Theory of electron multiple scattering

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A technique to calculate the T matrix exactly for N scatterers from the individual T matrices in the elastic-electron-scattering process is developed based on the multicenter-expansion method. A summing formula for the sets of T matrices is also derived to handle large systems without an accumulation of significant error. Furthermore, it is applied to the study of multiple scattering of a photoelectron and electron scattering by an adsorbate on solid surface.

I. INTRODUCTION

Electron scattering plays one of the major roles in many scientific disciplines. Especially with the recent rapid progress of surface science, it has become one of the important tools in surface studies due to its relatively big cross section. In the energy domain of 10–40 keV, reflection high-energy electron diffraction (RHEED) (Ref. 1) is routinely adopted as a structural analysis technique. RHEED is based on the plane-wave expansion. On the other hand, in the low-energy domain of 20–200 eV, we usually use low-energy electron diffraction (LEED),[2,3] which is essentially the layer Korringa-Kohn-Rostoker method.[4,5] Its theoretical basis is the spherical-wave expansion method. Their difference originates in the handling of the singularities of the scattering potentials. In order to handle the scattering problems, the T matrix[6] is commonly used, since physical interpretation of the scattering processes can be obtained quite straightforwardly. It is relatively easy to calculate the T matrix for a single scatterer. However, the calculation of the T matrix for many scatterers still remains the main issue in most cases. Practical techniques have been developed and applied to various problems only for systems having translational invariance. Especially, in the LEED analysis, many powerful assembling techniques of T matrices have been developed by Van Hove and Tong,[2] Pendry,[3] and others since structural analysis requires accurate and efficient techniques. On the other hand, without the translational invariance, the scattering problem cannot be transformed to that within a unit cell, and usually it tends to become a complicated problem. It is the reason why the random systems are being studied only approximately.[8] The difficulty originates from the fact that a good approximation to scattering-state functions is given not by plane waves but by spherical waves.

Recently, we developed a method for calculating precisely the total T matrix from the T matrices for two nonoverlapping scatterers in the elastic process.[9] Furthermore, we applied it to a study of the focusing of the electron scattering. In this paper, we generalize it to a system of N scatterers. Our previously developed method can also handle it, but the error could accumulate as the number of scatterers increases, since the single-center expansion is involved in its repetition process. On the other hand, the method to be discussed here can present the total T matrix as accurately as individual T matrices. Therefore, it can be used, for example, for the study of the random systems, the structure analysis of microclusters, or the electron scattering by gas molecules, as well.[10] This method can also be straightforwardly applied to the study of the multiple scattering of a photoelectron.

A discussion of the present paper is as follows. First, we report an approach to the calculation of the T matrix for many-scatterer systems in the elastic process by assembling the T matrices for the individual scatterers in Sec. II. The multiple scattering of a photoelectron is discussed in Sec. III. Finally, in Sec. IV we apply the present theory to the problem of the focusing effect of electron scattering. Discussions are given in Sec. V.

II. GENERAL THEORY OF THE ELECTRON MULTIPLE SCATTERING

Formally, the T matrix for N scatterers can be written as follows using the individual T matrices t^{α} ($\alpha=1,\ldots,N$):[7]

$$T=\sum_{\alpha} t^{\alpha}+\sum_{\alpha\neq\beta} t^{\alpha}G_0t^{\beta}+\sum_{\substack{\alpha\neq\beta,\\ \beta\neq\gamma}} t^{\alpha}G_0t^{\beta}G_0t^{\gamma}+\cdots , \tag{1}$$

where G_0 is the free Green's function, and $\alpha,\beta,\gamma,\ldots=1,2,\ldots,N$. When $\mathbf{k}_i$ and $\mathbf{k}_f$ are the incident and scattered wave vectors, respectively, the T matrix can be expanded in terms of the spherical harmonics Y_L as

$$T(\mathbf{k}_f,\mathbf{k}_i)=(4\pi)^2\sum_{L,L'} T_{LL'}Y_L(\hat{\mathbf{k}}_f)Y^*_{L'}(\hat{\mathbf{k}}_i) , \tag{2}$$

where $L=(l,m)$, and the caret indicates a unit vector.

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The transition probability from $\mathbf{k}_i$ to $\mathbf{k}_f$ is proportional to $|T(\mathbf{k}_f,\mathbf{k}_i)|^2$. In the elastic scattering, $|\mathbf{k}_i|=|\mathbf{k}_f|=k=(2m_eE/\hbar^2)^{1/2}$, where E is the kinetic energy of an electron, m_e is the electron mass, and $\hbar$ is the Planck constant. Generalizing the case of the elastic scattering for $N=2$, which we have investigated in detail before,[9] we can derive the following expression for the N-scatterer case as

$$T(\mathbf{k}_f,\mathbf{k}_i)\equiv\langle\mathbf{k}_f|T|\mathbf{k}_i\rangle=(4\pi)^2\sum_{L,L'}Y_L(\hat{\mathbf{k}}_f)[K_fT_tK_i^\dagger+K_fT_tGT_tK_i^\dagger+K_fT_tGT_tGT_tK_i^\dagger+\cdots]_{LL'}Y_{L'}^*(\hat{\mathbf{k}}_i)$$
$$=(4\pi)^2\sum_{L,L'}[K_fT_t(\mathcal{I}-GT_t)^{-1}K_i^\dagger]_{LL'}Y_L(\hat{\mathbf{k}}_f)Y_{L'}^*(\hat{\mathbf{k}}_i)\ , \tag{3}$$

where

$$T_t=\begin{pmatrix}\tilde{t}^1&\tilde{0}&\tilde{0}&\cdots&\tilde{0}\\\tilde{0}&\tilde{t}^2&&&\tilde{0}\\\tilde{0}&&\ddots&&\\\vdots&&&&\\\tilde{0}&\tilde{0}&&&\tilde{t}^N\end{pmatrix}\ , \tag{4}$$

$$G=\begin{pmatrix}\tilde{0}&\tilde{G}^{12}&\tilde{G}^{13}&\cdots&\tilde{G}^{1N}\\\tilde{G}^{21}&\tilde{0}&&&\tilde{G}^{2N}\\\tilde{G}^{31}&&\ddots&&\\\vdots&&&&\\\tilde{G}^{N1}&\tilde{G}^{N2}&&\tilde{G}^{NN-1}&\tilde{0}\end{pmatrix}\ , \tag{5}$$

$$K_f=(e^{-i\mathbf{k}_f\cdot\mathbf{R}_1}\tilde{I}e^{-i\mathbf{k}_f\cdot\mathbf{R}_2}\tilde{I}\cdots e^{-i\mathbf{k}_f\cdot\mathbf{R}_N}\tilde{I})\ , \tag{6}$$

$$K_i^\dagger=\begin{pmatrix}e^{i\mathbf{k}_i\cdot\mathbf{R}_1}\tilde{I}\\\vdots\\e^{i\mathbf{k}_i\cdot\mathbf{R}_N}\tilde{I}\end{pmatrix}\ , \tag{7}$$

$$\mathcal{I}=\begin{pmatrix}\tilde{I}&\tilde{0}&\tilde{0}&\cdots&\tilde{0}\\\tilde{0}&\tilde{I}&&&\tilde{0}\\\tilde{0}&&\ddots&&\\\vdots&&&&\\\tilde{0}&\tilde{0}&&&\tilde{I}\end{pmatrix}\ , \tag{8}$$

a tilde signifies a matrix, rows and columns of which are labeled $L=(l,m)$, and $\tilde{I}$ is the unit matrix. Furthermore,

$$G_{LL'}^{\alpha\beta}=-\frac{8\pi m_eik}{\hbar^2}\sum_{L''}i^{l''}(-1)^{m''}C_{L'\bar{L}''}^{L}h_{l''}^{(1)}(k|\mathbf{R}_\alpha-\mathbf{R}_\beta|)Y_{L''}(\hat{\mathbf{R}}_{\alpha,\beta})\ , \tag{9}$$

$$t_{LL'}^{\alpha}(k)=i^{-(l-l')}\int_0^\infty\rho_1^2d\rho_1\int d\Omega_{\rho_1}\int_0^\infty\rho_2^2d\rho_2\int d\Omega_{\rho_2}j_1(k\rho_1)Y_L^*(\hat{\boldsymbol{\rho}}_1)t^\alpha(\boldsymbol{\rho}_1,\boldsymbol{\rho}_2)Y_{L'}(\hat{\boldsymbol{\rho}}_2)j_{l'}(k\rho_2)\ , \tag{10}$$

where

$$\hat{\mathbf{R}}_{\alpha,\beta}=(\mathbf{R}_\alpha-\mathbf{R}_\beta)/|\mathbf{R}_\alpha-\mathbf{R}_\beta|\ ,$$

and the free Green's function in real space is expressed as[11]

$$G_0(\mathbf{r}_1-\mathbf{r}_2)=\sum_{L,L'}G_{LL'}^{\alpha\beta}i^{l-l'}j_1(k\rho_1)j_{l'}(k\rho_2)Y_L(\hat{\boldsymbol{\rho}}_1)Y_{L'}^*(\hat{\boldsymbol{\rho}}_2) \tag{11}$$

as far as the condition $|\boldsymbol{\rho}_1-\boldsymbol{\rho}_2|\le|\mathbf{R}_\alpha-\mathbf{R}_\beta|$ is satisfied, where $\mathbf{r}_1=\boldsymbol{\rho}_1+\mathbf{R}_\alpha$ and $\mathbf{r}_2=\boldsymbol{\rho}_2+\mathbf{R}_\beta$. The Gaunt's number $C_{L'L''}^{L}$ is defined by

$$C_{L'L''}^{L}=\int d\Omega_\rho Y_L^*(\hat{\boldsymbol{\rho}})Y_{L'}(\hat{\boldsymbol{\rho}})Y_{L''}(\hat{\boldsymbol{\rho}})\ . \tag{12}$$

In the above identities, $\mathbf{R}_\alpha$ ($\alpha=1,\ldots,N$) are positions of the scatterers, and they correspond to the origins of each coordinate where $t^\alpha_{LL'}(k)$ are calculated, $j_l(k\rho)$, $h_l^{(1)}(k\rho)$, spherical Bessel, and Hankel function of the first kind, respectively, and finally, $\bar{L}=(l,-m)$.

Comparison between Eqs. (2) and (3) indicates the T matrix in the angular momentum space as

$$T_{LL'}(\mathbf{k}_f,\mathbf{k}_i)=\left[(e^{-i\mathbf{k}_f\cdot\mathbf{R}_1}\tilde{I}e^{-i\mathbf{k}_f\cdot\mathbf{R}_2}\tilde{I}\cdots e^{-i\mathbf{k}_f\cdot\mathbf{R}_N}\tilde{I})T_t(\mathcal{J}-GT_t)^{-1}\begin{bmatrix}e^{i\mathbf{k}_i\cdot\mathbf{R}_1}\tilde{I}\\ \vdots\\ e^{i\mathbf{k}_i\cdot\mathbf{R}_N}\tilde{I}\end{bmatrix}\right]_{LL'}, \tag{13}$$

or

$$T_{LL'}(\mathbf{k}_f,\mathbf{k}_i)=\sum_{\alpha,\beta}T^{\alpha\beta}_{LL'}(\mathbf{k}_f,\mathbf{k}_i)\ , \tag{14a}$$

$$T^{\alpha\beta}_{LL'}(\mathbf{k}_f,\mathbf{k}_i)=[T_t(\mathcal{J}-GT_t)^{-1}]_{\alpha L,\beta L'}e^{-\mathbf{k}_f\cdot\mathbf{R}_\alpha}e^{i\mathbf{k}_i\cdot\mathbf{R}_\beta}\ . \tag{14b}$$

Equation (13) has a very clear physical meaning. When the multiple scattering is neglected (kinematic case), it can be written as

$$T_{LL'}(\mathbf{k}_f,\mathbf{k}_i)=\sum_\alpha e^{-i(\mathbf{k}_f-\mathbf{k}_i)\cdot\mathbf{R}_\alpha}t^\alpha_{LL'}(k)\ . \tag{15}$$

Equation (15) can be understood as the individual T matrices are expanded at each scattering center $\mathbf{R}^\alpha$ ($\alpha=1,\ldots,N$); then they are shifted back to the origin $\mathbf{r}=\mathbf{0}$ to form the T matrix of the system. Namely, Eq. (13) corresponds to the T matrix obtained by the multicenter expansion method including the multiple scattering. Therefore, the angular momentum space of the combined system is still as small as those of the individual T matrices. When we use

$$[g(\mathbf{k}_i)]_{\alpha L,\beta L'}\equiv g^{\alpha\beta}_{LL'}(\mathbf{k}_i)\equiv G^{\alpha\beta}_{LL'}e^{-i\mathbf{k}_i\cdot(\mathbf{R}_\alpha-\mathbf{R}_\beta)}\ ,$$

Eq. (13) can be also summed up as

$$T_{LL'}(\mathbf{k}_f,\mathbf{k}_i)=\sum_\alpha e^{-i(\mathbf{k}_f-\mathbf{k}_i)\cdot\mathbf{R}_\alpha}T^\alpha_{LL'}(\mathbf{k}_i)\ , \tag{16a}$$

$$T^\alpha_{LL'}(\mathbf{k}_i)=\sum_\beta\{T_t[\mathcal{J}-g(\mathbf{k}_i)T_t]^{-1}\}_{\alpha L,\beta L'}\ . \tag{16b}$$

In general, the dimension of the matrix in Eq. (13) rapidly increases with the number of scatterers. Therefore, in order to handle the large system, we have to divide it into subgroups of scatterers, calculate their T matrices, then sum them up. Such a summing formula of T matrices can also be deduced from Eq. (3). Assuming that the number of subgroups is n, and defining $\mathbf{d}_s$ as the origin of sth group of scatterers, Eq. (13) is also expressed as

$$\tilde{T}(\mathbf{k}_f,\mathbf{k}_i)=(e^{-i\mathbf{k}_f\cdot\mathbf{d}_1}\tilde{I}\cdots e^{-i\mathbf{k}_f\cdot\mathbf{d}_n}\tilde{I})\times[T^{fi}+T^f(\mathcal{J}-GT^0)^{-1}]\begin{bmatrix}e^{i\mathbf{k}_i\cdot\mathbf{d}_1}\tilde{I}\\ \vdots\\ e^{i\mathbf{k}_i\cdot\mathbf{d}_n}\tilde{I}\end{bmatrix}, \tag{17}$$

where we have introduced the following definitions:

$$T^{fi}=\begin{bmatrix}\tilde{T}^{fi(1)} & \tilde{0} & \tilde{0} & \cdots & \tilde{0}\\ \tilde{0} & \tilde{T}^{fi(2)} & & & \tilde{0}\\ \tilde{0} & & \ddots & & \\ \vdots & & & & \\ \tilde{0} & \tilde{0} & & & \tilde{T}^{fi(n)}\end{bmatrix}, \tag{18a}$$

$$\tilde{T}^{fi(s)}=(e^{-i\mathbf{k}_f\cdot\mathbf{R}^{(s)}_1}\tilde{I}\cdots e^{-i\mathbf{k}_f\cdot\mathbf{R}^{(s)}_N}\tilde{I})T^{(s)}_w\begin{bmatrix}e^{i\mathbf{k}_i\cdot\mathbf{R}^{(s)}_1}\tilde{I}\\ \vdots\\ e^{i\mathbf{k}_i\cdot\mathbf{R}^{(s)}_N}\tilde{I}\end{bmatrix}, \tag{18b}$$

$$T^{(s)}_w=T^{(s)}_t(\mathcal{J}-G^{(s)}T^{(s)}_t)^{-1}\ , \tag{19}$$

$$T^i=\begin{bmatrix}\tilde{T}^{i(1)} & \tilde{0} & \tilde{0} & \cdots & \tilde{0}\\ \tilde{0} & \tilde{T}^{i(2)} & & & \tilde{0}\\ \tilde{0} & & \ddots & & \\ \vdots & & & & \\ \tilde{0} & \tilde{0} & & & \tilde{T}^{i(n)}\end{bmatrix}, \tag{20a}$$

$$\tilde{T}^{i(s)}=[\tilde{P}(-\mathbf{R}^{(s)}_1)\cdots\tilde{P}(-\mathbf{R}^{(s)}_N)]T^{(s)}_w\begin{bmatrix}e^{i\mathbf{k}_i\cdot\mathbf{R}^{(s)}_1}\tilde{I}\\ \vdots\\ e^{i\mathbf{k}_i\cdot\mathbf{R}^{(s)}_N}\tilde{I}\end{bmatrix}, \tag{20b}$$

$$T^f=\begin{bmatrix}\tilde{T}^{f(1)} & \tilde{0} & \tilde{0} & \cdots & \tilde{0}\\ \tilde{0} & \tilde{T}^{f(2)} & & & \tilde{0}\\ \tilde{0} & & \ddots & & \\ & & & & \\ \vdots & & & & \\ \tilde{0} & \tilde{0} & & & \tilde{T}^{f(n)}\end{bmatrix}, \tag{21a}$$

$$\tilde{T}^{f(s)}=(e^{-i\mathbf{k}_f\cdot\mathbf{R}^{(s)}_1}\tilde{I}\cdots e^{-i\mathbf{k}_f\cdot\mathbf{R}^{(s)}_N}\tilde{I})T^{(s)}_w\begin{bmatrix}\tilde{P}(\mathbf{R}^{(s)}_1)\\ \vdots\\ \tilde{P}(\mathbf{R}^{(s)}_N)\end{bmatrix}, \tag{21b}$$

$$T^0=\begin{bmatrix} \tilde{T}^{0(1)} & \tilde{0} & \tilde{0} & \cdots & \tilde{0} \\ \tilde{0} & \tilde{T}^{0(2)} & & & \tilde{0} \\ \tilde{0} & & \ddots & & \\ \vdots & & & & \\ \tilde{0} & \tilde{0} & & & \tilde{T}^{0(n)} \end{bmatrix}, \qquad (22a)$$

$$G=\begin{bmatrix} \tilde{0} & \tilde{G}^{12} & \tilde{G}^{13} & \cdots & \tilde{G}^{1n} \\ \tilde{G}^{21} & \tilde{0} & & & \tilde{G}^{2n} \\ \tilde{G}^{31} & & \ddots & & \\ \vdots & & & & \\ \tilde{G}^{n1} & \tilde{G}^{n2} & & \tilde{G}^{nn-1} & \tilde{0} \end{bmatrix},$$

$$\tilde{T}^{0(s)}=[\tilde{P}(-\mathbf{R}_1^{(s)})\cdots\tilde{P}(-\mathbf{R}_N^{(s)})]T_w^{(s)}\begin{bmatrix} \tilde{P}(\mathbf{R}_1^{(s)}) \\ \vdots \\ \tilde{P}(\mathbf{R}_N^{(s)}) \end{bmatrix}, \qquad (22b)$$

$$T_t^{(s)}=\begin{bmatrix} \tilde{t}^{1(s)} & \tilde{0} & \tilde{0} & \cdots & \tilde{0} \\ \tilde{0} & \tilde{t}^{2(s)} & & & \tilde{0} \\ \tilde{0} & & \ddots & & \\ \vdots & & & & \\ \tilde{0} & \tilde{0} & & & \tilde{t}^{N(s)} \end{bmatrix}, \qquad (23)$$

$$G^{st}_{LL'}=-\frac{8\pi m_e ik}{\hbar^2}\sum_{L''} i^{l''}(-1)^{m''}C^{L}_{L'\bar{L}''} \times h^{(1)}_{l''}(k|\mathbf{d}_s-\mathbf{d}_t|)Y_{L''}(\hat{\mathbf{d}}_{s,t}), \qquad (24a)$$

where

$$\hat{\mathbf{d}}_{s,t}=(\mathbf{d}_s-\mathbf{d}_t)/|\mathbf{d}_s-\mathbf{d}_t|,$$

$$G^{(s)}=\begin{bmatrix} \tilde{0} & \tilde{G}^{12(s)} & \cdots & \tilde{G}^{1N(s)} \\ \tilde{G}^{21(s)} & \tilde{0} & & \tilde{G}^{2N(s)} \\ \vdots & & \ddots & \\ \tilde{G}^{N1(s)} & \tilde{G}^{N2(s)} & \tilde{G}^{NN-1(s)} & \tilde{0} \end{bmatrix}, \qquad (25a)$$

$$G^{\alpha\beta(s)}_{LL'}=-\frac{8\pi m_e ik}{\hbar^2}\sum_{L''} i^{l''}(-1)^{m''}C^{L}_{L'\bar{L}''}h^{(1)}_{l''}(k|\mathbf{R}_\alpha^{(s)}-\mathbf{R}_\beta^{(s)}|)Y_{L''}(\hat{\mathbf{R}}^{(s)}_{\alpha,\beta}), \qquad (25b)$$

where

$$\hat{\mathbf{R}}^{(s)}_{\alpha,\beta}=(\mathbf{R}_\alpha^{(s)}-R_\beta^{(s)})/|\mathbf{R}_\alpha^{(s)}-\mathbf{R}_\beta^{(s)}|,$$

and

$$P_{LL'}(\mathbf{R})=\int d\Omega_k e^{i\mathbf{k}\cdot\mathbf{R}}Y^*_L(\hat{\mathbf{k}})Y_{L'}(\hat{\mathbf{k}})=\sum_{L''}4\pi(-1)^{m''}C^{L}_{L'\bar{L}''}i^{l''}j_{l''}(kR)Y_{L''}(\hat{\mathbf{R}}). \qquad (26)$$

In the derivation of Eq. (17), we have used the identity relationship

$$G_0(\boldsymbol{\rho}_1+\mathbf{R}_\alpha^{(s)}+\mathbf{d}_s-\boldsymbol{\rho}_2-\mathbf{R}_\beta^{(t)}-\mathbf{d}_t)=\sum_{L,L'}\sum_{L_1L_2}P_{LL_1}(\mathbf{R}_\alpha^{(s)})G^{st}_{L_1L_2}P_{L_2L'}(-\mathbf{R}_\beta^{(t)})i^{l-l'}j_l(k\rho_1)j_{l'}(k\rho_2)Y_L(\hat{\boldsymbol{\rho}}_1)Y^*_{L'}(\hat{\boldsymbol{\rho}}_2). \qquad (27)$$

Equation (27) is valid when the condition $|\boldsymbol{\rho}_1+\mathbf{R}_\alpha^{(s)}-\boldsymbol{\rho}_2-\mathbf{R}_\beta^{(t)}|\le|\mathbf{d}_s-\mathbf{d}_t|$ is satisfied.

When the scatterer is rotated, the T matrix is transformed by[11]

$$t'_{LL'}=\sum_{m',m''}t_{l_1m',l_2m''}D^{l_1}_{m_1m'}(\alpha\beta\gamma)D^{*l_2}_{m_2m''}(\alpha\beta\gamma), \qquad (28)$$

where D stands for the Wigner's D function and α,β,γ are Euler angles which correspond to the rotation of a scatterer. In the presence of the translational invariance, Eq. (3) can be summed up as

$$T(\mathbf{k}_f,\mathbf{k}_i)=(4\pi)^2\sum_{L,L'}Y_L(\mathbf{k}_f)Y^*_{L'}(\hat{\mathbf{k}}_i)\left[\sum_\alpha e^{-i(\mathbf{k}_f-\mathbf{k}_i)\cdot\mathbf{R}_\alpha}\tilde{t}+\sum_\alpha e^{-i(\mathbf{k}_f-\mathbf{k}_i)\cdot\mathbf{R}_\alpha}\tilde{t}\sum_{\beta(\neq\alpha)}\tilde{G}^{\alpha\beta}e^{-i\mathbf{k}_i\cdot(\mathbf{R}_\alpha-\mathbf{R}_\beta)}\tilde{t}+\cdots\right]_{LL'}$$

$$=(4\pi)^2\sum_\alpha e^{-i(\mathbf{k}_f-\mathbf{k}_i)\cdot\mathbf{R}_\alpha}\sum_{L,L'}Y_L(\mathbf{k}_f)Y^*_{L'}(\hat{\mathbf{k}}_i)[\tilde{t}\{\tilde{I}-\tilde{B}(\mathbf{k}_i)\tilde{t}\}^{-1}]_{LL'}, \qquad (29)$$

where

$$[\tilde{B}(\mathbf{k}_i)]_{LL'} \equiv B_{LL'}(\mathbf{k}_i) = \sum_{\mathbf{R}_\beta \neq 0} G_{LL'}(\mathbf{R}_\beta) e^{-i\mathbf{k}_i \cdot \mathbf{R}_\beta} . \tag{30}$$

Comparison between Eqs. (2) and (29) gives

$$T_{LL'} = \sum_\alpha e^{-i(\mathbf{k}_f - \mathbf{k}_i)\cdot \mathbf{R}_\alpha} [\tilde{t}\{\tilde{I} - \tilde{B}(\mathbf{k}_i)\tilde{t}\}^{-1}]_{LL'} . \tag{31}$$

Equation (31) has a very similar form to Eq. (15). Namely, if $\tilde{t}\{\tilde{I} - \tilde{B}(\mathbf{k}_i)\tilde{t}\}^{-1}$ is taken as the T matrix for a unit cell, the effect of the multiple scattering among the different cells does not appear explicitly. This effect only appears through $\tilde{B}(\mathbf{k}_i)$. For this reason, the physical discussion can be confined within a unit cell in the presence of the translational invariance.

Next, let us consider the case of more than one atom in a unit cell. Introducing the condition of the translational invariance into Eq. (17), we can modify it as

$$\begin{aligned} \tilde{T}(\mathbf{k}_f, \mathbf{k}_i) = & (e^{-i(\mathbf{k}_f - \mathbf{k}_i)\cdot \mathbf{d}_1} \tilde{I} \cdots e^{-i(\mathbf{k}_f - \mathbf{k}_i)\cdot \mathbf{d}_n} \tilde{I}) \\ & \times \left[(e^{-i(\mathbf{k}_f - \mathbf{k}_i)\cdot \mathbf{R}_1} \tilde{I} \cdots e^{-i(\mathbf{k}_f - \mathbf{k}_i)\cdot \mathbf{R}_N} \tilde{I}) T_w(\mathbf{k}_i) [\mathcal{I} - X(\mathbf{k}_i) T_w(\mathbf{k}_i)]^{-1} \begin{bmatrix} \tilde{I} \\ \vdots \\ \tilde{I} \end{bmatrix} (1) \right] \begin{bmatrix} \tilde{I} \\ \vdots \\ \tilde{I} \end{bmatrix} (1) \\ & \qquad \begin{matrix} \\ \\ (N) \end{matrix} \qquad \begin{matrix} \\ \\ (n) \end{matrix} \\ = & \sum_s e^{-i(\mathbf{k}_f - \mathbf{k}_i)\cdot \mathbf{d}_s} \sum_\alpha e^{-i(\mathbf{k}_f - \mathbf{k}_i)\cdot \mathbf{R}_\alpha} T^\alpha_{LL'}(\mathbf{k}_i) , \end{aligned} \tag{32}$$

where

$$T^\alpha_{LL'}(\mathbf{k}_i) = \sum_{\beta=1}^{N} \{T_w(\mathbf{k}_i)[\mathcal{I} - X(\mathbf{k}_i) T_w(\mathbf{k}_i)]^{-1}\}_{\alpha L, \beta L'} , \tag{33}$$

$$T_w(\mathbf{k}_i) = T_t [\mathcal{I} - g(\mathbf{k}_i) T_t]^{-1} , \tag{34}$$

$$[X(\mathbf{k}_i)]_{\alpha L, \beta L'} \equiv \sum_{\mathbf{d}_t \neq 0} G_{LL'}(\mathbf{d}_t + \mathbf{R}_\alpha - \mathbf{R}_\beta) e^{-i\mathbf{k}_i \cdot (\mathbf{d}_t + \mathbf{R}_\alpha - \mathbf{R}_\beta)} , \tag{35}$$

and

$$G_{LL'}(\mathbf{R}) = -\frac{8\pi m_e i k}{\hbar^2} \sum_{L''} i^{l''} (-1)^{m''} C^{L}_{L'\bar{L}''} h^{(1)}_{l''}(kR) Y_{L''}(\hat{\mathbf{R}}) . \tag{36}$$

In Eq. (32), the number of atoms in a unit cell is assumed to be N, and we have used the following identity relationship:

$$\left[\begin{bmatrix} \tilde{P}(\mathbf{R}_1) \\ \vdots \\ \tilde{P}(\mathbf{R}_N) \end{bmatrix} \tilde{G}^{st} (\tilde{P}(-\mathbf{R}_1) \cdots \tilde{P}(-\mathbf{R}_N)) \right]_{\alpha L, \beta L'} = G_{LL'}(\mathbf{d}_s - \mathbf{d}_t + \mathbf{R}_\alpha - \mathbf{R}_\beta) . \tag{37}$$

Substituting Eq. (32) into Eq. (2), we can obtain the expression for $T(\mathbf{k}_f, \mathbf{k}_i)$. The difference between Eqs. (33) and (16b) clearly shows the role of the translational invariance. Equations (13), (17), (28), (31), and (32) constitute the general framework of the electron multiple-scattering theory. Especially, in the presence of the two-dimensional translational invariance, Eqs. (31) and (32) can reproduce the LEED wave functions[3] (see Appendix A for details). In the case of muffin-tin potentials, the T matrix given by Eq. (10) can be written as follows:

$$t^\alpha_{LL'}(k) = t^\alpha_l(k) \delta_{LL'} = -\frac{\hbar^2}{2m_e k} e^{i\delta^\alpha_l} (\sin\delta^\alpha_l) \delta_{LL'} \quad (\alpha = 1, \ldots, N) , \tag{38}$$

where δ^α_l is the phase shift. The method of calculating the phase shift for a spherically symmetric potential can be found in any standard quantum-mechanics textbook. For a nonspherical potential, we presented a technique for calculating its T matrix,[11] and methods for obtaining $t_{LL'}(k)$ for molecules have been developed by Takatsuka and McKoy,[12] and others.[13–15] It is possible, then, to study various electron scattering problems with Eq. (13) or Eq. (17).

III. MULTIPLE SCATTERING OF A PHOTOELECTRON

In this section, we investigate the problem of the multiple scattering of a photoelectron. It is known as the central issue of the angle-resolved x-ray photoelectron spectroscopy (XPS). In general, the photoelectron wave function is written as[16,17]

$$\phi^{\rm opt}(\mathbf{r})=-\frac{2m_e ik}{\hbar^2}\sum_L A_L i^l h_l^{(1)}(k|\mathbf{r}-\mathbf{R}_s|) \times Y_L((\mathbf{r}-\mathbf{R}_s)/|\mathbf{r}-\mathbf{R}_s|)\ , \tag{39}$$

where $\mathbf{R}_s$ is the position of the emitter of a photoelectron. The major difference from the previous case is that here the incident wave is not the plane wave but the spherical wave. In order to obtain the T matrix for a photoelectron, let us determine its derivation by writing the similarities and the differences explicitly. Using the following relationship:

$$h_l^{(1)}(k|\mathbf{r}-\mathbf{R}_s|)Y_L((r-R_s)/|\mathbf{r}-\mathbf{R}_s|)=-\frac{\hbar^2}{2m_e ik}\sum_{L'} G_{L'L}^{\alpha s} i^{l'-l} j_{l'}(k|\mathbf{r}-\mathbf{R}_\alpha|)Y_{L'}((\mathbf{r}-\mathbf{R}_\alpha)/|\mathbf{r}-\mathbf{R}_\alpha|)\ , \tag{40}$$

Eq. (33) can be modified as

$$\phi^{\rm opt}(\mathbf{r})=\sum_{L,L'}[i^{l'}j_{l'}(k|\mathbf{r}-\mathbf{R}_\alpha|)Y_{L'}((\mathbf{r}-\mathbf{R}_\alpha)/|\mathbf{r}-\mathbf{R}_\alpha|)]G_{L'L}^{\alpha s}A_L\ . \tag{41}$$

On the other hand, from Eqs. (3), (10), (11), and the identity relationship

$$e^{i\mathbf{k}\cdot\mathbf{r}}=e^{i\mathbf{k}\cdot\mathbf{R}_\alpha}e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{R}_\alpha)} \tag{42a}$$

or

$$\sum_L[4\pi Y_L^*(\hat{\mathbf{k}})][i^l j_l(kr)Y_L(\hat{\mathbf{r}})]=\sum_L[4\pi Y_L^*(\hat{\mathbf{k}})][e^{i\mathbf{k}\cdot\mathbf{R}_\alpha}i^l j_l(k|\mathbf{r}-\mathbf{R}_\alpha|)Y_L((\mathbf{r}-\mathbf{R}_\alpha)/|\mathbf{r}-\mathbf{R}_\alpha|)]\ , \tag{42b}$$

we can easily recognize that (a) $\{i^l j_l(kr)Y_L(\hat{\mathbf{r}})\}$ corresponds to the base set of the electron-scattering state in both cases, (b) $4\pi Y_L(\hat{\mathbf{k}}_f)$ and $4\pi Y_L^*(\hat{\mathbf{k}}_i)$ in Eq. (3) come from the scattered and the incident plane waves, respectively, and (c) $\{e^{i\mathbf{k}\cdot\mathbf{R}_\alpha}\}$ in Eq. (13) also originate in the plane waves. Taking all of these into account and comparing Eqs. (35) and (36b), we can deduce the T matrix for a photoelectron as

$$T^{\rm opt}(\mathbf{k}_f,\phi^{\rm opt})\equiv\langle\mathbf{k}_f|T|\phi^{\rm opt}\rangle=\sum_{L,L'}4\pi Y_L(\hat{\mathbf{k}}_f)Q_{LL'}\ , \tag{43a}$$

$$\tilde{Q}=(e^{-i\mathbf{k}_f\cdot\mathbf{R}_1}\tilde{I}\cdots e^{-i\mathbf{k}_f\cdot\mathbf{R}_N}\tilde{I})T_t(\mathcal{J}-GT_t)^{-1}G\begin{pmatrix}\tilde{0}\\ \tilde{A}\\ \tilde{0}\\ \vdots\\ \tilde{0}\end{pmatrix}(s)\ , \tag{43b}$$

where $(\tilde{A})_{LL'}=A_L\delta_{LL'}$. Using the following relationship:

$$h_l^{(1)}(kr)=(-i)^{l+1}\frac{e^{ikr}}{kr}\quad(r\to\infty)\ , \tag{44}$$

and neglecting the effect of multiple scattering, we can reproduce the standard expression for the scattered wave function of the XPS from Eq. (37) (see Appendix A for details).

A summing formula for $\tilde{Q}$, which corresponds to Eq. (17) for $\tilde{T}$, can also be deduced as

$$\tilde{Q}=(e^{-i\mathbf{k}_f\cdot\mathbf{d}_1}\tilde{I}\cdots e^{-i\mathbf{k}_f\cdot\mathbf{d}_n}\tilde{I}) \times(T^{fo}+T^f(\mathcal{J}-GT^0)^{-1}GT^{io})\begin{pmatrix}\tilde{I}\\ \tilde{0}\\ \tilde{0}\\ \vdots\\ \tilde{0}\end{pmatrix}\ , \tag{45}$$

where

$$T^{fo}=\begin{pmatrix}\tilde{T}^{fo(1)} & \tilde{0} & \tilde{0} & \cdots & \tilde{0}\\ \tilde{0} & \tilde{0} & & & \tilde{0}\\ \tilde{0} & & \ddots & & \\ \vdots & & & & \\ \tilde{0} & \tilde{0} & & & \tilde{0}\end{pmatrix}\ , \tag{46a}$$

$$\tilde{T}^{fo(1)}=(e^{-i\mathbf{k}_f\cdot\mathbf{R}_1^{(1)}}\tilde{I}\cdots e^{-i\mathbf{k}_f\cdot\mathbf{R}_N^{(1)}}\tilde{I})T_w^{(1)}G^{(1)}\begin{pmatrix}\tilde{0}\\ \tilde{A}\\ \tilde{0}\\ \vdots\\ \tilde{0}\end{pmatrix}(s)\ , \tag{46b}$$

$$T^{io}=\begin{pmatrix}\tilde{T}^{fo(1)} & \tilde{0} & \tilde{0} & \cdots & \tilde{0}\\ \tilde{0} & \tilde{0} & & & \tilde{0}\\ \tilde{0} & & \ddots & & \\ \vdots & & & & \\ \tilde{0} & \tilde{0} & & & \tilde{0}\end{pmatrix}\ , \tag{47a}$$

and

$$\tilde{T}^{io(1)}=[\tilde{P}(-\mathbf{R}_1^{(1)})\cdots\tilde{P}(-\mathbf{R}_N^{(1)})]T_w^{(1)}G^{(1)}\begin{bmatrix}\tilde{0}\\ \tilde{A}\\ \tilde{0}\\ \vdots\\ \tilde{0}\end{bmatrix}(s) \quad . \quad (47b)$$

In Eq. (39), the emitter of a photoelectron is assumed to be the sth atom of group "1." T^0, T^f, T_w, G, and other matrices have been defined in Sec. II.

IV. APPLICATION TO THE FOCUSING OF THE ELECTRON SCATTERING

Recently, we have studied the problem of the focusing of the electron scattering using two atoms.[9] Due to the present work, we are now in a position to be able to find the proper configuration using an arbitrary number of atoms. Here, using up to ten periodically placed Si atoms in a row, we have studied two cases. Namely, the incident direction is parallel to the Si row [see Fig. 1(a) (case I)], or perpendicular to it [see Fig. 2(a) (case II)]. When every atom is of the same type, if we neglect the multiple scattering (kinematic case), Eq. (13) becomes

$$T_{LL'}=\sum_\alpha e^{-i(\mathbf{k}_f-\mathbf{k}_i)\cdot\mathbf{R}_\alpha}t_{LL'} \quad . \quad (48)$$

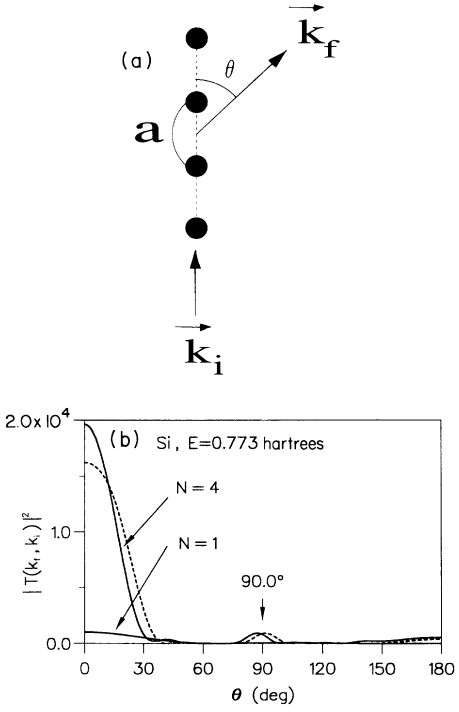

FIG. 1. Electron multiple scattering by Si atoms. (a) Schematic view of the scattering. (b) Differential cross section as a function of θ. Solid lines represent results of the present theory, the dotted line represents results of the kinematic theory. Incident electron energy $E=0.773$ hartrees, $a=5.05a_0$, N is the number of Si atoms, and a_0 is the Bohr radius.

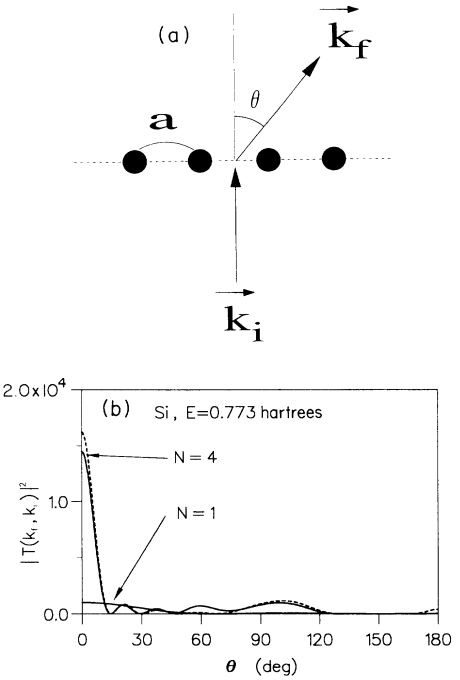

FIG. 2. Same as Fig. 1.

Then, we have

$$|T(\mathbf{k}_f,\mathbf{k}_i)|^2=\left|\sum_\alpha e^{-i(\mathbf{k}_f-\mathbf{k}_i)\cdot\mathbf{R}_\alpha}\right|^2|t(\mathbf{k}_f,\mathbf{k}_i)|^2 \quad (49)$$

or

$$|T(\mathbf{k}_i,\mathbf{k}_i)|^2=N^2|t(\mathbf{k}_i,\mathbf{k}_i)|^2$$

for the forward scattering. Namely, in the kinematic case the forward scattering by N scatterers is enhanced by N^2 compared with that of one scatterer. In Figs. 1(b) and 2(b), we show the comparison between the present theory (solid lines) and the kinetic case (dotted lines). Varying from $N=1$ to 10, we have investigated the effect of the multiple scattering. For simplicity, we show only the case of $N=4$ here. Well-defined peaks show up and grow with the number of scatterers at around

$$\theta=\tan^{-1}\{[k^2-(k_z+g_z)^2]^{1/2}/(k_z+g_z)\} \quad \text{(case I)} \, ,$$

and

$$\theta=\tan^{-1}[g_z/(k^2-g_z^2)^{1/2}] \quad \text{(case II)} \, ,$$

which correspond to those of the infinite one-dimensional system. At $E=0.773$ hartrees, they are $\theta=0°$ and 90.0° (case I), and $\theta=0°$ (case II), where g_z is the one-dimensional reciprocal lattice vector. The maximum value in case I was 2.89×10^4 at $N=6$, and that in case II was 8.63×10^4 at $N=10$. But as far as the forward scattering is concerned, its intensity is not significantly enhanced compared with that of the kinetic case in general. Namely, the multiple scattering does not always work favorably for the enhancement of the forward scattering. Furthermore, we have investigated the case presented in Fig. 3, where the T matrix can be calculated

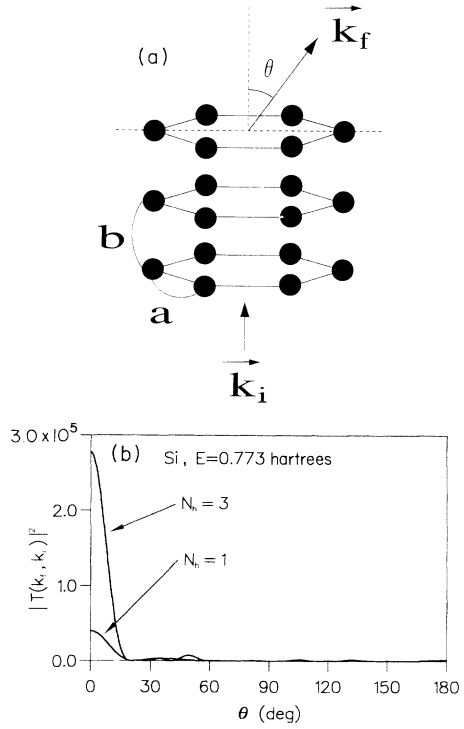

FIG. 3. Electron multiple scattering by Si hexagon clusters. (a) Schematic view of the scattering. (b) Differential cross section as a function of θ. $E=0.773$ hartrees, $a=5.05a_0$, $b=11.8a_0$, and N_h is the number of hexagons.

with Eq. (13) directly, or with Eq. (17) by utilizing the T matrix as a hexagon cluster.

V. DISCUSSIONS

We have developed a formalism to calculate the T matrix for a system of arbitrary numbers of scatterers as described by Eqs. (13) and (32). The important point here is that the T matrix is obtained through the multicenter-expansion method. Therefore, the angular momentum space does not expand even after assembling the individual T matrices. The summing formula for the sets of T matrices represented by Eq. (17) was also derived. It is then possible to handle large systems with Eq. (17). Furthermore, if the system consists of the collection of the basic structures, total computing time can be reduced dramatically using Eq. (17). Although we have used only atoms of the same type in Sec. IV to demonstrate the present theory, Eqs. (13), (17), and (32) can accept T matrices of any kind as long as they are prepared separately. We have also extended the present theory to the study of the multiple scattering of a photoelectron.

In this paper, we have discussed only the elastic process. In the inelastic scattering, general situations may not be as simple as the elastic process. The problem of inelastic electron scattering by an adsorbate is briefly discussed in Appendix B. We plan to present a study of electron multiple scattering in the general inelastic process in the near future.

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APPENDIX A: SCATTERED ELECTRON WAVE FUNCTIONS

In the framework of the Lippman-Schwinger equation,[18] the scattered-electron wave function is written as

$$\psi_{\text{scatt}}=G_0 T\phi_{\text{in}} , \tag{A1}$$

where $\phi_{\text{in}}=e^{i\mathbf{k}_i\cdot\mathbf{r}}$ is the incident wave. The free Green's function can be written as

$$G_0(\mathbf{r}-\mathbf{r}')=-\frac{2m_e}{\hbar^2}\frac{1}{4\pi}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}$$
$$\rightarrow-\frac{2m_e}{\hbar^2}\frac{1}{4\pi}\frac{e^{ikr}}{r}e^{-i\mathbf{k}_f\cdot\mathbf{r}'}\quad(r\rightarrow\infty) . \tag{A2}$$

Then, Eq. (A1) for the scattering by a cluster becomes

$$\psi_{\text{scatt}}(\mathbf{r})=-\frac{2m_e}{\hbar^2}\frac{1}{4\pi}\frac{e^{ikr}}{r}\langle\mathbf{k}_f|T|\mathbf{k}_i\rangle . \tag{A3}$$

On the other hand, in the presence of the two-dimensional translational invariance, using

$$G_0(\mathbf{r}-\mathbf{r}')=\frac{2m_e}{\hbar^2}\int\frac{d\mathbf{q}}{(2\pi)^3}\frac{e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}}{k^2-q^2+i\eta} , \tag{A4}$$

$$\sum_\alpha e^{i(\mathbf{k}_f-\mathbf{k}_i)\cdot\mathbf{R}_\alpha}=(2\pi)^2\sum_{\mathbf{g}}\delta(\mathbf{k}_{f\parallel}-\mathbf{k}_{i\parallel}-\mathbf{g}) , \tag{A5}$$

and Eq. (29), Eq. (A1) becomes

$$\psi_{\text{scatt}}(\mathbf{r})=\frac{2m_e}{\hbar^2}\int\frac{d\mathbf{k}_f}{(2\pi)^3}\frac{e^{i\mathbf{k}_f\cdot\mathbf{r}}}{k^2-k_f^2+i\eta}\langle\mathbf{k}_f|T|\mathbf{k}_i\rangle$$
$$=-\frac{m_e i}{\hbar^2}\sum_{\mathbf{g}}\frac{e^{i\mathbf{k}_{\mathbf{g}}\cdot\mathbf{r}}}{k_z(\mathbf{g})}\langle\mathbf{k}_{\mathbf{g}}|t|\mathbf{k}_i\rangle , \tag{A6}$$

where

$$\langle\mathbf{k}_{\mathbf{g}}|t|\mathbf{k}_i\rangle=(4\pi)^2\sum_{L,L'}Y_L(\hat{\mathbf{k}}_{\mathbf{g}})Y_{L'}^*(\hat{\mathbf{k}}_i)$$
$$\times[\tilde{t}\{\tilde{I}-\tilde{B}(\mathbf{k}_i)\tilde{t}\}^{-1}]_{LL'} , \tag{A7}$$
$$\mathbf{k}_{\mathbf{g}}=[\mathbf{k}_{i\parallel},k_z(\mathbf{g})] ,$$
$$k_z(\mathbf{g})=\text{sgn}(z)[k^2-(\mathbf{k}_{i\parallel}+\mathbf{g})^2]^{1/2} ,$$

$\mathbf{g}$ is the two-dimensional reciprocal-lattice vector, $\text{sgn}(z)=1$ for $z\geq 0$ and -1 for $z<0$, $\mathbf{k}_{i\parallel}$ is the parallel component of the incident wave vector. Equation (A6) corresponds to the LEED wave function. Similarly, using Eq. (32) the LEED wave function for the composite layer can be derived easily.

In the case of the scattering of a photoelectron, the incident wave becomes the spherical wave, namely, $\phi_{\text{in}}=\phi^{\text{opt}}(\mathbf{r})$. The corresponding scattered wave then becomes

$$\psi_{\text{scatt}}(\mathbf{r})=-\frac{2m_e}{\hbar^2}\frac{1}{4\pi}\frac{e^{ikr}}{r}\langle \mathbf{k}_f|T|\phi^{\text{opt}}\rangle \quad (r\to\infty)\,. \tag{A8}$$

On the other hand, substituting Eq. (44) into Eq. (39), we have

$$\phi^{\text{opt}}(\mathbf{r})=-\frac{2m_e}{\hbar^2}\sum_L A_L Y_L(\mathbf{k}_f)\frac{e^{ikr}}{r} \quad (r\to\infty)\,. \tag{A9}$$

The total wave function then becomes

$$\begin{aligned}\psi_{\text{total}}(\mathbf{r})&=\phi^{\text{opt}}(\mathbf{r})+\psi_{\text{scatt}}(\mathbf{r})\\&=-\frac{2m_e}{\hbar^2}\frac{e^{ikr}}{r}\left[\sum_L A_L Y_L(\hat{\mathbf{k}}_f)+\frac{1}{4\pi}\langle \mathbf{k}_f|T|\phi^{\text{opt}}\rangle\right]\\&=-\frac{2m_e}{\hbar^2}\frac{e^{ikr}}{r}\sum_{L,L'} Y_L(\hat{\mathbf{k}}_f)[\tilde{A}+\tilde{Q}]_{LL'}\,.\end{aligned} \tag{A10}$$

Equation (A10) is the generalized wave function for the photoelectron of the XPS.

APPENDIX B: INELASTIC ELECTRON SCATTERING BY AN ADSORBATE

Elastic scattering by an adsorbate on the solid surface can easily be handled by Eq. (13). Let us generalize the present theory further to the inelastic process.[19] Assigning 1 to the adsorbate responsible for the inelastic scattering, the T matrix corresponding to Eq. (3) becomes

$$\begin{aligned}T(\mathbf{k}_f,\mathbf{k}_i)=(4\pi)^2\sum_{L,L'} Y_L(\mathbf{k}_f)[K_f(\mathcal{J}-T_t^f G^f)^{-1}T_t^{fi}\\ \times(\mathcal{J}-G^i T_t^i)^{-1}K_i^+]_{LL'}\\ \times Y_{L'}^*(\hat{\mathbf{k}}_i)\,,\end{aligned} \tag{B1}$$

where

$$T_t^{fi}=\begin{bmatrix}\tilde{t}_1^{fi} & \tilde{0} & \tilde{0} & \cdots & \tilde{0}\\ \tilde{0} & \tilde{0} & & & \tilde{0}\\ \tilde{0} & & \ddots & & \\ \vdots & & & & \\ \tilde{0} & \tilde{0} & & & \tilde{0}\end{bmatrix}, \tag{B2}$$

and $\tilde{t}_1^{fi}$ is the T matrix in the angular momentum space for inelastic scattering by an adsorbate. In Eqs. (B1) and (B2), i and f stand for the initial (E_i) and final (E_f) electron energy states before and after the inelastic scattering by an adsorbate, respectively. T_t^f and T_t^i are T matrices for the elastic process, and G^f and G^i are free Green's functions. Their corresponding energies are E_i and E_f, respectively.

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