

## Multiple-scattering theory of low-energy electron diffraction for a nonspherical scattering potential

Seido Nagano and S. Y. Tong

*Laboratory for Surface Studies and Department of Physics, University of Wisconsin—Milwaukee, Milwaukee, Wisconsin 53201*

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We present a multiple-scattering theory of low-energy electron diffraction (LEED) in which the scattering from nonspherical atomic potentials is expressed in terms of full scattering matrices  $t_{LL'}(k)$ . These scattering matrices  $t_{LL'}(k)$  are evaluated through numerical integration and solving coupled equations. The method of Sams and Kourie is used. We also present formulas for the rotation and the temperature correction of  $t_{LL'}(k)$ . The atomic scattering  $t_{LL'}(k)$  are then incorporated into standard multiple-scattering theories of LEED, and the method becomes suitable for calculating intensity-energy spectra of semiconductor surfaces and some open faces of metals.

### I. INTRODUCTION

The multiple-scattering theory of low-energy electron diffraction (LEED) has been used to determine the surface structure of many clean and adsorbate-covered metal and semiconductor surfaces.<sup>1-5</sup> However, existing theories of LEED all use the so-called muffin-tin approximation for individual scattering potentials. In the muffin-tin approximation, the potential inside a radial distance  $R_{MT}$  from the nucleus of an atom is spherically symmetrized, and the potential in the interstitial region between atomic spheres is assumed to be flat. While the muffin-tin approximation works well at LEED energies for many metal and semiconductor surfaces, we nevertheless expect that its use could produce large errors on some open faces of metals and on some semiconductor surfaces. To assess the applicability of the muffin-tin approximation and to improve the accuracy of LEED theory, it is important to formulate a multiple scattering theory of LEED that incorporates nonspherical individual scattering potentials.

In this paper, we present such a multiple-scattering theory of LEED. We first divide a crystal into layers of periodic arrays of unit cells. Each unit cell may contain one or more nonspherical individual potentials. We assume that the electron scattering from a nonspherical individual potential can be expressed by a finite-dimensional nondiagonal  $t$  matrix  $t_{LL'}(k)$ , where  $L=(l,m)$  and  $L'=(l',m')$ , and  $k=[(2m/\hbar^2)E]^{1/2}$ . In the muffin-tin approximation,  $t_{LL'}(k)$  simplifies to a diagonal matrix  $t_l$  dependent only on  $l$ . Thus, given a nonspherical potential for example, from an all-electron full-potential linearized augmented-plane-wave (FLAPW) calculation,<sup>6,7</sup> we would expand it in angular-momentum space and solve for  $t_{LL'}(k)$ . Since a self-consistent FLAPW calculation is rather time consuming, and since a nonspherical potential is calculated relative to a given orientation, it would be useful to be able to transform a  $t_{LL'}(k)$  calculated relative to one orientation into that of another (e.g., from a [100] orientation to a [111] orientation). In Sec. II we present the steps leading to the evaluation of  $t_{LL'}(k)$  of individual nonspherical potentials. The transformation of  $t_{LL'}(k)$  under rotation and inversion

operations is presented in Sec. III. Temperature corrections for nonspherical potentials are presented in Sec. IV. In Sec. V the individual  $t_{LL'}(k)$  are incorporated into the multiple-scattering slab method of LEED.<sup>8-10</sup> Just as in a conventional LEED calculation with spherical potentials, the present theory does not itself produce the potentials for the surface and deeper layer atoms. These have to be generated independently from (self-consistent) full-potential calculations. Also, a straight refraction condition is assumed for the electron at the vacuum-solid interface,<sup>8</sup> with image-potential effects neglected. Image-potential scattering effects are important only at very low energies (e.g.,  $E \leq 10$  eV).<sup>11</sup>

### II. SCATTERING BY INDIVIDUAL NONSPHERICAL POTENTIAL

Starting with an individual nonspherical scattering potential

$$V(\mathbf{r}) = \sum_L V_L(r) Y_L(\hat{\mathbf{r}}), \quad (2.1)$$

we can write the Lippmann-Schwinger equation as follows:

$$\psi(\mathbf{r}) = \phi(\mathbf{r}) + \int G_0(\mathbf{r}-\mathbf{r}_1) V(\mathbf{r}_1) \psi(\mathbf{r}_1) d\mathbf{r}_1. \quad (2.2)$$

Here  $\phi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}$  is an incident wave,  $\mathbf{k}$  a wave vector,  $G_0(\mathbf{r}-\mathbf{r}_1)$  a single-particle Green's function, and  $\psi(\mathbf{r})$  the total wave function. The  $t$  matrix is defined by

$$\int t(\mathbf{r}_1, \mathbf{r}_2) \phi(\mathbf{r}_2) d\mathbf{r}_2 = V(\mathbf{r}_1) \psi(\mathbf{r}_1). \quad (2.3)$$

We can rewrite Eq. (2.2) using the angular-momentum representation. By substituting into it the following expressions:

$$\phi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_L 4\pi i^l j_l(kr) Y_L(\hat{\mathbf{r}}) Y_L^*(\hat{\mathbf{k}}), \quad (2.4)$$

$$\psi(\mathbf{r}) = \sum_{L,L'} 4\pi i^L F_{LL'}(r) Y_L(\hat{\mathbf{r}}) Y_{L'}^*(\hat{\mathbf{k}}), \quad (2.5)$$

and using the orthogonality of spherical harmonics, namely,

$$G_0(\mathbf{r}-\mathbf{r}_1) = -\frac{2mik}{\hbar^2} \sum_L j_L(kr_<) h_L^{(1)}(kr_>) Y_L(\hat{\mathbf{r}}) Y_L^*(\hat{\mathbf{r}}_1), \quad \int Y_L(\hat{\mathbf{r}}) Y_{L'}^*(\hat{\mathbf{r}}) d\Omega_r = \delta_{LL'}, \quad (2.7)$$

(2.6) we obtain

$$F_{LL'}(r) = j_L(kr) \delta_{LL'} - \frac{2mik}{\hbar^2} \sum_{L_2, L_3} C_{L_2 L_3}^L \int_0^\infty (r')^2 dr' j_L(kr_<) h_L^{(1)}(kr_>) V_{L_2}^{L'}(r') F_{L_3 L}(r'). \quad (2.8)$$

The Gaunt's number  $C_{L_2 L_3}^L$  is defined by

$$C_{L_2 L_3}^L = \int d\Omega_r Y_{L_2}^*(\hat{\mathbf{r}}) Y_{L_3}(\hat{\mathbf{r}}) Y_L(\hat{\mathbf{r}}). \quad (2.9)$$

Here  $Y_L(\hat{\mathbf{r}})$ ,  $Y_L(\hat{\mathbf{k}})$  are spherical harmonics,  $j_L(kr)$ ,  $h_L^{(1)}(kr)$  are spherical Bessel and Hankel functions of the first kind, respectively, and  $r_> = \max(r, r')$ ,  $r_< = \min(r, r')$ ,  $|\mathbf{k}| = k$ ,  $m$  is the electron mass, and  $\hbar$  is Planck's constant.

In order to simplify Eq. (2.8), let us introduce a matrix:

$$U_{LL_3}(r) = -\frac{2mik}{\hbar^2} \sum_{L_2} C_{L_2 L_3}^L r^2 V_{L_2}^L(r). \quad (2.10)$$

Then, we can write Eq. (2.8) as

$$F_{LL'}(r) = j_L(kr) \delta_{LL'} + \sum_{L_3} \int_0^\infty dr' j_L(kr_<) h_L^{(1)}(kr_>) U_{LL_3}(r') F_{L_3 L}(r'). \quad (2.11)$$

The integral in Eq. (2.11) contains both  $r_>$  and  $r_<$  and would be very difficult to treat numerically. It can be simplified by the following scheme. First, we rewrite Eq. (2.11) as follows:

$$F_{LL'}(r) = j_L(kr) \left[ \delta_{LL'} + \int_0^\infty dr' h_L^{(1)}(kr') [\tilde{U}(r') \cdot \tilde{F}(r')]_{LL'} \right] + \int_0^r dr' [j_L(kr') h_L^{(1)}(kr) - j_L(kr) h_L^{(1)}(kr')] [\tilde{U}(r') \cdot \tilde{F}(r')]_{LL'}. \quad (2.12)$$

or

$$\tilde{F}(r) = \tilde{J}(kr) \cdot \left[ \tilde{I} + \int_0^\infty dr' \tilde{H}(kr') \cdot \tilde{U}(r') \cdot \tilde{F}(r') \right] + \int_0^r dr' [\tilde{J}(kr') \cdot \tilde{H}(kr) - \tilde{J}(kr) \cdot \tilde{H}(kr')] \cdot \tilde{U}(r') \cdot \tilde{F}(r'), \quad (2.12')$$

where we have used the matrix representation for the quantities involved, and  $J_{LL}(kr) = j_L(kr) \delta_{LL'}$ ,  $H_{LL}(kr) = h_L(kr) \delta_{LL'}$ ,  $I_{LL} = \delta_{LL'}$ . Since there is the freedom to split  $\tilde{F}(r)$  into two parts, we can define a constant matrix  $\tilde{C}$  by

$$\tilde{F}(r) = \tilde{f}(r) \cdot \tilde{C}. \quad (2.13)$$

Substituting Eq. (2.13) into Eq. (2.12'), we have

$$\tilde{f}(r) \cdot \tilde{C} = \tilde{J}(kr) \cdot \left[ \tilde{I} + \int_0^\infty dr' \tilde{H}(kr') \cdot \tilde{U}(r') \cdot \tilde{f}(r') \cdot \tilde{C} \right] + \int_0^r dr' [\tilde{J}(kr') \cdot \tilde{H}(kr) - \tilde{J}(kr) \cdot \tilde{H}(kr')] \cdot \tilde{U}(r') \cdot \tilde{f}(r') \cdot \tilde{C}. \quad (2.14)$$

A judicious choice of  $\tilde{C}$  would eliminate it from Eq. (2.14). Thus if we set

$$\tilde{I} + \int_0^\infty dr' \tilde{H}(kr') \cdot \tilde{U}(r') \cdot \tilde{f}(r') \cdot \tilde{C} = \tilde{C}, \quad (2.15)$$

we obtain

$$\tilde{f}(r) = \tilde{J}(kr) + \int_0^r dr' [\tilde{J}(kr') \cdot \tilde{H}(kr) - \tilde{J}(kr) \cdot \tilde{H}(kr')] \cdot \tilde{U}(r') \cdot \tilde{f}(r'), \quad (2.16)$$

and from Eq. (2.15) we have

$$\tilde{C} = \left[ \tilde{I} - \int_0^\infty dr' \tilde{H}(kr') \cdot \tilde{U}(r') \cdot \tilde{f}(r') \right]^{-1}. \quad (2.17)$$

Equation (2.16) takes the form of coupled integral equations of the Volterra type. Its numerical evaluation, as pointed out by Sams and Kourie,<sup>12</sup> can be done by boot-strapping and is simplified by the fact that  $j_L(kr') h_L(kr) - j_L(kr) h_L(kr') = 0$  at  $r' = r$ .

The  $t$ -matrix expansion in terms of spherical harmonics is given by

$$t(\mathbf{r}_1, \mathbf{r}_2) = \sum_{LL'} t_{LL'}(r_1 r_2) Y_L(\hat{\mathbf{r}}_1) Y_{L'}^*(\hat{\mathbf{r}}_2). \quad (2.18)$$

Substituting Eqs. (2.5) and (2.18) into Eq. (2.3) and using Eq. (2.7), we obtain

$$\int_0^\infty r_2^2 dr_2 t_{LL'}(r_1 r_2) j_{l'}(kr_2) = \sum_{L_2, L_3} C_{L_2 L_3}^L V_{L_2}(r_1) F_{L_3 L'}(r_1). \quad (2.19)$$

The  $t$  matrix as a function of wave vector  $k$  is given by

$$t_{LL'}(k) = i^{-(l-l')} \int_0^\infty r_1^2 dr_1 \int_0^\infty r_2^2 dr_2 j_l(kr_1) t_{LL'}(r_1 r_2) j_{l'}(kr_2). \quad (2.20)$$

For the muffin-tin potential model  $t_{LL'}(k) = t_l(k) \delta_{LL'}$ , and the definition given in Eq. (2.20) agrees with the standard definition of the diagonal  $t$  matrix.<sup>8</sup> Therefore from Eq. (2.19) we obtain

$$t_{LL'}(k) = \frac{\hbar^2}{2m} \frac{i}{k} i^{-(l-l')} \int_0^\infty dr [\tilde{J}(kr) \cdot \tilde{U}(r) \cdot \tilde{F}(r)]_{LL'}. \quad (2.21)$$

The numerical procedure for evaluating  $t_{LL'}(k)$  follows the following sequence: We start with a given nonspherical potential and use Eqs. (2.16), (2.17), and (2.13) to solve for  $\tilde{f}(r)$ ,  $\tilde{C}$ , and  $\tilde{F}(r)$ , respectively. Then  $t_{LL'}(k)$  can be obtained from Eq. (2.21). Although the matrix inversion in Eq. (2.16) is avoided, the number of coupled equations in Eq. (2.16) is  $(l_m+1)^4$ , compared to  $l_m+1$  decoupled equations for the muffin-tin potential case. Here,  $l_m$  is the maximum  $l$  value used in the calculation. With the use of symmetry,  $t_{LL'}(k)$  block-diagonalizes into a number of smaller square matrices, and consequently, the computation time is substantially reduced.

### III. ROTATION AND INVERSION OF $t_{LL'}(k)$

The  $t$  matrix of a nonspherical potential depends on the orientation of the potential. The calculation of self-consistent nonspherical potentials is itself a lengthy numerical problem, and usually it takes more time to generate the potential than to calculate the scattering LEED spectra. Thus it is highly desirable to be able to generate  $t$  matrices of arbitrary orientations from one calculated for a particular orientation. For example, one may want to calculate the  $t_{LL'}(k)$  relative to the [111] direction from that of the [100] direction. This would save the computation time of recalculating a nonspherical  $V(\mathbf{r})$  relative to the [100] direction and going through the steps of Eqs. (2.16), (2.17), and (2.13).

To do this, we need to find a relation between the rotated  $t$  matrix,  $t_{L_1 L_2}$  and the original  $t$  matrix,  $t_{L_1 L_2}$ . We start with the real-space representation of  $t_{L_1 L_2}$ :

$$t(\mathbf{r}_1, \mathbf{r}_2) = V(\mathbf{r}_1) \delta(\mathbf{r}_1 - \mathbf{r}_2) + V(\mathbf{r}_1) G_0(\mathbf{r}_1 - \mathbf{r}_2) V(\mathbf{r}_2) + \int d\mathbf{r}_3 V(\mathbf{r}_1) G_0(\mathbf{r}_1 - \mathbf{r}_3) V(\mathbf{r}_3) G_0(\mathbf{r}_3 - \mathbf{r}_2) V(\mathbf{r}_2) + \dots, \quad (3.1)$$

which can be expressed in a more convenient form:

$$t(\mathbf{r}_1, \mathbf{r}_2) = V(\mathbf{r}_1) [\delta(\mathbf{r}_1 - \mathbf{r}_2) - G_0(\mathbf{r}_1 - \mathbf{r}_2) V(\mathbf{r}_2)]^{-1}. \quad (3.1')$$

Then, from Eq. (2.18), we have

$$\begin{aligned} t_{L_1 L_2}(r_1 r_2) &= \int d\Omega r_1 \int d\Omega r_2 Y_{L_1}^*(\hat{\mathbf{r}}_1) Y_{L_2}(\hat{\mathbf{r}}_2) t(\mathbf{r}_1, \mathbf{r}_2) \\ &= \int d\Omega r_1 \int d\Omega r_2 Y_{L_1}^*(\hat{\mathbf{r}}_1) Y_{L_2}(\hat{\mathbf{r}}_2) V(\mathbf{r}_1) [\delta(\mathbf{r}_1 - \mathbf{r}_2) - G_0(\mathbf{r}_1 - \mathbf{r}_2) V(\mathbf{r}_2)]^{-1}. \end{aligned} \quad (3.2)$$

As an atom is rotated, the new  $t$  matrix becomes

$$t_{L_1 L_2}(r_1 r_2) = \int d\Omega r_1 \int d\Omega r_2 Y_{L_1}^*(\hat{\mathbf{r}}_1) Y_{L_2}(\hat{\mathbf{r}}_2) \hat{R} V(\mathbf{r}_1) [\delta(\mathbf{r}_1 - \mathbf{r}_2) - G_0(\mathbf{r}_1 - \mathbf{r}_2) \hat{R} V(\mathbf{r}_2)]^{-1}, \quad (3.3)$$

where  $\hat{R}$  stands for the rotation operator. However, we know that

$$\hat{R} V(\mathbf{r}) = V(\hat{R}^{-1} \mathbf{r}), \quad (3.4)$$

therefore Eq. (3.3) can be rewritten as

$$t_{L_1 L_2}(r_1 r_2) = \int d\Omega r_1 \int d\Omega r_2 Y_{L_1}^*(\hat{\mathbf{r}}_1) Y_{L_2}(\hat{\mathbf{r}}_2) V(\hat{R}^{-1} \mathbf{r}_1) [\delta(\mathbf{r}_1 - \mathbf{r}_2) - G_0(\mathbf{r}_1 - \mathbf{r}_2) V(\hat{R}^{-1} \mathbf{r}_2)]^{-1}. \quad (3.5)$$

Since  $G_0(\mathbf{r}_1 - \mathbf{r}_2) = G_0(|\mathbf{r}_1 - \mathbf{r}_2|)$  and  $\delta(\mathbf{r}_1 - \mathbf{r}_2) = \delta(|\mathbf{r}_1 - \mathbf{r}_2|)$ , the Green's function and  $\delta$  function are invariant under rotation. Therefore Eq. (3.5) becomes

$$t_{L_1 L_2}(r_1 r_2) = \int d\Omega r_1 \int d\Omega r_2 Y_{L_1}^*(\hat{\mathbf{r}}_1) Y_{L_2}(\hat{\mathbf{r}}_2) V(\hat{R}^{-1} \mathbf{r}_1) [\delta(\hat{R}^{-1} \mathbf{r}_1 - \hat{R}^{-1} \mathbf{r}_2) - G_0(\hat{R}^{-1} \mathbf{r}_1 - \hat{R}^{-1} \mathbf{r}_2) V(\hat{R}^{-1} \mathbf{r}_2)]^{-1}. \quad (3.6)$$

If we change variables  $\mathbf{r}_1, \mathbf{r}_2$  to  $\hat{R} \mathbf{r}_1, \hat{R} \mathbf{r}_2$ , respectively, we obtain

$$t_{L_1 L_2}(r_1 r_2) = \int d\Omega r_1 \int d\Omega r_2 Y_{L_1}^*(\hat{R} \hat{\mathbf{r}}_1) Y_{L_2}(\hat{R} \hat{\mathbf{r}}_2) V(\mathbf{r}_1) [\delta(\mathbf{r}_1 - \mathbf{r}_2) - G_0(\mathbf{r}_1 - \mathbf{r}_2) V(\mathbf{r}_2)]^{-1}, \quad (3.7)$$

where  $\int d\Omega r_1$  and  $\int d\Omega r_2$  are invariant because they cover the whole solid angle. Using Eqs. (3.1') and (2.18) again, we find

$$\begin{aligned} \epsilon_{L_1 L_2}(r_1 r_2) &= \int d\Omega r_1 \int d\Omega r_2 Y_{L_1}^*(\hat{R}\hat{r}_1) Y_{L_2}(\hat{R}\hat{r}_2) t(r_1, r_2) \\ &= \sum_{L'_1, L'_2} t_{L'_1 L'_2}(r_1 r_2) \int d\Omega r_1 Y_{L'_1}^*(\hat{R}\hat{r}_1) Y_{L'_1}(\hat{r}_1) \int d\Omega r_2 Y_{L_2}(\hat{R}\hat{r}_2) Y_{L'_2}^*(\hat{r}_2). \end{aligned} \quad (3.8)$$

But since

$$\begin{aligned} Y_{lm}(\hat{r}) &= \langle \hat{r} | lm \rangle, \\ Y_{lm}^*(\hat{r}) &= \langle lm | \hat{r} \rangle, \end{aligned} \quad (3.9)$$

we can derive the following relations:<sup>13</sup>

$$\begin{aligned} Y_{l_1 m_1}^*(\hat{R}\hat{r}_1) &= \langle l_1 m_1 | \hat{R}\hat{r}_1 \rangle = \sum_{m'} \langle l_1 m_1 | \hat{R} | l_1 m' \rangle \langle l_1 m' | \hat{r}_1 \rangle \\ &= \sum_{m'} D_{m_1 m'}^{l_1}(\alpha\beta\gamma) Y_{l_1 m'}^*(\hat{r}_1), \end{aligned} \quad (3.10)$$

and

$$\begin{aligned} Y_{l_2 m_2}(\hat{R}\hat{r}_2) &= \langle \hat{R}\hat{r}_2 | l_2 m_2 \rangle = \sum_{m''} \langle \hat{r}_2 | l_2 m'' \rangle \langle l_2 m'' | \hat{R}^{-1} | l_2 m_2 \rangle \\ &= \sum_{m''} \langle \hat{r}_2 | l_2 m'' \rangle \langle l_2 m_2 | \hat{R} | l_2 m'' \rangle^* \\ &= \sum_{m''} Y_{l_2 m''}(\hat{r}_2) D_{m_2 m''}^{*l_2}(\alpha\beta\gamma). \end{aligned} \quad (3.11)$$

Here,  $\alpha$ ,  $\beta$ , and  $\gamma$  are the Euler angles which correspond to the rotation operator  $\hat{R}$ , and

$$D_{mm'}^{l_1}(\alpha\beta\gamma) = \langle lm | \hat{R} | lm' \rangle \quad (3.12)$$

is the Wigner's  $D$  function. Then using Eq. (2.7), we obtain

$$\int d\Omega r_1 Y_{L_1}^*(\hat{R}\hat{r}_1) Y_{L'_1}(\hat{r}_1) = \sum_{m'} D_{m_1 m'}^{L_1}(\alpha\beta\gamma) \delta_{l_1 l'} \delta_{m_1 m'}, \quad (3.13)$$

and

$$\int d\Omega r_2 Y_{L_2}(\hat{R}\hat{r}_2) Y_{L'_2}^*(\hat{r}_2) = \sum_{m''} D_{m_2 m''}^{*L_2}(\alpha\beta\gamma) \delta_{l_2 l'_2} \delta_{m_2 m''}. \quad (3.14)$$

Therefore, we can rewrite (3.8) as

$$\epsilon_{L_1 L_2}(r_1 r_2) = \sum_{m', m''} t_{l_1 m' l_2 m''}(r_1 r_2) D_{m_1 m'}^{l_1}(\alpha\beta\gamma) D_{m_2 m''}^{*l_2}(\alpha\beta\gamma) \quad (3.15)$$

or, using Eq. (2.20), we obtain

$$\epsilon_{L_1 L_2}(k) = \sum_{m', m''} t_{l_1 m' l_2 m''}(k) D_{m_1 m'}^{l_1}(\alpha\beta\gamma) D_{m_2 m''}^{*l_2}(\alpha\beta\gamma). \quad (3.16)$$

Equation (3.16) is then the general relationship that connects a rotated  $\epsilon_{L_1 L_2}(k)$  to the original  $t_{L_1 L_2}(k)$ . As a specific example, the inversion of an atomic potential can be found by means of the inversion operator  $\hat{I}$ . Thus we have

$$\epsilon_{L_1 L_2}(r_1 r_2) = \sum_{L'_1 L'_2} t_{L'_1 L'_2}(r_1 r_2) \int d\Omega r_1 Y_{L'_1}^*(\hat{I}r_1) Y_{L'_1}(r_1) \int d\Omega r_2 Y_{L_2}(\hat{I}r_2) Y_{L'_2}(r_2). \quad (3.17)$$

If we use the relations of  $Y_{lm}(\hat{r})$  under inversion, we obtain

$$Y_{L_1}^*(\hat{I}\hat{r}_1) = Y_{L_1}^*(\pi - \theta_1, \phi_1 + \pi) = (-1)^{l_1} Y_{L_1}^*(\theta_1, \phi_1) \quad (3.18)$$

and

$$Y_{L_2}(\hat{I}\hat{r}_2) = Y_{L_2}(\pi - \theta_2, \phi_2 + \pi) = (-1)^{l_2} Y_{L_2}(\theta_2, \phi_2). \quad (3.19)$$

Then we have

$$\epsilon_{L_1 L_2}(r_1 r_2) = (-1)^{l_1 + l_2} t_{L_1 L_2}(r_1 r_2) \quad (3.20)$$

or

$$t_{L_1 L_2}(k) = (-1)^{l_1 + l_2} t_{L_1 L_2}(k). \quad (3.21)$$

These simple relations are useful for a slab of the Si(111) crystal, in which the two atomic potentials within each unit cell are inverted from one another.

#### IV. TEMPERATURE EFFECT ON ELASTIC SCATTERING

Let us introduce the  $t$  matrix in momentum space in order to discuss the temperature effect:

$$t(T, \mathbf{k}', \mathbf{k}) = \int \int e^{-i\mathbf{k}' \cdot \mathbf{r}_1} t(\mathbf{r}_1 - \mathbf{R}, \mathbf{r}_2 - \mathbf{R}) e^{i\mathbf{k} \cdot \mathbf{r}_2} d\mathbf{r}_1 d\mathbf{r}_2, \quad (4.1)$$

where  $\mathbf{R}$  is the position of the nucleus of an atom and  $\mathbf{k}, \mathbf{k}'$  are incident and scattered wave-number vectors, respectively. After a change of variables, Eq. (4.1) becomes

$$t(T, \mathbf{k}', \mathbf{k}) = e^{-i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{R}} \int \int e^{-i\mathbf{k}' \cdot \boldsymbol{\rho}_1} t(\boldsymbol{\rho}_1, \boldsymbol{\rho}_2) e^{i\mathbf{k} \cdot \boldsymbol{\rho}_2} d\boldsymbol{\rho}_1 d\boldsymbol{\rho}_2. \quad (4.2)$$

Writing  $\mathbf{R}$  as a sum of the equilibrium position  $\mathbf{R}_0$  and the thermal displacement  $\Delta\mathbf{R}$ , we have

$$t(T, \mathbf{k}', \mathbf{k}) = e^{-i(\mathbf{k}' - \mathbf{k}) \cdot \Delta\mathbf{R}} t(0, \mathbf{k}', \mathbf{k}), \quad (4.3)$$

where

$$t(0, \mathbf{k}', \mathbf{k}) = e^{-i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{R}_0} \int \int e^{-i\mathbf{k}' \cdot \boldsymbol{\rho}_1} t(\boldsymbol{\rho}_1, \boldsymbol{\rho}_2) e^{i\mathbf{k} \cdot \boldsymbol{\rho}_2} d\boldsymbol{\rho}_1 d\boldsymbol{\rho}_2, \quad (4.4)$$

and it is independent of temperature. Therefore the temperature effect is included in the exponential factor  $e^{-i(\mathbf{k}' - \mathbf{k}) \cdot \Delta\mathbf{R}}$ . In general, the thermal displacements of an atom are angularly asymmetric. Here, just as in the case of the muffin-tin potential, we shall use the Debye model for the temperature correction of the  $t$  matrix.<sup>8</sup> The Debye approximation assumes isotropic displacements, and Eq. (4.3) becomes

$$t(T, \mathbf{k}', \mathbf{k}) = t(0, \mathbf{k}', \mathbf{k}) \exp(-\alpha |\mathbf{k} - \mathbf{k}'|^2) \quad (4.5)$$

where

$$\alpha = \frac{3\hbar^2 T}{mk_B \Theta^2} \quad (4.6)$$

and  $\Theta, T$  are the Debye and the current temperatures,  $k_B$  the Boltzmann constant, and the high-temperature limit is used in Eq. (4.6). By expanding the  $t$  matrix and  $e^{-\alpha |\mathbf{k} - \mathbf{k}'|^2}$  in terms of spherical harmonics, we obtain

$$t(T, \mathbf{k}', \mathbf{k}) = (4\pi)^2 \sum_{L, L'} t_{LL'}(k, T) Y_L(\hat{\mathbf{k}}') Y_{L'}^*(\hat{\mathbf{k}}), \quad (4.7)$$

$$t(0, \mathbf{k}', \mathbf{k}) = (4\pi)^2 \sum_{L_2, L_3} t_{L_2 L_3}(k, 0) Y_{L_2}(\hat{\mathbf{k}}') Y_{L_3}^*(\hat{\mathbf{k}}), \quad (4.8)$$

and

$$e^{-\alpha |\mathbf{k} - \mathbf{k}'|^2} = \exp(-2\alpha k^2) \sum_{L_4} 4\pi i^{l_4} j_{l_4}(-2i\alpha k^2) Y_{L_4}^*(\hat{\mathbf{k}}') Y_{L_4}(\hat{\mathbf{k}}). \quad (4.9)$$

Here, the definitions of  $t_{LL'}(k, T)$  and  $t_{LL'}(k, 0)$  are the same as in Eq. (2.20) except for the temperature dependence (details of the expressions are given in Appendix A). Inserting Eqs. (4.7) and (4.9) into Eq. (4.5), and using the orthogonality condition Eq. (2.7) for the spherical harmonics, we obtain

$$\begin{aligned} t_{LL'}(k, T) &= 4\pi \exp(-2\alpha k^2) \sum_{L_2, L_3, L_4} t_{L_2 L_3}(k, 0) i^{l_4} j_{l_4}(-2i\alpha k^2) \int d\Omega_{\mathbf{k}'} Y_{L_2}(\hat{\mathbf{k}}') Y_{L_4}^*(\hat{\mathbf{k}}') Y_{L'}^*(\hat{\mathbf{k}}') \\ &\quad \times \int d\Omega_{\mathbf{k}} Y_{L_3}^*(\hat{\mathbf{k}}) Y_{L_4}(\hat{\mathbf{k}}) Y_L(\hat{\mathbf{k}}) \\ &= 4\pi \exp(-2\alpha k^2) \sum_{L_2, L_3, L_4} t_{L_2 L_3}(k, 0) (-1)^{m_4} i^{l_4} j_{l_4}(-2i\alpha k^2) C_{L_2 L_4}^L C_{L_4 L'}^{L_3}, \end{aligned} \quad (4.10)$$

where  $C_{L_2 L_3}^{L_1}$  is the Gaunt number and  $\bar{L}_4 = (l_4, -m_4)$ . Equation (4.10) can be used to obtain the temperature correction based on the simple isotropic vibrational model.

### V. MULTIPLE SCATTERING BY A CRYSTAL SLAB

Once the  $t$  matrices  $t_{LL'}(k)$  for individual nonspherical potentials are calculated, it follows standard multiple scattering theory of LEED to incorporate them into layer-scattering matrices. The computation times for the remaining steps are essentially the same as those of existing LEED theories. Thus we divide a crystal slab into layers parallel to the surface. Atoms in each layer are grouped into subplanes such that all subplanes have the same two-dimensional periodic structure. Each subplane has one atom per unit cell and atoms in each subplane are of the same element. The subplane scattering matrix  $\tau_{LL'}(\mathbf{k}_i)$  is given by<sup>1,8,9,14</sup>

$$\tau_{LL'}(\mathbf{k}_i) = t_{LL'}(k) + \sum_{L_1 L_2} t_{LL_1}(k) G_{L_1 L_2}^{\text{sp}}(\mathbf{k}_i) \tau_{L_2 L'}(k). \quad (5.1)$$

Or, in matrix notation,

$$\tilde{\tau} = (\tilde{I} - \tilde{t} \tilde{G}^{\text{sp}})^{-1} \tilde{t}. \quad (5.2)$$

In Eq. (5.1) or (5.2), the structural propagators are given by<sup>8</sup>

$$G_{LL'}^{\text{sp}}(\mathbf{k}_i) = \sum_{\mathbf{p} \neq 0} G_{LL'}(\mathbf{p}) e^{-i\mathbf{k}_i \cdot \mathbf{p}} \quad (5.3)$$

and

$$G_{LL'}(\mathbf{p}) = -\frac{8\pi m i k}{\hbar^2} \sum_{L_3} i^{l_3} a(LL'L_3) h_{l_3}^{(1)}(kp) Y_{L_3}(\hat{\mathbf{p}}). \quad (5.4)$$

The summation of  $\mathbf{p}$  is over atomic sites within a subplane, and

$$a(L_1 L_2 L_3) = (-1)^{m_3} C_{L_2 L_3}^{L_1}. \quad (5.5)$$

The different subplanes are assembled into a slab via  $\mathbf{k}$ -space multiple scattering techniques such as RFS or layer-doubling.<sup>3</sup> In the case of multiple atoms per unit cell or subplanes which are closely spaced, the combined-space method can be used to assemble them into a slab.<sup>1,10,15</sup>

Before closing this section, we wish to discuss an assumption taken in the derivation of Eq. (5.1). In deriving Eq. (5.1) we have expanded the Green's function in terms of spherical harmonics as follows:

$$G_0(\rho_1 + \mathbf{R}_1 - \rho_2 - \mathbf{R}_2) = -\frac{8\pi m i k}{\hbar^2} \sum_{L_1, L_2, L_3} i^{l_1 - l_2 + l_3} a(L_1 L_2 L_3) h_{l_3}^{(1)}(k | \mathbf{R}_1 - \mathbf{R}_2 |) j_{l_1}(k\rho_1) j_{l_2}(k\rho_2) \\ \times Y_{L_1}(\hat{\rho}_1) Y_{L_2}^*(\hat{\rho}_2) Y_{L_3}(\hat{\mathbf{R}}_{12}), \quad (5.6)$$

where  $\mathbf{R}_1$  and  $\mathbf{R}_2$  are coordinates of the center of atoms,  $\rho_1$  and  $\rho_2$  are vectors from the nucleus to points within the potential, and  $\mathbf{R}_{12} = \mathbf{R}_1 - \mathbf{R}_2$ . Equation (5.6) is valid only if the condition  $|\rho_1 - \rho_2| \leq |\mathbf{R}_1 - \mathbf{R}_2|$  is satisfied. This condition is satisfied in the case of nonoverlapping muffin-tin potentials. It is violated in an area between neighboring atoms for nonspherical potentials (see Fig. 1). However, this area is usually quite small and the approximation may not be a serious one<sup>16</sup> (see discussion in Appendix B).

### VI. DISCUSSION

A multiple-scattering theory of LEED is presented which includes the scattering from nonspherical potentials. Ironically, the major position of the computation time is in the evaluation of  $t_{LL'}(k)$ . The use of the rotation formula for  $t_{LL'}(k)$  [Eq. (3.16)] saves some computation time as it allows new  $t$  matrices to be generated from existing ones. At the surface, probably a different set of  $t$  matrices has to be calculated, corresponding to different surface potentials. The basic assumption used in our scheme is that the scattering from a nonspherical poten-

tial can be expressed in terms of a  $t$  matrix expanded in angular-momentum space, with a finite number of partial waves (usually,  $l_{\text{max}} \leq 7$ ). We plan to test this scheme on semiconductor and metal surfaces.

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### APPENDIX A: PARTIAL WAVE EXPANSION OF $t(\mathbf{k}, \mathbf{k}_i)$

To derive the expansion given in Eq. (4.8), we use Dirac's notation and write

$$\langle \mathbf{r}_1 | t | \mathbf{r}_2 \rangle = \sum_{L_1, L_2} \langle \hat{\mathbf{r}}_1 | L_1 \rangle \langle L_1 | t | L_2 \rangle \langle L_2 | \hat{\mathbf{r}}_2 \rangle \quad (A1)$$

or

$$t(\mathbf{r}_1, \mathbf{r}_2) = \sum_{L_1, L_2} t_{L_1 L_2}(r_1, r_2) Y_{L_1}(\hat{\mathbf{r}}_1) Y_{L_2}^*(\hat{\mathbf{r}}_2), \quad (A2)$$

where

$$\langle \hat{\mathbf{r}}_1 | L_1 \rangle = Y_L(\hat{\mathbf{r}}_1)$$

and

$$\langle L_2 | \hat{\mathbf{r}}_2 \rangle = \langle \hat{\mathbf{r}}_2 | L_2 \rangle^* = Y_{L_2}^*(\hat{\mathbf{r}}_2). \quad (\text{A3})$$

Since  $t(\mathbf{k}, \mathbf{k}_i)$  is the Fourier transform of  $t(\mathbf{r}_1, \mathbf{r}_2)$ , we have

$$\langle \mathbf{k} | t | \mathbf{k}_i \rangle = \int d\mathbf{r}_1 \int d\mathbf{r}_2 \langle \mathbf{k} | \mathbf{r}_1 \rangle \langle \mathbf{r}_1 | t | \mathbf{r}_2 \rangle \langle \mathbf{r}_2 | \mathbf{k}_i \rangle \quad (\text{A4})$$

or

$$t(\mathbf{k}, \mathbf{k}_i) = \int d\mathbf{r}_1 \int d\mathbf{r}_2 e^{-i\mathbf{k} \cdot \mathbf{r}_1} t(\mathbf{r}_1, \mathbf{r}_2) e^{i\mathbf{k}_i \cdot \mathbf{r}_2}, \quad (\text{A5})$$

where

$$\langle \mathbf{r}_2 | \mathbf{k}_i \rangle = e^{i\mathbf{k}_i \cdot \mathbf{r}_2}$$

and

$$\langle \mathbf{k} | \mathbf{r}_1 \rangle = \langle \mathbf{r}_1 | \mathbf{k} \rangle^* = e^{-i\mathbf{k} \cdot \mathbf{r}_1}. \quad (\text{A6})$$

Substituting Eq. (A2) into Eq. (A5) and using the expression in Eq. (2.4), we obtain

$$\begin{aligned} t(\mathbf{k}, \mathbf{k}_i) &= \int d\mathbf{r}_1 \int d\mathbf{r}_2 e^{-i\mathbf{k} \cdot \mathbf{r}_1} \sum_{L_1, L_2} t_{L_1 L_2}(r_1 r_2) Y_{L_1}(\hat{\mathbf{r}}_1) Y_{L_2}^*(\hat{\mathbf{r}}_2) e^{i\mathbf{k}_i \cdot \mathbf{r}_2} \\ &= (4\pi)^2 \sum_{L, L'} t_{LL'}(k) Y_L(\hat{\mathbf{k}}) Y_{L'}^*(\hat{\mathbf{k}}_i), \end{aligned} \quad (\text{A7})$$

which is the expansion in Eq. (4.8).

## APPENDIX B: GREEN'S-FUNCTION EXPANSION AND NONSPHERICAL POTENTIALS

The expansion in Eq. (5.6) is rigorous only for nonoverlapping potentials. As an illustration let us adopt honeycomb unit cells shown in Fig. 1. In the figure,  $\rho_1$ ,  $\rho_2$ , and  $\rho_3$  cover regions within each unit cell. The condition  $|\rho_1 - \rho_2| \leq |\mathbf{R}_1 - \mathbf{R}_2|$  is violated only if

(a)  $\rho_1$  and  $\rho_2$  belong to nearest neighbor unit cells, and

(b)  $\rho_1$  and  $\rho_2$  are in (or near) the edge areas (shaded regions in Fig. 1) and that they point in essentially opposite directions.

Since  $t_{LL'}(k)$  is evaluated based on integrated values over the entire unit cell, the condition  $|\rho_1 - \rho_2| \leq |\mathbf{R}_1 - \mathbf{R}_2|$  is violated only in very limited regions. When the condition is violated, we can estimate the magnitude of the error in the expansion. Thus we expand

$$G_0(\rho_1 - \rho_2 + \mathbf{R}_1 - \mathbf{R}_2) = -\frac{2mik}{\hbar^2} \sum_L j_L(k |\rho_1 - \rho_2|) h_L^{(1)}(k |\mathbf{R}_1 - \mathbf{R}_2|) Y_L^*(\hat{\rho}_{12}) Y_L(\hat{\mathbf{R}}_{12}) \quad (\text{B1})$$

for  $|\rho_1 - \rho_2| \leq |\mathbf{R}_1 - \mathbf{R}_2|$ , and

$$G_0(\rho_1 - \rho_2 + \mathbf{R}_1 - \mathbf{R}_2) = -\frac{2mik}{\hbar^2} \sum_L j_L(k |\mathbf{R}_1 - \mathbf{R}_2|) h_L^{(1)}(k |\rho_1 - \rho_2|) Y_L^*(\hat{\rho}_{12}) Y_L(\hat{\mathbf{R}}_{12}) \quad (\text{B2})$$

for  $|\rho_1 - \rho_2| > |\mathbf{R}_1 - \mathbf{R}_2|$ . In Eqs. (B1) and (B3),  $\rho_{12} = \rho_1 - \rho_2$  and  $\mathbf{R}_{12} = \mathbf{R}_1 - \mathbf{R}_2$ . The difference in the two expansions [i.e., Eq. (B2) minus (B1)] is

$$S = -\frac{2mik}{\hbar^2} \sum_L [j_L(k |\mathbf{R}_1 - \mathbf{R}_2|) h_L^{(1)}(k |\rho_1 - \rho_2|) - j_L(k |\rho_1 - \rho_2|) h_L^{(1)}(k |\mathbf{R}_1 - \mathbf{R}_2|)] Y_L^*(\hat{\rho}_{12}) Y_L(\hat{\mathbf{R}}_{12}). \quad (\text{B3})$$

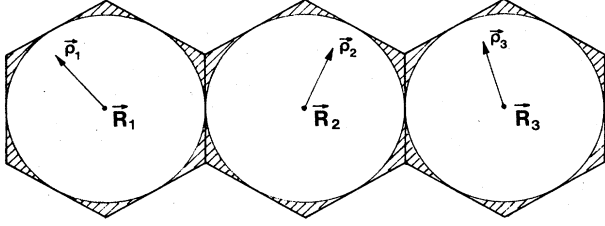
To estimate this difference, we note that  $|\rho_1 - \rho_2| \sim |\mathbf{R}_1 - \mathbf{R}_2|$  and  $k |\mathbf{R}_1 - \mathbf{R}_2| \gg 1$ . Thus

$$j_L(k |\mathbf{R}_1 - \mathbf{R}_2|) h_L^{(1)}(k |\rho_1 - \rho_2|) - j_L(k |\rho_1 - \rho_2|) h_L^{(1)}(k |\mathbf{R}_1 - \mathbf{R}_2|) \sim \frac{i(|\rho_1 - \rho_2| - |\mathbf{R}_1 - \mathbf{R}_2|)}{k |\rho_1 - \rho_2| |\mathbf{R}_1 - \mathbf{R}_2|} \ll 1, \quad (\text{B4})$$

and the error is small. Finally, on substituting the relation

$$j_L(k |\rho_1 - \rho_2|) Y_L^*(\hat{\rho}_{12}) = 4\pi \sum_{L_1, L_2} i^{l_1 - l_2 - l} a(L_1 L_2 L) j_{L_1}(k \rho_1) j_{L_2}(k \rho_2) Y_{L_1}(\hat{\rho}_1) Y_{L_2}^*(\hat{\rho}_2) \quad (\text{B5})$$

into Eq. (B1), we obtain the expansion in Eq. (5.6).

FIG. 1. Schematic diagram of unit cells and radial vector  $\rho_i$ .

### APPENDIX C: NUMERICAL ALGORITHM FOR EVALUATION OF $\tilde{f}(r)$

To evaluate Eq. (2.16) numerically, we introduce

$$\tilde{I}_1(r) = \int_0^r dr' \tilde{J}(r') \cdot \tilde{U}(r') \cdot \tilde{f}(r'), \quad (C1)$$

$$\tilde{I}_2(r) = \tilde{I} - \int_0^r dr' \tilde{H}(r') \cdot \tilde{U}(r') \cdot \tilde{f}(r'), \quad (C2)$$

then Eqs. (2.16) and (2.21) become

$$\tilde{f}(r) = \tilde{H}(r) \cdot \tilde{I}_1(r) + \tilde{J}(r) \cdot \tilde{I}_2(r) \quad (C3)$$

and

$$\begin{aligned} \tilde{K}_1(r_i) &= \tilde{K}_1(r_{i-1} + \Delta r_i) = \tilde{I}_1(r_{i-1} + \Delta r_i) - \tilde{J}(r_i) \cdot \tilde{U}(r_i) \cdot \tilde{f}(r_i) \frac{\Delta r_i}{2} \\ &= \tilde{I}_1(r_{i-1}) + \int_{r_{i-1}}^{r_i} dr' \tilde{J}(r') \cdot \tilde{U}(r') \cdot \tilde{f}(r') - \tilde{J}(r_i) \cdot \tilde{U}(r_i) \cdot \tilde{f}(r_i) \frac{\Delta r_i}{2} \\ &= \tilde{I}_1(r_{i-1}) + \frac{\Delta r_i}{2} \tilde{J}(r_{i-1}) \cdot \tilde{U}(r_{i-1}) \cdot \tilde{f}(r_{i-1}) \\ &= \tilde{K}_1(r_{i-1}) + \frac{1}{2} (\Delta r_i + \Delta r_{i-1}) \tilde{J}(r_{i-1}) \cdot \tilde{U}(r_{i-1}) \cdot \tilde{f}(r_{i-1}) \end{aligned} \quad (C6)$$

and

$$\tilde{K}_2(r_i) = \tilde{K}_2(r_{i-1}) - \frac{1}{2} (\Delta r_i + \Delta r_{i-1}) \tilde{H}(r_{i-1}) \cdot \tilde{U}(r_{i-1}) \cdot \tilde{f}(r_{i-1}). \quad (C7)$$

The radial position  $r_1$  is very close to the nucleus. Then  $U_{LL}(r_1)$  is dominated by the  $l=0$  Coulomb potential. Thus, for Eq. (2.10) and using a Coulomb potential of  $V_0(r) = -Ze^2/r$ , we obtain

$$U_{LL}(r_1) = \frac{2mik}{\hbar^2} r_1 Ze^2 \delta_{LL'}. \quad (C8)$$

If we now use

$$j_l(kr_1) \sim \frac{(kr_1)^l}{(2l+1)!!}, \quad (C9)$$

$$h_l^{(1)}(kr_1) \sim -i \frac{(2l-1)!!}{(kr_1)^{l+1}}, \quad (C10)$$

$$\tilde{f}_{LL'}(0) = j_l(0) \delta_{LL'}, \quad (C11)$$

$$t_{LL}(k) = \frac{\hbar^2}{2m} \frac{i}{k} i^{-(l-l')} [\tilde{I}_1(\infty) \cdot \tilde{I}_2^{-1}(\infty)]_{LL'}, \quad (C4)$$

respectively. Here we have abbreviated  $k$  in the arguments of  $\tilde{J}$  and  $\tilde{H}$ . It is clear that we cannot evaluate  $\tilde{I}_1(r), \tilde{I}_2(r)$  without knowing  $\tilde{f}(r)$ , which is itself the quantity we try to calculate. We can rewrite Eq. (C3) to avoid this problem,

$$\begin{aligned} \tilde{f}(r_i) &= \tilde{H}(r_i) \cdot \left[ \tilde{I}_1(r_i) - \tilde{J}(r_i) \cdot \tilde{U}(r_i) \cdot \tilde{f}(r_i) \frac{\Delta r_i}{2} \right] \\ &\quad + \tilde{J}(r_i) \cdot \left[ \tilde{I}_2(r_i) + \tilde{H}(r_i) \cdot \tilde{U}(r_i) \cdot \tilde{f}(r_i) \frac{\Delta r_i}{2} \right] \\ &\equiv \tilde{H}(r_i) \cdot \tilde{K}_1(r_i) + \tilde{K}(r_i) \cdot \tilde{K}_2(r_i), \end{aligned} \quad (C5)$$

where  $\tilde{K}_1(r_i)$  and  $\tilde{K}_2(r_i)$  are defined in Eq. (C5). Here  $r_0, r_1, \dots$  are radial distances which start from the nucleus, and  $\Delta r_i = r_i - r_{i-1}$ . In writing Eq. (C5), we have used the trapezoidal rule for the integration of Eqs. (C1) and (C2). With the help of Eqs. (C1) and (C2), the recursion relations for  $\tilde{K}_1$  and  $\tilde{K}_2$  are

we obtain

$$\tilde{K}_1(r_1) = \frac{r_1}{2} [\tilde{J}(r) \cdot \tilde{U}(r) \cdot \tilde{f}(r)]_{r=0} = 0 \quad (C12)$$

and

$$\begin{aligned} \tilde{K}_2(r_1) &= \tilde{I} - \frac{1}{2} r_1 [\tilde{H}(r) \cdot \tilde{U}(r) \cdot \tilde{f}(r)]_{r=0} \\ &= \left[ 1 - \frac{Ze^2}{2l+1} \frac{m}{\hbar^2} \right] r_1 \tilde{I}. \end{aligned} \quad (C13)$$

Thus if we start the calculation at the center of the atom, we can evaluate  $\tilde{K}_1(r_1), \tilde{K}_2(r_1)$ , and then  $\tilde{f}(r_1)$  using Eq. (C5). Iterating this process, we reach a point where the potential vanishes. By finding  $\tilde{I}_1$  and  $\tilde{I}_2$  from  $\tilde{K}_1$  and  $\tilde{K}_2$ , we obtain the  $t$  matrix from Eq. (C4).



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