$

If  $V_0$  is nonlocal, the dominant  $k_3$  dependence comes from  $e^{i\bar{k}\cdot(\bar{x}'-\bar{x})}$  in the second term. If  $V_0$  is local, the dominant  $k_3$  dependence comes from  $k_3^n$  in the first term. In either case, we have (12.2a).

Suppose that the  $k_3$  dependence arising from  $\bar{u}^\dagger$  and  $u$  in (13.4) can be disregarded as  $|\text{Im}k_3| \rightarrow \infty$ . Also suppose that  $V_0(\bar{x}, \bar{x}')$  is nonzero only for  $|x_3 - x_3'| \leq x_0$ . Then as  $|\text{Im}k_3| \rightarrow \infty$ ,

$$\epsilon(\bar{k}n) \propto e^{2\pi x_0 |\text{Im}k_3|}, \quad V_0 \text{ nonlocal}, \quad (13.5)$$

$$\epsilon(\bar{k}n) \propto k_3^n, \quad V_0 \text{ local}. \quad (13.6)$$

We expect (13.5) to be typical for phonons or electrons in a localized representation (in models where the force constants or overlap integrals are truncated), and (13.6) with  $n=2$  to be typical for electrons satisfying the Schrödinger equation (in models where the potential is local).

Finally, we turn to requirement (iii) of Sec. XII. In view of (4.4b),  $u(\bar{x})$  can be expanded in a Fourier series:

$$u(\bar{x}; \bar{k}n) = \sum_{\bar{K}} e^{i\bar{K}\cdot\bar{x}}u(\bar{K}; \bar{k}n). \quad (13.7)$$

Then (4.6) becomes

$$\sum_{\bar{K}'} H_0(\bar{K}\bar{K}'; \bar{k}) \cdot u(\bar{K}'; \bar{k}n) = \epsilon(\bar{k}n)u(\bar{K}; \bar{k}n), \quad (13.8)$$

with

$$\begin{aligned} H_0(\bar{K}\bar{K}'; \bar{k}) &\equiv \frac{1}{\nu} \int_{\nu} d\bar{x} \int_{\nu} d\bar{x}' e^{-i(\bar{k}+\bar{K})\cdot\bar{x}} \\ &\quad \times H_0(\bar{x}, \bar{x}')e^{i(\bar{k}+\bar{K}')\cdot\bar{x}'}. \end{aligned} \quad (13.9)$$

Since

$$H_0(\bar{K} - \bar{K}_0, \bar{K}' - \bar{K}_0, \bar{k} + \bar{K}_0) = H_0(\bar{K}\bar{K}'; \bar{k}), \quad (13.10)$$

$u(\bar{K} - \bar{K}_0; \bar{k} + \bar{K}_0, n)$  satisfies the same equation as  $u(\bar{K}; \bar{k}n)$ . Then we can take

$$\epsilon(\bar{k} + \bar{K}, n) = \epsilon(\bar{k}n), \quad (13.11)$$

$$u(\bar{K} - \bar{K}_0; \bar{k} + \bar{K}_0, n) = Au(\bar{K}; \bar{k}n), \quad (13.12)$$

where  $A$  is a constant. Equations (13.7) and (13.12) give

$$u(\bar{x}; \bar{k} + \bar{K}, n) = A_{\bar{K}}(\bar{k}n)e^{-i\bar{k}\cdot\bar{x}}u(\bar{x}; \bar{k}n) \quad (13.13)$$

or

$$\psi(\bar{x}; \bar{k} + \bar{K}, n) = A_{\bar{K}}(\bar{k}n)\psi(\bar{x}; \bar{k}n). \quad (13.14a)$$

Similarly,

$$\bar{\psi}(\bar{x}; \bar{k} + \bar{K}, n) = \bar{A}_{\bar{K}}(\bar{k}n)\bar{\psi}(\bar{x}; \bar{k}n). \quad (13.14b)$$

The normalization condition (4.32b) then yields

$$\bar{A}_{\bar{K}}(\bar{k}n)A_{\bar{K}}(\bar{k}n) = 1, \quad (13.15)$$

so

$$\begin{aligned} \psi(\bar{x}; \bar{k} + \bar{K}, n)\bar{\psi}^\dagger(\bar{x}'; \bar{k} + \bar{K}, n) &= \psi(\bar{x}; \bar{k}n)\bar{\psi}^\dagger(\bar{x}'; \bar{k}n). \\ & \quad (13.16) \end{aligned}$$

One expects that  $\Psi(\bar{x}; \bar{k}n)\bar{\Psi}^\dagger(\bar{x}'; \bar{k}n)$  will ordinarily have the same properties as  $\psi(\bar{x}; \bar{k}n)\bar{\psi}^\dagger(\bar{x}'; \bar{k}n)$  as a function of  $\bar{k}$ . One can investigate the behavior of  $\Psi$  for a given perturbation  $H - H_0$  by making use of the Lippmann-Schwinger equation.<sup>14</sup>

#### XIV. EVALUATION OF GREEN'S FUNCTION

In this section I treat only  $G_0$  explicitly, but the procedure and final result are valid for  $\mathfrak{G}_0$  as well if  $\Sigma_0(\bar{k})$  is an analytic function of  $k_3$ . (The arguments of the preceding section still apply if  $H_0 \rightarrow H_0 + \Sigma_0 - \mu$ .) My final result also holds for  $G$  and  $\mathfrak{G}$ , with  $\psi \rightarrow \Psi$ , provided that  $\Psi(\bar{k}n)$  meets the requirements of Sec. XII.

It is assumed that the eigenfunctions of  $H_0$  or  $H_0 + \Sigma_0 - \mu$  (or  $H$  or  $H + \Sigma - \mu$ ) for real  $\bar{k}$  comprise a complete set:

$$\frac{1}{N} \sum_{\bar{k}n} \psi(\bar{x}; \bar{k}n)\bar{\psi}^\dagger(\bar{x}'; \bar{k}n) = \delta(\bar{x} - \bar{x}'), \quad (14.1)$$

with  $\bar{k}$  ranging over the first Brillouin zone. The



factor of  $1/N$  results from our normalization convention (4.32). Equation (5.1) will then be satisfied by

$$G_0(\bar{x}\bar{x}'; \epsilon) = \frac{1}{N} \sum_{\bar{k}n} \frac{\psi(\bar{x}; \bar{k}n) \bar{\psi}^\dagger(\bar{x}'; \bar{k}n)}{\epsilon - \epsilon(\bar{k}n)}. \quad (14.2)$$

Letting the values of  $\bar{k}$  become continuous (so that  $N^{-1} \sum_{\bar{k}n} \rightarrow \int_{\text{BZ}} d\bar{k} \int_{-1/2}^{1/2} dk_3$ ), we have

$$G_0^*(\bar{x}\bar{x}'; \epsilon) = \int_{\text{BZ}} d\bar{k} G_0^*(\bar{x}\bar{x}'; \bar{k}\epsilon), \quad (14.3a)$$

$$G_0^*(\bar{x}\bar{x}'; \bar{k}\epsilon) \equiv \sum_n G_0^*(\bar{x}\bar{x}'; \bar{k}n\epsilon), \quad (14.3b)$$

$$G_0^*(\bar{x}\bar{x}'; \bar{k}n\epsilon) \equiv \int_{-1/2}^{1/2} dk_3 \frac{\psi(\bar{x}; \bar{k}n) \bar{\psi}^\dagger(\bar{x}'; \bar{k}n)}{\epsilon - \epsilon(\bar{k}n) + i\delta}, \quad (14.3c)$$

where we are now temporarily restricting the treatment to the retarded Green's function  $G_0^*$ ; the general case will be considered at the end of this section.

We evaluate the integral of (14.3c) by using the contour  $C$  shown in Fig. 1(a) of Ref. 1, for  $\text{sgn}(x_3 - x'_3) = +1$ , or in Fig. 1(b), for  $\text{sgn}(x_3 - x'_3) = -1$ . [Translate the notation of Ref. 1 by letting  $k_2 \rightarrow k_3$  and  $\pi/a \rightarrow \frac{1}{2}$ . Also note that one is free to choose  $\text{sgn}(0) = +1$  or  $-1$ .] Let

$$\begin{aligned} G_{\text{BC}}(\bar{x}\bar{x}'; \bar{k}n\epsilon) \\ \equiv -\text{sgn}(x_3 - x'_3) \int_C dk_3 \frac{\psi(\bar{x}; \bar{k}k_3n) \bar{\psi}^\dagger(\bar{x}'; \bar{k}k_3n)}{\epsilon - \epsilon(\bar{k}k_3n)}, \end{aligned} \quad (14.4)$$

where  $C'$  consists of curves around the branch points of  $\epsilon(k_3)$  and  $\psi(k_3)\bar{\psi}^\dagger(k_3)$ , as indicated in Fig. 1 of Ref. 1. Then

$$\begin{aligned} G_0^* = G_{\text{BC}} + G_V + G_\infty + \text{sum of residues at poles} \\ \times 2\pi i \text{sgn}(x_3 - x'_3), \end{aligned} \quad (14.5)$$

where  $G_V$  and  $G_\infty$  are defined by (14.4), with  $C'$  replaced by the vertical segments of  $C$  or the horizontal segment at infinity.

Equations (12.2) and (12.3), respectively, imply that  $G_\infty = 0$  and  $G_V = 0$ . By analogy with (3.4) of Ref. 1, there is a residue

$$-\psi(\bar{x}; \bar{k}k_{n1}n) \bar{\psi}^\dagger(\bar{x}'; \bar{k}k_{n1}n) / v_3(\bar{k}, k_{n1} + \delta k_{n1}, n) \quad (14.6)$$

at each pole  $k_{n1} + \delta k_{n1}$ , where  $\epsilon(k_{n1} + \delta k_{n1}) = \epsilon + i\delta$ . Application of the argument involving (3.6)–(3.8) of Ref. 1 then gives

$$\begin{aligned} G_0^*(\bar{x}\bar{x}'; \bar{k}n\epsilon) = -2\pi i \sum_t \frac{\psi(\bar{x}; \bar{k}k_{n1}n) \bar{\psi}^\dagger(\bar{x}'; \bar{k}k_{n1}n)}{v_3(\bar{k}k_{n1}n)} \\ \times \text{sgn}(x_3 - x'_3) + G_{\text{BC}}(\bar{x}\bar{x}'; \bar{k}n\epsilon), \end{aligned} \quad (14.7)$$

where the  $k_{n1}$  are those values of  $k_3$  satisfying

$$\epsilon(\bar{k}k_{n1}n) = \epsilon \quad (14.8)$$

for which

$$\text{Re} v_3(\bar{k}k_{n1}n) \text{sgn}(x_3 - x'_3) > 0, \quad k_{n1} \text{ real}, \quad (14.9a)$$

$$\text{Im} k_{n1} \text{sgn}(x_3 - x'_3) > 0, \quad k_{n1} \text{ complex}. \quad (14.9b)$$

Consider a branch point of order 1 (in the terminology of Ref. 10) connecting the  $n$ th and  $(n+1)$ th Riemann sheets, as depicted in Fig. 1 of Ref. 1. The values of

$$\psi(k_3)\bar{\psi}^\dagger(k_3) / [\epsilon - \epsilon(k_3)]$$

on the right-hand, downward side of  $C'$  for the  $n$ th sheet are the same as those for the left-hand, upward side of  $C'$  for the  $(n+1)$ th sheet, and vice versa. [If the order of the branch point is greater than 1, then more than two sheets have to be brought into the argument, but the conclusion (14.10) is unchanged.] The same is true for a branch point connecting the  $n$ th and  $(n-1)$ th sheets. Therefore

$$\sum_n G_{\text{BC}}(\bar{x}\bar{x}'; \bar{k}n\epsilon) = 0, \quad (14.10)$$

so (14.3b) and (14.7) give

$$\begin{aligned} G_0^*(\bar{x}\bar{x}'; \bar{k}\epsilon) = -2\pi i \sum_{n1} \frac{\psi(\bar{x}; \bar{k}k_{n1}n) \bar{\psi}^\dagger(\bar{x}'; \bar{k}k_{n1}n)}{v_3(\bar{k}k_{n1}n)} \\ \times \text{sgn}(x_3 - x'_3). \end{aligned} \quad (14.11)$$

The general Green's function  $G_0(\bar{x}\bar{x}'; \bar{k}\epsilon)$  is obtained by simply adding a general nonsingular part:

$$\begin{aligned} G_0(\bar{x}\bar{x}'; \bar{k}\epsilon) = -2\pi i \sum_{n1} \frac{\psi(\bar{x}; \bar{k}k_{n1}n) \bar{\psi}^\dagger(\bar{x}'; \bar{k}k_{n1}n)}{v_3(\bar{k}k_{n1}n)} \\ \times \text{sgn}(x_3 - x'_3) + G_0^{\text{NS}}(\bar{x}\bar{x}'; \bar{k}\epsilon). \end{aligned} \quad (14.12)$$

This is identical in form to (7.10). There is one apparent difference, in that the  $k_{n1}$  of the present section have been partitioned in a particular way according to (14.9). One can alter the constants  $\alpha$  in (7.9c), however, so as to go from the original partitioning of the  $k_{n1}$  to any other partitioning. That is, if we want to remove  $k_3$  from the set of  $k_{n1}^+$  and place it among the set of  $k_{n1}^-$ , we just let

$$\alpha(\bar{x}'; \bar{k}k_3n) - \alpha(\bar{x}; \bar{k}k_3n) \pm 2\pi i \bar{\psi}^\dagger(\bar{x}'; \bar{k}k_3n) / v_3(\bar{k}k_3n). \quad (14.13)$$

The present result and the result of Sec. VII are thus completely equivalent.

## XV. SUMMARY

The main result of this paper is a simple expression<sup>15</sup>:

$$G^S(\vec{x}\vec{x}'; \vec{k}\epsilon) = -2\pi i \sum_{n\Gamma} \frac{\Psi(\vec{x}; \vec{k}k_{n\Gamma}) \bar{\Psi}^*(\vec{x}'; \vec{k}k_{n\Gamma})}{v_3(\vec{k}k_{n\Gamma})} \times \text{sgn}(x_3 - x'_3), \quad (15.1)$$

where  $\vec{k} = (k_1, k_2)$  and

$$v_3(\vec{k}n) \equiv \frac{\partial \epsilon(\vec{k}n)}{\partial k_3}. \quad (15.2)$$

This is the contribution from one planar wave vector  $\vec{k}$  to the singular part of the Green's function  $G(\vec{x}\vec{x}'; \epsilon)$  that goes with the eigenvalue equation

$$H\Psi(\vec{k}n) = \epsilon(\vec{k}n)\Psi(\vec{k}n). \quad (15.3a)$$

The adjoint problem is

$$\bar{H}\bar{\Psi}(\vec{k}n) = \epsilon^*(\vec{k}n)\bar{\Psi}(\vec{k}n). \quad (15.3b)$$

If  $H$  is formally self-adjoint, i.e., if  $\bar{H} = H$ , then

$$\bar{\Psi}(\vec{k}n) = \Psi(\vec{k}^*n). \quad (15.4)$$

The  $k_{n\Gamma}$  are those values of  $k_3$  for which

$$\epsilon(\vec{k}k_{n\Gamma}) = \epsilon. \quad (15.5)$$

They are arbitrarily partitioned into two sets  $k_{n\Gamma}^+$  and  $k_{n\Gamma}^-$  (with no overlap between the sets); it is understood that the sum of (15.1) is over the  $k_{n\Gamma}^+$  if  $\text{sgn}(x_3 - x'_3) = +1$ , and the  $k_{n\Gamma}^-$  if  $\text{sgn}(x_3 - x'_3) = -1$ .

Written more completely and explicitly, my result for the Green's function is

$$G(\vec{x}\vec{x}'; \epsilon) = \int_{BZ} d\vec{k} G(\vec{x}\vec{x}'; \vec{k}\epsilon), \quad (15.6a)$$

$$G(\vec{x}\vec{x}'; \vec{k}\epsilon) = -2\pi i \left( \sum_{n\Gamma} \frac{\Psi(\vec{x}; \vec{k}k_{n\Gamma}^+) \bar{\Psi}^*(\vec{x}'; \vec{k}k_{n\Gamma}^+)}{v_3(\vec{k}k_{n\Gamma}^+)} \theta(x_3 - x'_3) - \sum_{n\Gamma} \frac{\Psi(\vec{x}; \vec{k}k_{n\Gamma}^-) \bar{\Psi}^*(\vec{x}'; \vec{k}k_{n\Gamma}^-)}{v_3(\vec{k}k_{n\Gamma}^-)} \theta(x'_3 - x_3) \right) + \sum_{n\Gamma} [\alpha(\vec{x}'; \vec{k}k_{n\Gamma}^+) \Psi(\vec{x}; \vec{k}k_{n\Gamma}^+) + \alpha(\vec{x}; \vec{k}k_{n\Gamma}^-) \Psi(\vec{x}'; \vec{k}k_{n\Gamma}^-)]. \quad (15.6b)$$

The integral of (15.6a) is over the first two-dimensional Brillouin zone. The values of the coefficients  $\alpha(\vec{x}'; \vec{k}k_{n\Gamma}^+)$  are determined by the boundary conditions (or dispersion relation<sup>7</sup>) imposed on  $G(\vec{x}\vec{x}'; \epsilon)$  at fixed  $\vec{x}'$  and  $\epsilon$ . With the right choice for the partitioning of the  $k_{n\Gamma}$  into  $k_{n\Gamma}^+$  and  $k_{n\Gamma}^-$ , one can frequently eliminate the last, nonsingular term in (15.6b). For example, the "retarded" Green's function  $G^*$  is given by (15.6) without the last term when we choose

$$\text{Im}k_{n\Gamma}^+ \geq 0, \quad k_{n\Gamma}^+ \text{ complex}, \quad (15.7a)$$

$$\text{Re}v_3(\vec{k}k_{n\Gamma}^+) \geq 0, \quad k_{n\Gamma}^+ \text{ real}. \quad (15.7b)$$

The exact Green's function  $\mathcal{G}(\vec{x}\vec{x}'; \epsilon)$  is given by (15.6) with  $\Psi(\vec{x}; \vec{k}n) \rightarrow \Psi(\vec{x}; \vec{k}n\epsilon)$ , etc., where

$$[H + \Sigma(\epsilon) - \mu]\Psi(\vec{k}n\epsilon) = \epsilon(\vec{k}n\epsilon)\Psi(\vec{k}n\epsilon), \quad (15.8a)$$

$$[\bar{H} + \bar{\Sigma}(\epsilon) - \mu]\bar{\Psi}(\vec{k}n\epsilon) = \epsilon^*(\vec{k}n\epsilon)\bar{\Psi}(\vec{k}n\epsilon), \quad (15.8b)$$

$$v_3(\vec{k}n\epsilon) \equiv \frac{\partial \epsilon(\vec{k}n\epsilon)}{\partial k_3}. \quad (15.8c)$$

$G$  and  $\mathcal{G}$  are the Green's functions for a system with an interface. (There are actually two Green's functions  $G^<$  and  $G^>$ , corresponding to the two media on opposite sides of the interface.) The bulk Green's functions  $G_0$  and  $\mathcal{G}_0$  are given by (15.6) with  $\Psi \rightarrow \psi$ , where  $\psi$  is a solution to (15.3)

with  $H \rightarrow H_0$  (or  $H_0 + \Sigma_0 - \mu$ ).

As we have seen, two independent approaches lead to the same expression (15.6). The first approach, valid for partial differential eigenvalue equations, requires that  $\epsilon(k_3)$  be differentiable and  $\psi(k_3)$  continuous at  $k_3 = k_{n\Gamma}$ . The second approach, valid for more general eigenvalue equations, requires that  $\epsilon(k_3)$  and  $\psi(k_3)$  be analytic functions of  $k_3$  everywhere except at branch points. As we showed, in extending the results of Ref. 12, this will be the case if  $H_0(\vec{k})$  is an analytic function of  $k_3$ .

This paper was concerned exclusively with time-independent Green's functions. To get from our result for, e.g.,  $G(\vec{x}\vec{x}'; \epsilon(\omega))$  to the result for the time-dependent Green's function  $G(\vec{x}\vec{x}'; t - t')$ , one would have to perform an inverse Fourier transform with respect to the frequency  $\omega$ . [Ordinarily,  $\epsilon(\omega) = \omega$  or  $\omega^2$ .] Similarly, to get the temperature Green's function  $G(\vec{x}\vec{x}'; \tau)$ , one would have to evaluate a Fourier series involving  $G(\vec{x}\vec{x}'; \epsilon(i\omega_n))$ ,  $\omega_n = n\pi/\beta\hbar$ .<sup>8</sup> In application, however, it is usually more convenient just to work directly with  $G(\epsilon(\omega))$  or  $G(\epsilon(i\omega_n))$ .

Our closed-form expression for  $G(\epsilon)$ —i.e., Eq. (15.6)—should prove useful in both numerical calculations for particular systems<sup>16</sup> and analytical studies of the general properties of interfaces.<sup>1, 17</sup>

- <sup>1</sup>R. E. Allen, Phys. Rev. B 19, 917 (1979).
- <sup>2</sup>P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), Chap. 7.
- <sup>3</sup>B. Friedman, *Principles and Techniques of Applied Mathematics* (Wiley, New York, 1956), Chap. 3.
- <sup>4</sup>J. T. Cushing, *Applied Analytical Mathematics for Physical Scientists* (Wiley, New York, 1975), Chap. 8.
- <sup>5</sup>(a) C. Kittel, *Quantum Theory of Solids* (Wiley, New York, 1963), pp. 193-4; (b) R. A. Smith, *Wave Mechanics of Crystalline Solids* (Chapman and Hall, London, 1961), pp. 122-124.
- <sup>6</sup>P. J. Feibelman, Phys. Rev. B 13, 4403 (1976).
- <sup>7</sup>V. L. Bonch-Bruевич and S. V. Tyablikov, *The Green Function Method in Statistical Mechanics* (North-Holland, Amsterdam, 1962), Sec. 9.
- <sup>8</sup>A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971).
- <sup>9</sup>A. J. Layzer, Phys. Rev. 129, 897 (1963).
- <sup>10</sup>W. Kohn, Phys. Rev. 115, 809 (1959); Phys. Rev. B 7, 2285 (1973).
- <sup>11</sup>E. I. Blount, Solid State Phys. 13, 305 (1962), see Appendix C.
- <sup>12</sup>J. B. Krieger, Phys. Rev. 156, 776 (1967).
- <sup>13</sup>J. E. Avron and B. Simon, Ann. Phys. (N.Y.) 110, 85 (1978).
- <sup>14</sup>P. J. Feibelman, Phys. Rev. B 12, 806 (1975).
- <sup>15</sup>This expression was previously presented in a talk: R. E. Allen, Bull. Am. Phys. Soc. 23, 258 (1978).
- <sup>16</sup>J. Pollmann and S. T. Pantelides, Phys. Rev. B 18, 5524 (1978).
- <sup>17</sup>D. C. Mattis, Ann. Phys. (N.Y.) 113, 184 (1978).