# Note on the Theory of Elastic Low-Energy-Electron Diffraction from a Vibrating Lattice*

C. B. Duke and D. L. Smith
*Department of Physics, Materials Research Laboratory, and Coordinated Science Laboratory, University of Illinois, Urbana, Illinois* 61801

and

B. W. Holland
*School of Physics, University of Warwick, Coventry, England*

(Received 8 November 1971)

The multiple-scattering series for the elastic electron-solid differential cross section is reduced to a set of coupled equations for layer scattering amplitudes by first performing the partial-wave decomposition of this series and subsequently defining the layer amplitudes as subsums of the complete series. The resulting equations are identical to those derived by Laramore and Duke in a recent paper. However, Laramore and Duke's derivation, in which the subsums of the multiple-scattering series were performed prior to the partial-wave decomposition, contains an ambiguity in the latter step which is avoided by our analysis.

In a recent set of papers,[1,2] Duke and Laramore constructed a general theory of electron scattering from a vibrating lattice[1] (hereafter referred to as DL) and applied this theory to evaluate the temperature dependence of the elastic-scattering differential cross sections[2] (hereafter referred to as LD). The essence of the second analysis is the reduction of an infinite series of mulitple-scattering integrals to a set of coupled algebraic equations for the elastic-scattering amplitudes of the electron from individual planar "layers" of scatterers. In their derivation LD proceeded by first deriving a set of coupled integral equations for the layer scattering amplitudes and subsequently reducing these integral equations to algebraic equations by a partial-wave expansion technique. However, their derivation[2] of Eq. (33) from Eq. (32) [and implicitly of Eq. (49) from Eqs. (3), (32), (33), and (48)] is not clear. The problem with their presentation lies in the apparent assumption of the validity of a partial-wave expansion of the layer ("subplane") scattering amplitudes [e.g., $\tau_\lambda(\vec{k}_f, \vec{k}_i, E)$ in the case of Eq. (33)] in the process of deriving a matrix equation for the expansion coefficients [e.g., the $\tau_\lambda^{LL'}(k_f, k_i)$] which contain matrix elements that depend explicitly on the direction of $\vec{k}_i$ [e.g., via $G^{sp}(\vec{k}, \vec{k}_i; E)$ in Eq. (33)].

In fact, the subplane scattering amplitudes for both a single subplane (i.e., the $\tau_\lambda^{LL'}$) and an array of subplanes (i.e., the $T_\lambda^{LL'}$) depend on the direction as well as magnitude of the wave vector $\vec{k}_i$ of the incident electron. Our purpose in this paper is to provide an explicit derivation of this result for a partial-wave expansion by performing the partial-wave expansion *prior* to the conversion of the multiple-scattering series to a set of coupled equations for layer scattering amplitudes. In our approach, the $\tau_\lambda^{LL'}$ and $T_\lambda^{LL'}$ are *defined* as the sum of certain series whose terms depend explicitly on $\vec{k}_i$. Therefore one is never led to suspect that their dependence on the direction of $\vec{k}_i$ might be incompatible with their definition as matrix elements (labeled by $L$ and $L'$) in a partial-wave expansion.

We find that $\tau_\lambda^{LL'}$ and $T_\lambda^{LL'}$ satisfy the equations derived by LD,[2] a result which implies that their derivation is not in error. Equations (32) in LD, and its analog for $T_\lambda^{LL'}$ obtained from Eq. (48), may be regarded as matrix eigenvalue equations associated with the spherical harmonics $Y_L(\Omega)$ as eigenvectors. The procedure followed by LD was to construct a solution to the resulting zero-eigenvalue determinental equation by requiring that all the matrix elements vanish individually. Our analysis verifies that the $\tau_\lambda^{LL'}$ and $T_\lambda^{LL'}$ generated in this manner are identical to those obtained from a straightforward summation of the multiple-scattering series following an angular momentum decomposition of the scattering amplitudes of the individual electron–ion-core scattering amplitudes.

The starting point of our calculation is Eq. (63) in DL for the multiple-scattering series for the elastic electron-solid scattering amplitude $R(\vec{k}_f, \vec{k}_i, E)$:

$$R(\vec{k}_f, \vec{k}_i; E) = \sum_n B(n; \vec{k}_f, \vec{k}_i; E) + \sum_{n \neq m} \sum_{\vec{k}_1} B(n; \vec{k}_1, \vec{k}_i; E) G(\vec{k}_1, E) B(m; \vec{k}_f, \vec{k}_1; E)$$

$$+\sum_{n\neq m;m\neq l}\sum_{\vec{k}_1,\vec{k}_2} B(n;\vec{k}_1,\vec{k}_i;E)G(\vec{k}_1,E)B(m;\vec{k}_2,\vec{k}_1,E)G(\vec{k}_2,E)\,B(l;\vec{k}_f,\vec{k}_2;E)+\cdots \quad . \tag{1}$$

The $B(n;\vec{k}',\vec{k};E)$ are the renormalized electron–ion-core interaction vertices defined by Eq. (60) in DL. It is convenient to rewrite Eq. (1) as

$$R(\vec{k}_f,\vec{k}_i;E)=\sum_{j=0}^{\infty} R_j(\vec{k}_f,\vec{k}_i;E) \quad , \tag{2a}$$

$$R_0(\vec{k}_f,\vec{k}_i;E)=\sum_n B(n;\vec{k}_f,\vec{k}_i;E) \quad , \tag{2b}$$

$$R_1(\vec{k}_f,\vec{k}_i;E)=\sum_{n\neq m}\sum_{\vec{k}_1} B(n;\vec{k}_1,\vec{k}_i;E)G(\vec{k}_1;E) \times B(m;\vec{k}_f,\vec{k}_1;E) \quad . \tag{2c}$$

The definition of the general term $R_n$ is evident from Eqs. (1) and (2) so we do not display it explicitly. Following Eq. (64) in DL, we define the reduced ion-core scattering vertices $b_n(\vec{k}_2,\vec{k}_1;E)$ according to

$$B(n;\vec{k}_2,\vec{k}_1;E)=e^{-i(\vec{k}_2-\vec{k}_1)\cdot\vec{R}_n^0}\,b_n(\vec{k}_2,\vec{k}_1;E) \quad . \tag{3}$$

We decompose $b_n(\vec{k}_2,\vec{k}_1;E)$ into partial waves via $[L\equiv(l,m)]$

$$b_n(\vec{k}_2,\vec{k}_1;E)=\sum_{L,L'} b_n^{LL'}(k_2,k_1;E)Y_L^*(\hat{k}_2)Y_{L'}(\hat{k}_1) \quad . \tag{4}$$

We proceed by examining the partial-wave decomposition of each term in the series specified by Eq. (2a) and subsequently performing partial summations of these terms to define appropriate planar scattering amplitudes. The results for $R_0$ are self-evident from Eqs. (2b) and (4):

$$R_0(\vec{k}_f,\vec{k}_i;E)=\sum_n e^{i(\vec{k}_i-\vec{k}_f)\cdot\vec{R}_n^0} \times\sum_{LL'} b_n^{LL'}(k_f,k_i;E)Y_L^*(\hat{k}_f)Y_{L'}(\hat{k}_i) \quad . \tag{5}$$

Turning to a consideration of $R_1$, we use Eqs. (2) and (3) to obtain

$$R_1(\vec{k}_f,\vec{k}_i;E)=\sum_{n\neq m}\int\frac{d^3k_1}{(2\pi)^3}\,e^{i(\vec{k}_i\cdot\vec{R}_n^0-\vec{k}_f\cdot\vec{R}_m^0)} \times b_n(\vec{k}_1;\vec{k}_i;E)G(\vec{k}_1,E)b_m(\vec{k}_f,\vec{k}_1,E) \times e^{-i\vec{k}_1\cdot(\vec{R}_n^0-\vec{R}_m^0)} \quad . \tag{6}$$

We substitute into Eq. (6) the partial-wave expansions for $b_n$ and $b_m$ [Eq. (4)]; the definition for $G(\vec{k}_1;E)$:

$$G(\vec{k}_1;E)=\lim_{\epsilon\to 0^+}(-2m/\hbar^2)[k_1^2-k^2(E)-i\epsilon]^{-1} \quad , \tag{7a}$$

$$k^2(E)=2m[E-\Sigma(E)]/\hbar^2 \quad ; \tag{7b}$$

and the partial-wave expansion for the exponential:

$$e^{-i\vec{k}\cdot\vec{R}}=\sum_L 4\pi(-i)^l j_l(kR)Y_L(\hat{R})Y_L^*(\hat{k}) \quad . \tag{8}$$

The quantity $\Sigma(E)$ is the one-electron proper self-energy associated with electron-electron interactions as described by Eqs. (81) and (82) in LD, postulated by Duke and Tucker,[3] and derived by Duke and Laramore.[4] Using Eqs. (7) and (8) in Eq. (6) gives

$$R_1(\vec{k}_f,\vec{k}_i;E)=\sum_{n\neq m}\exp[i(\vec{k}_i\cdot\vec{R}_n^0-\vec{k}_f\cdot\vec{R}_m^0)]\sum_{L'L_1}Y_{L'}(\hat{k}_i)Y_{L_1}^*(\hat{k}_f)\sum_{LL_1L_2}Y_{L_2}(\vec{R}_n^0-\vec{R}_m^0) \times\frac{(-i)^{l_2}m}{\pi^2\hbar^2}\int_0^\infty dk_1\,\frac{k_1^2 b_n^{LL'}(k_1,k_i;E)b_m^{L_1L_1'}(k_f,k_1;F)j_{l_2}(k_1|\vec{R}_n^0-\vec{R}_m^0|)}{k^2(E)-k_1^2+i\epsilon}\int d\Omega_{k_1}Y_L^*(\hat{k}_1)Y_{L_1'}(\hat{k}_1)Y_{L_2}^*(\hat{k}_1). \tag{9}$$

The integral over the directions of $\vec{k}_1$ is well known.[5] We designate it by[2]

$$I(L_1',L,L_2)=\int d\Omega_{k_1}Y_{L_1'}(\hat{k}_1)Y_L^*(\hat{k}_1)Y_{L_2}^*(\hat{k}_1) \tag{10}$$

and note its evaluation in Eqs. (42) and (43) in LD.

Turning to our consideration of the radial integral in Eq. (9), we recall from Eqs. (40) in LD

$$b_n^{LL'}(k_1,k_i;E)=(-1)^l\,b_n^{LL'}(-k_1,k_i;E) \quad , \tag{11a}$$

$$b_m^{L_1L_1'}(k_f,k_1;E)=(-1)^{l_1'}\,b_m^{L_1L_1'}(k_f,-k_1;E) \quad . \tag{11b}$$

From these equations, the relation

$$j_{l_2}(kr)=(-1)^{l_2}j_{l_2}(-kr) \quad , \tag{12}$$

and the fact that

$$I(L_1',L,L_2)=0 \quad \text{unless} \quad l_1'+l+l_2=2m \quad , \tag{13}$$

we conclude that the integral of the radial integral is an even function of $k_1$ so that we can extend the range of the integral from $-\infty$ to $+\infty$.

After extending the $k_1$ integral to the range $(-\infty,\infty)$, we evaluate it by contour integration. This evaluation requires that we know the analytic structure $b_n^{LL'}(k,k';E)$ in the complex $k(k')$ plane

holding $k'(k)$ and $E$ as fixed real variables. An assumption, consistent with the model used by LD and others,[6-8] is that the $b_n$ do not exhibit any singularities in the upper-half $k(k')$ plane. This assumption is analogous to (and consistent with) that of nonoverlapping spherical potentials in the coordinate representation analysis of the rigid-lattice version of the theory.[9] However, our momentum-representation analysis also is valid for overlapping (but finite-range) and vibrating spherical potentials. Using these assumptions about the $b_n$, the formulas

$$j_l(u) = \tfrac{1}{2}[h_l^{(1)}(u) + h_l^{(2)}(u)] \quad , \tag{14a}$$

$$h_l^{(2)}(-u) = (-1)^l h_l^{(1)}(u) \quad , \tag{14b}$$

in which the $h_l^{(i)}(u)$ are the spherical Hankel functions,[2,10] and Eq. (13), we obtain

$$\int_0^\infty dk_1 \, \frac{k_1^2 b_n^{LL'}(k_1, k_i; E) b_m^{L_1 L_1'}(k_f, k_1; E) j_{l_2}(k_1 |\vec{R}_n^0 - \vec{R}_m^0|)}{k_1^2 - k^2(E) - i\epsilon}$$

$$= \tfrac{1}{2} i\pi [k(E) b_n^{LL'}(k(E), k_i; E) b_m^{L_1 L_1'}(k_f, k(E); E) h_{l_2}^{(1)}(k(E) |\vec{R}_n^0 - \vec{R}_m^0|)] \quad . \tag{15}$$

Substituting Eqs. (10) and (15) into Eq. (9) gives

$$R_1(\vec{k}_f, \vec{k}_i; E) = \sum_{n \neq m} \exp[i(\vec{k}_i \cdot \vec{R}_n^0 - \vec{k}_f \cdot \vec{R}_m^0)]$$

$$\times \sum_{L'L_1} Y_{L'}(\hat{k}_i) Y_{L_1}^*(\hat{k}_f) \sum_{LL_1'} b_n^{LL'}(k(E), k_i; E) \, b_m^{L_1 L_1'}(k_f, k(E); E) G_{L_1' L}(\vec{R}_n^0 - \vec{R}_m^0; E) \quad , \tag{16}$$

in which we have used the definition of the matrix elements $G_{L'L}$ of the Green's function

$$G_{L'L}(\vec{R}; E) = \frac{-imk(E)}{2\pi\hbar^2} \times \sum_{L_2} (-i)^{l_2} I(L', L, L_2) h_{l_2}^{(1)}(k(E)|\vec{R}|) Y_{L_2}(\hat{R}) \quad . \tag{17}$$

The expression for $R_1$ given by Eq. (16) completes the specification of the first two terms in the sum for $R(\vec{k}_f, \vec{k}_i, E_i)$ defined in Eq. (2a). Using the expressions (dropping superscript "0" for convenience)

$$\exp[i(\vec{k}_i \cdot \vec{R}_0 - \vec{k}_f \cdot \vec{R}_n)] = \exp[i(\vec{k}_i - \vec{k}_f) \cdot \vec{R}_n + \vec{k}_i \cdot (\vec{R}_0 - \vec{R}_n)] \quad , \tag{18}$$

and changing our notation to read

$$\sum_n \rightarrow \sum_{\vec{R}_n} \quad ,$$

we can obtain the general term in Eq. (2a) by induction. The result is specified by

$$R_n(\vec{k}_f, \vec{k}_i; E) = \sum_{\vec{R}_0, \vec{R}_1, \ldots, \vec{R}_n} e^{i(\vec{k}_i - \vec{k}_f) \cdot \vec{R}_n} \sum_{LL', L_1 L_1', \ldots, L_n L_n'} Y_{L'}(\hat{k}_i) Y_{L_n}^*(\hat{k}_f)$$

$$\times b_{\vec{R}_0}^{LL'}(k(E), k_i; E) b_{\vec{R}_1}^{L_1 L_1'}(k(E), k(E); E) \cdots b_{\vec{R}_n}^{L_n L_n'}(k_f, k(E); E)$$

$$\times e^{i\vec{k}_i \cdot (\vec{R}_0 - \vec{R}_1)} G_{L_1' L}(\vec{R}_0 - \vec{R}_1; E) \cdots e^{i\vec{k}_i \cdot (\vec{R}_{n-1} - \vec{R}_n)} G_{L_n' L_{n-1}}(\vec{R}_{n-1} - \vec{R}_n; E) \quad , \quad n \geq 1 \quad . \tag{19}$$

Equations (2a), (5), (16), and (19) completely specify $R(\vec{k}_f, \vec{k}_i; E)$ to be given by the schematic expression

$$R(\vec{k}_f, \vec{k}_i; E) = \sum_{LL'} Y_{L'}(\hat{k}_i) Y_L^*(\hat{k}_f) \sum_{\vec{R}} e^{i(\vec{k}_i - \vec{k}_f) \cdot \vec{R}} \sum_{j=0}^{\infty} \Bigg( \sum_{\vec{R}_0, \vec{R}_1, \ldots, \vec{R}_{j-1}} \sum_{L_0; L_1 L_1'; \ldots; L_{j-1} L_{j-1}'; L_j'} b_{\vec{R}_0}^{L_0 L'}(k(E), k_i; E)$$

$$\times b_{\vec{R}_1}^{L_1 L_1'}(k(E), k(E); E) \cdots b_{\vec{R}}^{L L_j'}(k_f, k(E), E) \, e^{i\vec{k}_i \cdot (\vec{R}_0 - \vec{R}_1)} G_{L_1' L_0}(\vec{R}_0 - \vec{R}_1; E) \cdots$$

$$\times e^{i\vec{k}_i \cdot (\vec{R}_{j-1} - \vec{R})} G_{L_j' L_{j-1}}(\vec{R}_{j-1} - \vec{R}; E) \Bigg) \quad . \tag{20}$$

Equation (20) is the final result of the first step in our calculation: i.e., the reduction of the sum of multiple-scattering integrals given in Eq. (1) to a sum of matrix products whose matrix elements are labeled by the angular momentum quantum numbers $L$. It is the finite-temperature analog

of Beeby's expression for the cross section [Eq. (8) in Ref. 9] based on his analysis of the rigid-lattice muffin-tin model.

The second step in our calculation is the conversion of the sum given in Eq. (20) to a sum over layer scattering amplitudes $T_\lambda^{LL'}$ which satisfy a set of coupled algebraic equations. This is accomplished by a partial subsummation of Eq. (20) originally referred to[9] as the "summation over paths." In this method, the sum over positions $\vec{R}$ is decomposed into a sum over planes of atoms parallel to the exposed surface of the solid. The sum over positions in an individual plane is further divided into a sum over identical subplanes each exhibiting the space-group symmetry of the lattice for translation parallel to the surface and containing only one atom per unit cell. The $||T_\lambda^{LL'}||$ are the scattering matrices for the subplane labeled by $\lambda$. Our performance of this step of the calculation differs from Beeby's original analysis only in that because of the inclusion of the consequences of lattice vibrations, the $||b_R^{LL'}||$ matrices in Eq. (20) are not diagonal in the $L$ indices (unlike Beeby's $t$ matrices).

Turning to our examination of Eq. (20), we consider only "energy-shell" scattering for which

$$k_f = k_i = k(E) \tag{21}$$

and recall that the $b_R^{LL'}$ depend only on the subplane index $\lambda$ (i.e., to be independent of the scatterer's position in the subplane). We first sum over terms in Eq. (20) in which all the $\vec{R}_i$ lie in the same subplane. We define the subplane scattering matrix $||\tau_\lambda^{LL'}||$ via

$$\tau_\lambda^{LL'}(\vec{k}_i) = \sum_{j=0}^{\infty} \Bigg( \sum_{\substack{\vec{R}_0,\vec{R}_1,\ldots,\vec{R}_{j-1} \\ \text{(All } R\text{'s in } \lambda \text{ subplane)}}} \sum_{L_0;L_1L_1';\ldots;L_{j-1}L_{j-1}';L_j'} b_\lambda^{L_0L'}(k(E)) b_\lambda^{L_1L_1'}(k(E)) \cdots b_\lambda^{LL_j'}(k(E))$$

$$\times e^{i\vec{k}_i\cdot(\vec{R}_0-\vec{R}_1)} G_{L_1'L_0}(\vec{R}_0-\vec{R}_1;E)\, e^{i\vec{k}_i\cdot(\vec{R}_1-\vec{R}_2)} G_{L_2'L_1}(\vec{R}_1-\vec{R}_2;E) \cdots e^{i\vec{k}_i\cdot(\vec{R}_{j-1}-\vec{R})} G_{L_j'L_{j-1}}(\vec{R}_{j-1}-\vec{R};E) \Bigg) \ . \tag{22}$$

If we designate the Bravais net vectors of the (identical) subplanes by $\vec{P}$, the terms in Eq. (22) may be regrouped to give

$$\tau_\lambda^{LL'}(\vec{k}_i) = \sum_{j=0}^{\infty} \sum_{L_0;L_1L_1';\ldots;L_{j-1}L_j';L_j'} b_\lambda^{LL_j'}(k(E)) G_{L_j'L_{j-1}}^{sp}(\vec{k}_i)$$

$$\times b_\lambda^{L_{j-1}L_{j-1}'}(k(E)) G_{L_{j-1}'L_{j-2}}^{sp}(\vec{k}_i) \cdots b_\lambda^{L_1L_1'}(k(E)) G_{L_1'L_0}^{sp}(\vec{k}_i) b_\lambda^{L_0L'}(k(E)) \ , \tag{23}$$

in which we used the definition of the "subplane propagator" $G_{L'L}^{sp}$:

$$G_{LL'}^{sp}(\vec{k}_i) = \sum_{\vec{P}\neq 0} e^{i\vec{k}_i\cdot\vec{P}} G_{LL'}(\vec{P};E) \ . \tag{24}$$

Equation (23) is just a power-series expansion of the matrix equation of the $\tau_\lambda^{LL'}$ given by

$$\tau_\lambda^{LL'}(\vec{k}_i) = b_\lambda^{LL'}(k(E)) + \sum_{L_1L_0} b_\lambda^{LL_1}(k(E)) \times G_{L_1'L_0}^{sp}(\vec{k}_i) \tau_\lambda^{L_0L'}(\vec{k}_i) \ . \tag{25}$$

We next consider those terms in the sum in Eq. (20) for which all the $\vec{R}$'s are in the $\lambda$th subplane except $\vec{R}_0$, which is the in subplane $\lambda_0$ ($\lambda_0 \neq \lambda$). The expression in brackets in Eq. (20) becomes

$$S_0 = \sum_{j=0}^{\infty} \sum_{\lambda_0,\lambda_0\neq\lambda} \sum_{L_0L_1'} \{b_\lambda(k(E))[G^{sp}(\vec{k}_i) b_\lambda(k(E))]^{j-1}\}_{LL_1'}$$

$$\times \sum_{\vec{P}} \exp[i\vec{k}_i\cdot(\vec{d}_{\lambda_0}-\vec{d}_\lambda+\vec{P})] G_{L_1'L_0}(\vec{d}_{\lambda_0}-\vec{d}_\lambda+\vec{P};E)$$

$$\times b_{\lambda_0}^{L_0L'}(k(E)) \ . \tag{26}$$

We use the symbol $\vec{d}_\lambda$ to designate the location, relative to an external coordinate system, of the vector $\vec{P}\equiv 0$ in the sum over $\vec{P}$ in the subplane labeled by $\lambda$. If we define the matrix elements of the interplanar propagator, $G_{LL'}^{\lambda\lambda_0}$, via

$$G_{L_1'L_0}^{\lambda\lambda_0}(\vec{k}_i) = \sum_{\vec{P}} \exp[i\vec{k}_i\cdot(\vec{d}_{\lambda_0}-\vec{d}_\lambda+\vec{P})] \times G_{L_1'L_0}(\vec{d}_{\lambda_0}-\vec{d}_\lambda+\vec{P};E) \ , \tag{27}$$

then Eq. (26) for $S_0$ becomes

$$S_0 = \sum_{\lambda_0;\lambda_0\neq\lambda} [\tau_\lambda(\vec{k}_i) G^{\lambda\lambda_0}(\vec{k}_i) b_{\lambda_0}(\vec{k}_i)]_{LL'} \ .$$

It is now clear that when we sum all terms in the sum in Eq. (20) for which there are two different values of $\lambda$ (all the $R$'s lie in one of two subplanes) the expression in large parentheses in Eq. (20) becomes

$$S_1 = \sum_{\lambda_0;\lambda_0\neq\lambda} [\tau_\lambda(\vec{k}_i) G^{\lambda\lambda_0}(\vec{k}_i) \tau_{\lambda_0}(\vec{k}_i)]_{LL'} \ .$$

More generally, when we sum over all terms in the sum in Eq. (20) for which $n$ values of $\lambda$ occur, the

expression in large parentheses becomes

$$S_n = \sum_{\lambda_1\lambda_2\lambda_3\cdots\lambda_{n-1};\lambda_i\neq\lambda_{i+1}} [\tau_\lambda(\vec{k}_t)G^{\lambda\lambda_1}(\vec{k}_t) \times\tau_{\lambda_1}(\vec{k}_t)\cdots G^{\lambda_{n-2}\lambda_{n-1}}(\vec{k}_t)\tau_{\lambda_{n-1}}(\vec{k}_t)]_{LL'}.$$

Summing over all values of $n$ for the bracketed expressions in Eq. (20) leads to our definition of the matrix elements of the "layer" scattering matrix $||T_\lambda^{LL'}||$:

$$\Big(\tau_\lambda(\vec{k}_t) + \sum_{\lambda_1;\lambda_1\neq\lambda} \tau_\lambda(\vec{k}_t)G^{\lambda\lambda_1}(\vec{k}_t)\tau_{\lambda_1}(\vec{k}_t) + \sum_{\lambda_1,\lambda_2;\lambda_1\neq\lambda,\lambda_2\neq\lambda} \tau_\lambda(\vec{k}_t)G^{\lambda\lambda_1}(\vec{k}_t)\tau_{\lambda_1}(\vec{k}_t)G^{\lambda_1\lambda_2}(\vec{k}_t)\tau_{\lambda_2}(\vec{k}_t) + \cdots\Big)_{LL'} = T_\lambda^{LL'}(\vec{k}_t) \quad . \tag{28}$$

Equation (28) is just the power-series expansion of our desired coupled linear equations for the layer scattering matrices:

$$T_\lambda^{LL'}(\vec{k}_t) = \tau_\lambda^{LL'}(\vec{k}_t) + \sum_{\lambda';\lambda'\neq\lambda} \sum_{L_1L_2} \times\tau_\lambda^{LL_1}(\vec{k}_t)G_{L_1L_2}^{\lambda\lambda'}(\vec{k}_t)T_{\lambda'}^{L_2L'}(\vec{k}_t) \quad . \tag{29}$$

Insertion of Eq. (29) into Eq. (20) gives our final expression for the electron-solid scattering amplitude

$$R(\vec{k}_f,\vec{k}_i;E) = \sum_{LL'} Y_{L'}(\hat{k}_i)Y_L^*(\hat{k}_f)N_{\|}\sum_{\vec{g}}\delta(\vec{k}_i-\vec{k}_f+\vec{g}) \times\sum_\lambda e^{i(\vec{k}_i-\vec{k}_f)\cdot\vec{d}_\lambda}T_\lambda^{LL'}(\vec{k}_i) \quad , \tag{30}$$

in which the $\vec{g}$ are the reciprocal-lattice vectors of the Bravais net of the (identical) subplanes, and $N_{\|}$ is the number of cells per unit area.

Equations (25), (29), and (30) are identical to Eqs. (54), (55), and (2), respectively, in LD. Therefore, as noted earlier in the paper, the results of LD are correct, although the derivation given by LD of Eqs. (54) and (55) from Eqs. (32) and (48) is, perhaps, less transparent than the one given above.

*Research supported in part by the Advanced Research Projects Agency under Contract No. HC 15-67-C-0221.

[1]C. B. Duke and G. E. Laramore, Phys. Rev. B 2, 4765 (1970), referred to as DL in the text.

[2]G. E. Laramore and C. B. Duke, Phys. Rev. B 2, 4783 (1970), referred to as LD in the text.

[3]C. B. Duke and C. W. Tucker, Jr., Surface Sci. 15, 231 (1969).

[4]C. B. Duke and G. E. Laramore, Phys. Rev. B 3, 3183 (1971).

[5]See, for example, K. Gottfried, *Quantum Mechanics* (Benjamin, New York, 1966), p. 290.

[6]S. Y. Tong and T. N. Rhodin, Phys. Rev. Letters 26, 711 (1971).

[7]D. W. Jepsen, P. M. Marcus, and F. Jona, Phys. Rev. Letters 26, 1365 (1971).

[8]G. E. Laramore, C. B. Duke, A. Bagchi, and A. B. Kunz, Phys. Rev. B 4, 2058 (1971).

[9]J. L. Beeby, J. Phys. C 1, 82 (1968).

[10]H. A. Antosiewicz, Natl. Bur. Std. (U.S.) Appl. Math. Ser. 55, 435 (1964).

PHYSICAL REVIEW B VOLUME 5, NUMBER 8 15 APRIL 1972

# Off-Center Direction of Certain Atomic Impurities in Alkali Halide Matrices

G. K. Pandey and D. K. Shukla

*Physics Department, Allahabad University, Allahabad, India*

(Received 10 November 1971)

The direction of the off-center displacement of certain atomic impurities in alkali halide matrices has been determined through calculations of certain barrier parameters. The controversial results for the RbCl: $Ag^+$ system and other systems like KCl: $Li^+$ and NaCl: $Li^+$ have been suitably discussed in the light of present calculations.

Recent experiments[1,2] have presented strong evidence for the off-centered position of certain atomic impurities in alkali halide matrices. For the RbCl: $Ag^+$ system, however, controversial results have been obtained by Kirby *et al.*[1] and Kapphan and Lüty.[2] The latter authors could explain their results on the basis of a ⟨111⟩ displacement direction, whereas the multiplet structure of the far-infrared absorption[1] ruled out such a configuration and presented evidence for a displacement in the ⟨110⟩ direction. We, in the present note, wish to present certain calculations of the barrier parameters, which will throw important light on this controversy concerning the displacement direction. For the sake of completeness, we also present calculations for the KCl: $Li^+$ and NaCl: $Li^+$ systems and