# Dielectric matrix for aluminum*

S. P. Singhal
*Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803*
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The dielectric screening matrix $\epsilon_{GG'}(\vec{q})$ for aluminum is evaluated using realistic band energies and wave functions. The Bloch states are obtained from a self-consistent tight-binding calculation in which Gaussian orbitals are used as basis functions. Results are presented for three principal directions of $\vec{q}$, [100], [110], and [111], with 15 values for the reciprocal-lattice vectors $\vec{G}$ and $\vec{G}'$. It is found that the off-diagonal elements are, in general, small compared to the diagonal terms and that the diagonal terms show some directional effect in their monotonic decrease as $|\vec{q}+\vec{G}|$ increases.

## I. INTRODUCTION

The response of electrons to a potential causes readjustment of their distribution and gives rise to the screening of the potential involving the well-known quantity, the dielectric function. This quantity plays an important role in the study of various properties, e.g., transport phenomenon, lattice defects, and optical properties. Consequently, it has been the subject of many investigations.

The formal theory of dielectric screening provides an expression for the dielectric matrix,[1-4]

$$\epsilon(\vec{Q},\vec{Q}') = \delta_{\vec{Q}\vec{Q}'} - V(\vec{Q})\chi^{(0)}(\vec{Q},\vec{Q}'),$$
$$\vec{Q}=\vec{q}+\vec{G},\quad \vec{Q}'=\vec{q}+\vec{G}', \tag{1}$$

where $V(\vec{Q})$ is the Fourier transform of the effective electron-electron interaction given by

$$V(\vec{Q}) = \frac{V^{(0)}(\vec{Q})}{1+V^{(0)}(\vec{Q})G(\vec{Q})\chi^{(0)}(\vec{Q},\vec{Q})} \ . \tag{2}$$

The function $G(\vec{Q})$ corrects for exchange and correlation effects.[5] The quantity $\chi^{(0)}(\vec{Q},\vec{Q}')$ is the irreducible polarization part of the density response matrix given in terms of Bloch states.

Most studies have concentrated on evaluating only the diagonal part[6] of the dielectric matrix or have approximated the Bloch states by slightly modified plane waves[7] to evaluate the off-diagonal terms. Recently there have been several studies[8-11] to evaluate $\epsilon(\vec{q},\omega)$ (only diagonal terms in $\vec{q},\vec{q}'$) utilizing the real band structures. Off-diagonal parts of the dielectric matrix have been evaluated for diamond,[4] silicon,[12] and transition metals (Pd and Ni).[13] We present here a method to evaluate the complete dielectric matrix by using realistic band structure and wave functions obtained from a tight-binding self-consistent calculation.[14] Such an exhaustive study has never been done before for any metal.

The basic formalism is presented in Sec. II. We start from the random-phase-approximation (RPA) expression for the dielectric matrix, expand the Bloch states in terms of the set of Gaussian functions used for the band-structure calculation, and obtain an expression that can be attacked numerically with the available data. Section III provides a brief summary of the band-structure calculation and some of the details of the Brillouin-zone integration using the tetrahedron method.[15] Results are presented in Sec. IV for three principal directions, [100], [110], and [111], for $\vec{q}$ and 15 values for the reciprocal-lattice vectors $\vec{G}$ and $\vec{G}'$. Owing to symmetry relations [Appendix and Eq. (32)], we need to evaluate a much smaller number (than the 225) of elements for each value of $\vec{q}$.

## II. FORMALISM

The response of the free electrons to the oscillations of the ions of the lattice is described by the dielectric matrix $\epsilon$. In the random-phase approximation, we have the basic result[16]

$$\epsilon_{ts}(\vec{p}) = \epsilon(\vec{p}+\vec{K}_t,\vec{p}+\vec{K}_s)$$
$$= \delta_{st} - \frac{4\pi e^2}{N\Omega(\vec{p}+\vec{K}_t)^2}\sum_{n\vec{k},l\vec{q}}\frac{N_n(\vec{k})-N_l(\vec{q})}{E_n(\vec{k})-E_l(\vec{q})}$$
$$\times\langle l\vec{q}|e^{i(\vec{p}+\vec{K}_s)\cdot\vec{r}}|n\vec{k}\rangle\langle n\vec{k}|e^{-i(\vec{p}+\vec{K}_t)\cdot\vec{r}}|l\vec{q}\rangle \ , \tag{3}$$

where $E_n(\vec{k})$ and $N_n(\vec{k})$ are the energy and the occupation number, respectively, of an electron of momentum $\vec{k}$ and band $n$; $|n\vec{k}\rangle$ is the Bloch state for such an electron, and $N$ is the number of unit cells of volume $\Omega$ each. The summation over bands and momentum vectors $\vec{k}$ and $\vec{q}$ is obviously limited to cases where one band is occupied and the other one is empty; both $\vec{k}$ and $\vec{q}$ vary over the whole of the first Brillouin zone (FBZ).

One must make some assumption about the Bloch states to obtain numerical results from Eq. (3). In the present case, we expand the Bloch states in terms of Gaussian orbitals to be able to use the realistic bands and wave functions obtained by a self-consistent band calculation.[14] We write

$$|n\vec{k}\rangle = \frac{1}{\sqrt{N}}\sum_{i,\mu}e^{i\vec{k}\cdot\vec{R}_\mu}a_{ni}(\vec{k})u_i(\vec{r}-\vec{R}_\mu) \ , \tag{4}$$

where $u_i(\vec{r}-\vec{R}_\mu)$ is a member of the set of the Gaussian orbitals (consisting of 52 such orbitals:

nine of $s$-type symmetry, six each of the three $p$ types, and five each of the five $d$ types) centered around the lattice point $\vec{R}_\mu$ and $a_{ni}(\vec{k})$ is the mixing coefficient. The self-consistent band calculation provides us the values of these $a_{ni}$'s for various bands and $\vec{k}$ points in the Brillouin zone.

Using expression (4) for the Bloch states, we simplify the matrix elements in Eq. (3), i.e.,

$$\begin{aligned}\langle l\vec{q}|e^{i(\vec{p}+\vec{K}_s)\cdot\vec{r}}|n\vec{k}\rangle &= \frac{1}{N}\sum_{ij,\mu\nu} e^{-i\vec{q}\cdot\vec{R}_\nu} a^*_{lj}(\vec{q}) a_{ni}(\vec{k}) e^{i\vec{k}\cdot\vec{R}_\mu} \\ &\times \langle u_j(\vec{r}-\vec{R}_\nu)|e^{i(\vec{p}+\vec{K}_s)\cdot\vec{r}}|u_i(\vec{r}-\vec{R}_\mu)\rangle \\ &= \frac{1}{N}\sum_{i,j} a^*_{lj}(\vec{q}) P_{ji}(\vec{p}+\vec{K}_s,\vec{q}) a_{ni}(\vec{k}) \\ &\times \sum_\mu e^{i(\vec{p}+\vec{k}-\vec{q})\cdot\vec{R}_\mu} \quad , \end{aligned} \tag{5}$$

where we have defined the matrix $P$ by

$$P_{ji}(\vec{q}_1,\vec{q}_2) = \sum_\mu e^{-i\vec{q}_2\cdot\vec{R}_\mu}\langle u_j(\vec{r}-\vec{R}_\mu)|e^{i\vec{q}_1\cdot\vec{r}}|u_i(\vec{r})\rangle . \tag{6}$$

The summation over $\mu$ can be carried out independently, using the fact that such a sum is zero unless $\vec{p}+\vec{k}-\vec{q}$ happens to be a reciprocal-lattice vector, to give

$$\begin{aligned}\frac{1}{N}\sum_\mu e^{i(\vec{p}+\vec{k}-\vec{q})\cdot\vec{R}_\mu} &= \begin{cases}1 & \text{whenever } \vec{p}+\vec{k}-\vec{q}=\vec{G}\\ 0 & \text{otherwise}\end{cases} \\ &= \sum_{\vec{G}} \delta_{\vec{k},\vec{q}-\vec{p}+\vec{G}} \quad . \end{aligned} \tag{7}$$

However, since $\vec{q}$ and $\vec{k}$ are limited to within the FBZ and in the presence of $\vec{K}_s$, $\vec{K}_t$ to give off-diagonal elements, $\vec{p}$ is also restricted to this same region, for any given $\vec{k}$, $\vec{p}$, and $\vec{q}$ we can have only one value of $\vec{G}$ that will satisfy the $\delta$ function. Thus we have the result

$$\begin{aligned}\langle l\vec{q}|e^{i(\vec{p}+\vec{K}_s)\cdot\vec{r}}|n\vec{k}\rangle &= \sum_{i,j} a^*_{lj}(\vec{q}) P_{ji}(\vec{p}+\vec{K}_s,\vec{q}) \\ &\times a_{ni}(\vec{k})\delta_{\vec{k},(\vec{q}-\vec{p})_R} \quad , \end{aligned} \tag{8}$$

where

$$(\vec{q}-\vec{p})_R = \vec{q}-\vec{p}+\vec{G} \tag{8a}$$

and $\vec{G}$ is a reciprocal-lattice vector such that $\vec{q}-\vec{p}+\vec{G}$ is a vector in the FBZ.

We insert (8) and the corresponding expression for the other matrix element in Eq. (3),

$$\begin{aligned}\epsilon_{ts}(\vec{p}) = \delta_{st} &- \frac{4\pi e^2}{N\Omega(\vec{p}+\vec{K}_t)^2}\sum_{n\vec{k},l\vec{q}} \frac{N_n(\vec{k})-N_l(\vec{q})}{E_n(\vec{k})-E_l(\vec{q})}\delta_{\vec{k},(\vec{q}-\vec{p})_R} \\ &\times\left(\sum_{ij} a^*_{lj}(\vec{q})P_{ji}(\vec{p}+\vec{K}_s,\vec{q})a_{ni}(\vec{k})\right) \\ &\times\left(\sum_{j'i'} a^*_{lj'}(\vec{q})P_{j'i'}(\vec{p}+\vec{K}_t,\vec{q})a_{ni'}(\vec{k})\right)^* \quad . \end{aligned} \tag{9}$$

The $\vec{k}$ sum can be performed immediately. The expression can be simplified by defining a matrix of the wave-function coefficients. If we form a matrix $A(\vec{k})$ such that its $n$th column consists of the coefficients for the $n$th band, i.e.,

$$A_{in}(\vec{k}) = a_{ni}(\vec{k}) \quad , \tag{10a}$$

we can define a new set of matrix elements,

$$\begin{aligned} m_{ln}(\vec{p},\vec{K}_s,\vec{q}) &= \sum_{ij} a^*_{lj}(\vec{q})P_{ji}(\vec{p}+\vec{K}_s,\vec{q})a_{ni}((\vec{q}-\vec{p})_R) \\ &= [A^\dagger(\vec{q})P(\vec{p}+\vec{K}_s,\vec{q})A((\vec{q}-\vec{p})_R)]_{ln} \quad , \end{aligned} \tag{10b}$$

and we have the simplified expression

$$\begin{aligned}\epsilon_{ts}(\vec{p}) = \delta_{st} &- \frac{4\pi e^2}{N\Omega(\vec{p}+\vec{K}_t)^2}\sum_{nl,\vec{q}} \frac{N_n((\vec{q}-\vec{p})_R)-N_l(\vec{q})}{E_n((\vec{q}-\vec{p})_R)-E_l(\vec{q})} \\ &\times m_{ln}(\vec{p},\vec{K}_s,\vec{q})m^*_{ln}(\vec{p},\vec{K}_t,\vec{q}) \quad . \end{aligned} \tag{11}$$

From the definition of the matrix $m$ [Eq. (10b)] and the value of $(\vec{q}-\vec{p})_R$, it is obvious that $m_{ln}$ depends on $\vec{p}+\vec{K}_s$ rather than individual values of $\vec{p}$ and $\vec{K}_s$, i.e.,

$$m_{ln}(\vec{p},\vec{K}_s,\vec{q}) = m_{ln}(\vec{p}+\vec{K}_s,\vec{q}) \quad . \tag{12}$$

It does not change the energy or occupation number of a state if the wave vector is shifted by a reciprocal-lattice vector. This fact can be used with Eq. (12) to rewrite Eq. (11) in the form

$$\begin{aligned}\epsilon(\vec{p}_t,\vec{p}_s) = \delta_{st} &- \frac{4\pi e^2}{N\Omega\vec{p}_t^{\,2}}\sum_{nl,\vec{q}} \frac{N_n((\vec{q}-\vec{p}_s)_R)-N_l(\vec{q})}{E_n((\vec{q}-\vec{p}_s)_R)-E_l(\vec{q})} \\ &\times m_{ln}(\vec{p}_s,\vec{q})m^*_{ln}(\vec{p}_t,\vec{q}) \quad , \end{aligned} \tag{13}$$

where $\vec{p}_s$ and $\vec{p}_t$ differ only by a reciprocal-lattice vector. Thus we may have

$$\vec{p}_s = \vec{p}+\vec{K}_s, \quad \vec{p}_t = \vec{p}+\vec{K}_t$$

and of course $(\vec{q}-\vec{p}_s)_R = (\vec{q}-\vec{p}_t)_R = (\vec{q}-\vec{p})_R$. Since the sum for $\vec{q}$ is over all values in the FBZ, Eq. (13) in combination with the transformation (A7) gives a fundamental symmetry relation for the matrix elements $\epsilon_{st}$:

$$\epsilon(\gamma\vec{p}_s,\gamma\vec{p}_t) = \epsilon(\vec{p}_s,\vec{p}_t); \tag{14}$$

i.e., when both values of the wave vector in the matrix elements of $\epsilon$ are rotated by the same operator, the result does not change. This property reduces substantially the number of $\epsilon$-matrix elements to be evaluated.

## III. MATHEMATICAL DETAILS

### A. Band structure

The linear-combination-of atomic-orbitals method is employed in a variational approach to obtain the band structure self-consistently.[14] The Bloch states are expanded in terms of the Gaussian orbitals [Eq. (4)], using a total of 52 basis functions of $s$, $p$, and $d$ types. The calculation is begun by constructing

a crystal potential from a superposition of overlapping neutral-atom charge densities, with the atoms assumed to be in the $3s^1 3p^2$ configuration. The wave functions used in forming the atomic charge density are taken from the Hartree-Fock self-consistent field calculation of Clementi.[17] Energy levels and wave functions are determined for this potential and used to initiate an iterative procedure leading to self-consistency. In this process corrected Fourier coefficients of the Coulomb potential are calculated using wave functions of the occupied states at 89 points in $\frac{1}{48}$ of the Brillouin zone resulting from the previous iteration. The exchange parameter for the Slater-type exchange potential was set at the value $\frac{2}{3}$.

This method uses Gaussian orbitals that are not orthogonal and as a result the coefficients $a_{ni}$ satisfy the orthogonality (with the overlap matrix)

$$A^\dagger(\vec{k})S(\vec{k})A(\vec{k}) = I \quad , \tag{15a}$$

where $A(\vec{k})$ is the matrix defined by (10a) and $S(\vec{k})$ is the overlap matrix

$$S_{ji}(\vec{k}) = \sum_\mu e^{-i\vec{k}\cdot\vec{R}_\mu}\langle u_j(\vec{r}-\vec{R}_\mu)\,|\,u_i(\vec{r})\rangle = P_{ji}(0,\vec{k}) \quad . \tag{15b}$$

The energies and wave functions are evaluated by diagonalizing the Hamiltonian matrix $H(\vec{k})$, i.e., solving the determinantal equation

$$|H_{ji}(\vec{k}) - E(\vec{k})S_{ji}(\vec{k})| = 0 \quad , \tag{16}$$

where $H_{ji}(\vec{k})$ are the matrix elements of the Hamiltonian given by

$$H_{ji}(\vec{k}) = \sum_\mu e^{-i\vec{k}\cdot\vec{R}_\mu}\langle u_j(\vec{r}-\vec{R}_\mu)\,|\,[-\vec{\nabla}^2 + V(\vec{r})]\,|\,u_i(\vec{r})\rangle . \tag{17}$$

A simple unitary transformation is introduced so that the Hamiltonian and overlap matrices will be real. Specifically,

$$S(\vec{k}) \rightarrow US(\vec{k})U^\dagger \quad ,$$

where

$$U = \begin{pmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & iI \end{pmatrix} \tag{18}$$

gives the unitary transformation in block form, the blocks referring to $d$, $s$, and $p$ types of Gaussian functions, respectively.

### B. Brillouin-zone integration

The sum over $\vec{q}$ in Eq. (13) is easily converted to an integral over the Brillouin zone by using

$$\frac{1}{N}\sum_{\vec{q}} \rightarrow \frac{\Omega}{(2\pi)^3}\int d^3q \quad . \tag{19}$$

We utilize the transformation property of the various quantities with respect to the cubic group to reduce the region of integration to the $\frac{1}{48}$ irreducible subzone (SZ) along with a sum over group operators ($\beta$). Any operator $\beta$ in the cubic group can be expressed as the product of two operators, one belonging to the group of the wave vector ($\gamma$ say) and the other a member of the set generating the star of $\vec{p}$ ($\alpha$), giving

$$\int_{BZ} d^3q\, f(\vec{p},\vec{q}) = \sum_{\gamma,\alpha}\int_{SZ} d^3q\, f(\vec{p},\gamma\alpha\vec{q}) \quad . \tag{19'}$$

The dielectric matrix elements are thus given by

$$\epsilon_{ts}(\vec{p}) = \delta_{st} - \frac{4\pi e^2}{\Omega(\vec{p}+\vec{K}_t)^2}Q_{ts}(\vec{p}) \quad , \tag{20}$$

where

$$Q_{ts}(\vec{p}) = \frac{\Omega}{(2\pi)^3}\sum_{nl,\beta}\int_{SZ} d^3q\, \frac{N_n((\beta\vec{q}-\vec{p})_R) - N_l(\beta\vec{q})}{E_n((\beta\vec{q}-\vec{p})_R) - E_l(\beta\vec{q})} \times m_{ln}(\vec{p}+\vec{K}_s,\beta\vec{q})m^*_{ln}(\vec{p}+\vec{K}_t,\beta\vec{q}) \quad , \tag{21}$$

and $Q_{ts}$ possesses the symmetry

$$Q_{ts}(\vec{p}) = Q_{st}(\vec{p}) \quad . \tag{22}$$

We can now make use of the fact that the energies are the same at all $\vec{q}$ values that are connected by an operator of the cubic group to reduce the $\beta$ sum to separate sums over the $\alpha$ and $\gamma$ operators. The $\vec{q}$ integral can, of course, be converted to a surface integral and an integral over energies to give

$$Q_{ts}(\vec{p}) = \frac{\Omega}{(2\pi)^3}\sum_{nl}\sum_{\alpha\in O_h/G(\vec{p})}\int\frac{dE}{E} \times \int ds\, \frac{N_n((\vec{q}-\alpha^{-1}\vec{p})_R) - N_l(\vec{q})}{|\mathrm{grad}\Delta_{nl}(\vec{q},\alpha^{-1}\vec{p})|} \times \sum_{\gamma\in G(\vec{p})} m_{ln}(\alpha^{-1}\gamma^{-1}(\vec{p}+\vec{K}_s),\vec{q}) \times m^*_{ln}(\alpha^{-1}\gamma^{-1}(\vec{p}+\vec{K}_t),\vec{q}) \quad , \tag{23}$$

where

$$\Delta_{nl}(\vec{q},\alpha^{-1}\vec{p}) = E_n((\vec{q}-\alpha^{-1}\vec{p})_R) - E_l(\vec{q}) \quad , \tag{24}$$

and the surface integral is over all $\vec{q}$ within the subzone satisfying the condition $\Delta_{nl} = E$.

The surface integral is performed by dividing the SZ into tetrahedrons[15] filling up the entire region. This method has the basic advantage that the occupation number in the integral is taken care of easily by reducing the tetrahedron into smaller ones that will contribute. The general integral involved is of the type

$$\int\frac{dS}{|\mathrm{grad}\Delta|}A(\vec{k})\Theta(E(\vec{k})-E_F) \quad . \tag{25}$$

The energies at the four corners of the tetrahedron are arranged in an increasing order, i.e.,

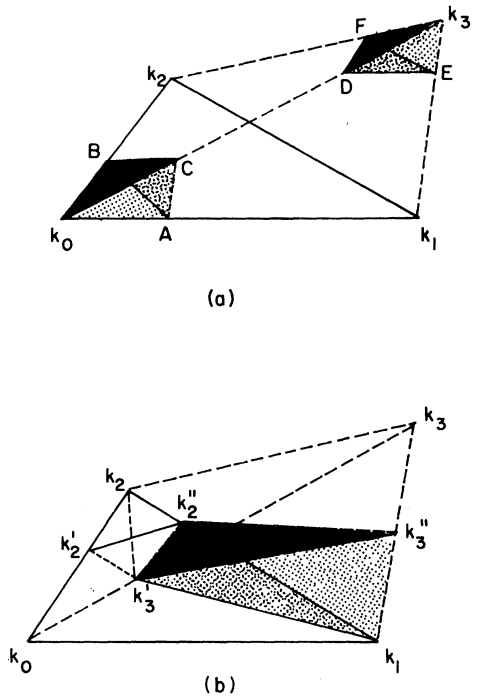


FIG. 1. (a) Division of the tetrahedron $k_0k_1k_2k_3$ to get the contributing part for cases when $E_{k_0} \le E_F \le E_{k_1}$ and $E_{k_2} \le E_F \le E_{k_3}$. (b) The case when $E_{k_1} \le E_F \le E_{k_2}$ gives three different tetrahedrons needed for the contributions.

$$E_0 \le E_1 \le E_2 \le E_3 \ ,$$

where

$$E_i = E(\vec{k}_i), \quad i = 0, 1, 2, 3 \ .$$

Depending upon the value of $E_F$, the portion of the tetrahedron that contributes is obtained in three separate cases:

1. $E_0 \le E_F \le E_1$. If $E_0 = E_F$, all of the tetrahedron has $\vec{k}$ points giving rise to $E(\vec{k}) > E_F$ and there is no contribution at all. Otherwise, we find points $A$, $B$, and $C$ [Fig. 1(a)] where $E(\vec{k}) = E_F$ given by

$$\vec{q}_i = \vec{k}_0 + \frac{E_F - E_0}{E_i - E_0}(\vec{k}_i - \vec{k}_0), \quad i = 1, 2, 3 \ .$$

It is then the tetrahedron ($k_0ABC$) that is relevant for the surface integral. When $E_F = E_1$, point $A$ coincides with $k_1$.

2. $E_2 \le E_F \le E_3$. Again, a simple case develops when $E_F = E_3$ and the whole of the tetrahedron contributes. Otherwise, we find points $D$, $E$, and $F$ [Fig. 1(a)] given by

$$\vec{q}_i = \vec{k}_3 + \frac{E_3 - E_F}{E_3 - E_i}(\vec{k}_i - \vec{k}_3), \quad i = 0, 1, 2 \ ,$$

with the resulting tetrahedron $DEFk_3$ being excluded from consideration (integral for tetrahedron $k_0k_1k_2k_3$ minus integral for tetrahedron $DEFk_3$).

3. $E_1 \le E_F \le E_2$. This final case is the most complicated and results in three smaller tetrahedrons [Fig. 1(b)]. First we find point $k_3'$ where $E(\vec{k}_3') = E_F$ along the $k_0k_3$ direction. This gives rise to two tetrahedrons: $k_0k_1k_2k_3'$ of the type 2 (here the energies are in the order $E_{k_0} \le E_{k_1} \le E_{k_3'} = E_F \le E_{k_2}$) and the tetrahedron $k_1k_3'k_2k_3$ of type 1. Thus we have the total contribution being that from tetrahedrons $k_1k_3'k_2''k_3''$ and $k_0k_1k_3'k_2$ minus that from $k_3'k_2'k_2''k_2$. All the primed $k$ points are obtained by linear interpolation between the corresponding directions to find the energy $E_F$.

Once the tetrahedron has been reduced to the contributing part without the $\Theta$ function, we have the straightforward surface integral of the type

$$I = \int_E \frac{dS}{|\mathrm{grad}\Delta|} A(\vec{k}) \tag{26}$$

for which we make the linear expansion both of $A(k)$ and $\Delta$ values,

$$A(\vec{k}) = A_0 + \vec{c} \cdot (\vec{k} - \vec{k}_0) \tag{27a}$$

and

$$\Delta(\vec{k}) = \Delta_0 + \vec{b} \cdot (\vec{k} - \vec{k}_0) \ , \tag{27b}$$

thereby reducing the integral in (26) to the form

$$I = \int \frac{dS}{|b|}[A_0 + \vec{c} \cdot (\vec{k} - \vec{k}_0)]$$

$$= \frac{f(E)}{|b|}\{\vec{A}_0 + \vec{c} \cdot [\vec{S}(E) - \vec{k}_0]\} \ , \tag{28}$$

where

$$f(E) = \int_E dS$$

gives the area of the constant-energy surface inside the tetrahedron and $\vec{s}$ is the first moment given by

$$f(E)\vec{S}(E) = \int_E \vec{k}\, dS \ .$$

The values of $\vec{S}(E)$ and $f(E)$ are obtained in different forms for the various cases of $E$ relative to the values of $\Delta$ at the four corners arranged in an increasing order. We have the following cases:

1. $\Delta_0 \le E \le \Delta_1$. If $E = \Delta_0$, the constant-energy surface ends up as a point, line, or a triangle. The only case with nonzero contribution will be

(i) $E = \Delta_0 = \Delta_1 = \Delta_2$:

$$\frac{f(E)}{|b|} = \frac{|v|}{2}\frac{1}{\Delta_3 - \Delta_0}$$

and

$$\vec{S}(E) = \vec{k}_0 + \tfrac{1}{3}[(\vec{k}_1 - \vec{k}_0) + (\vec{k}_2 - \vec{k}_0)] \ , \tag{29a}$$

where

$$v = [(\vec{k}_1 - \vec{k}_0) \times (\vec{k}_2 - \vec{k}_0)] \cdot (\vec{k}_3 - \vec{k}_0)$$

is six times the volume of the tetrahedron.

(ii) $\Delta_0 < E \leq \Delta_1$: We find the points $A$, $B$, and $C$ such that $\Delta = E$ along the three directions, just like for the case of occupation number. The results turn out to be

$$\frac{f(E)}{|b|} = \frac{|v|}{2} \times \begin{cases} \dfrac{(\Delta_3 - E)^2}{(\Delta_3 - \Delta_0)(\Delta_3 - \Delta_1)(\Delta_3 - \Delta_2)}, & E < \Delta_3 \\ \dfrac{1}{\Delta_3 - \Delta_0}, & E = \Delta_1 = \Delta_2 = \Delta_3 \\ 0, & \text{otherwise} \end{cases} \tag{30a}$$

and

$$\vec{S}(E) = \begin{cases} \vec{k}_3 + \dfrac{\Delta_3 - E}{3} \displaystyle\sum_{i=0,1,2} \frac{\vec{k}_i - \vec{k}_3}{\Delta_3 - \Delta_i}, & E < \Delta_3 \\ \vec{k}_0 + \frac{1}{3}[(\vec{k}_1 - \vec{k}_0) + (\vec{k}_2 - \vec{k}_0) + (\vec{k}_3 - \vec{k}_0)], & E = \Delta_1 = \Delta_2 = \Delta_3 \end{cases} \tag{30b}$$

3. $\Delta_1 \leq E \leq \Delta_2$. The constant-energy surface evaluated in the simple manner of case 1 above can extend outside the tetrahedron in this case and as a result we have the difference of the contributions from two such surfaces; i.e., we have

$$\frac{f(E)}{|b|} = \frac{f_0(E)}{|b|} - \frac{f_1(E)}{|b|} \tag{31a}$$

and

$$\vec{S}(E) = \frac{\vec{S}_0(E) f_0(E) - \vec{S}_1(E) f_1(E)}{f_0(E) - f_1(E)}, \tag{31b}$$

where $f_0(E)$ and $\vec{S}_0(E)$ are as given by Eq. (29b) and

$$\frac{f_1(E)}{|b|} = \frac{|v|}{2} \frac{(E - \Delta_1)^2}{(\Delta_1 - \Delta_0)(\Delta_2 - \Delta_0)(\Delta_3 - \Delta_1)} \tag{31c}$$

and

$$\vec{S}_1(E) = \vec{k}_1 + \frac{E - \Delta_1}{3} \sum_{i=0,2,3} \frac{\vec{k}_i - \vec{k}_1}{\Delta_i - \Delta_1}. \tag{31d}$$

However, when $\Delta_0 = \Delta_1 < E < \Delta_2$, it becomes impossible to find the closing point of the triangular surface of $\Delta = E$ in the $k_0 k_1$ direction. For that case, we have the limiting results

$$\frac{f(E)}{|b|} = \frac{|v|}{2} \frac{E - \Delta_0}{(\Delta_2 - \Delta_0)(\Delta_3 - \Delta_0)} \left( \frac{\Delta_2 - E}{\Delta_2 - \Delta_0} + \frac{\Delta_3 - E}{\Delta_3 - \Delta_0} \right) \tag{31e}$$

and

$$\vec{S}(E) = \vec{k}_0 + \left[ 3 \left( \frac{\Delta_2 - E}{\Delta_2 - \Delta_0} + \frac{\Delta_3 - E}{\Delta_3 - \Delta_0} \right) \right]^{-1} \left\{ (k_1 - k_0) \left[ \left( \frac{\Delta_2 - E}{\Delta_2 - \Delta_0} \right)^2 + \left( \frac{\Delta_3 - E}{\Delta_3 - \Delta_0} \right)^2 + \frac{\Delta_2 - E}{\Delta_2 - \Delta_0} \frac{\Delta_3 - E}{\Delta_3 - \Delta_0} \right] + (\vec{k}_2 - \vec{k}_0) \right.$$

$$\left. \times \left( \frac{\Delta_3 - E}{\Delta_3 - \Delta_0} + 2 \frac{\Delta_2 - E}{\Delta_2 - \Delta_0} \right) \frac{E - \Delta_0}{\Delta_2 - \Delta_0} + (\vec{k}_3 - \vec{k}_0) \right.$$

$$\left. \times \left( \frac{\Delta_2 - E}{\Delta_2 - \Delta_0} + 2 \frac{\Delta_3 - E}{\Delta_3 - \Delta_0} \right) \frac{E - \Delta_0}{\Delta_3 - \Delta_0} \right\}. \tag{31f}$$

When the two cases $E = \Delta_0 = \Delta_1 = \Delta_2$ and $E = \Delta_1 = \Delta_2 = \Delta_3$ involve an outer face of the original tetrahedron (before Fermi-function truncation), we must use an extra weight factor of $\frac{1}{2}$ for $f(E)$.

## IV. RESULTS AND DISCUSSION

We evaluated the matrix $Q_{ts}(\vec{p})$, given by Eq. (23), for three principal directions, $\Gamma X$, $\Gamma K$, and $\Gamma L$, for a total of nine values of $\vec{p}$. The reciprocal-lattice vectors $\vec{K}_s$ and $\vec{K}_t$ were allowed a range of 15 values [(0, 0, 0), eight variations of (1, 1, 1), and six variations of (2, 0, 0)]. The integration was done by using four-point division along the $\Gamma X$ line. The simplest case, $p = (2\pi/a)(\frac{1}{4}, 0, 0)$ and $\vec{K}_s = \vec{K}_t$ (0, 0, 0), was also evaluated by eight-point division and the results were found to agree within 6%.

Table I shows the values of $Q_{ts}(\vec{p})$ for $\vec{p}$ along the $\Gamma X$ line and those values of $\vec{K}_s$ and $\vec{K}_t$ that give rise to independent matrix elements (31 such cases). The complete matrix (15×15 in size) for $Q_{ts}(\vec{p})$ can be obtained by applying the symmetry relations

$$Q(\vec{p} + \vec{K}_s, \vec{p} + \vec{K}_t) = Q(\vec{p} + \vec{K}_t, \vec{p} + \vec{K}_s) \tag{32a}$$

and

$$Q(\gamma(\vec{p} + \vec{K}_s), \gamma(\vec{p} + \vec{K}_t)) = Q(\vec{p} + \vec{K}_s, \vec{p} + \vec{K}_t), \tag{32b}$$

where

TABLE I. Values of $Q_{ts}(\vec{p})$, defined by Eq. (23), for $\vec{p}$ in [100] direction. Only those values of $\vec{K}_s$ and $\vec{K}_t$ that give rise to independent matrix elements are shown. $\vec{K}_s$, $\vec{K}_t$, and $\vec{p}$ are in units of $\pi/2a$ and $Q_{ts}(\vec{p})$ in $\mathrm{Ry}^{-1}$.

| $\vec{K}_t$ | $\vec{K}_s$ | $\vec{p}$ (1, 0, 0) | (2, 0, 0) | (3, 0, 0) | (4, 0, 0) |
|---|---|---|---|---|---|
| (0, 0, 0) | (0, 0, 0) | −2.321 | −2.499 | −2.444 | −2.234 |
| | (4, 4, 4) | −0.0260 | −0.0283 | −0.0296 | −0.0464 |
| | ($\bar{4}$, 4, 4) | −0.0971 | −0.0729 | −0.0396 | −0.0628 |
| | (8, 0, 0) | 0.1472 | 0.0509 | 0.0315 | −0.0136 |
| | ($\bar{8}$, 0, 0) | −0.0659 | −0.2051 | −0.1885 | −0.5929 |
| | (0, 8, 0) | 0.0288 | 0.0265 | −0.0077 | 0.1269 |
| (4, 4, 4) | (4, 4, 4) | −1.154 | −0.928 | −0.607 | −0.2871 |
| | (4, 4, $\bar{4}$) | −0.1906 | −0.1332 | −0.0657 | −0.0284 |
| | (4, $\bar{4}$, $\bar{4}$) | −0.0424 | 0.0157 | 0.0293 | 0.0064 |
| | ($\bar{4}$, 4, 4) | 0.1311 | 0.1265 | 0.1673 | 0.1062 |
| | ($\bar{4}$, 4, $\bar{4}$) | 0.1478 | 0.1458 | 0.1311 | 0.0621 |
| | ($\bar{4}$, $\bar{4}$, $\bar{4}$) | 0.1574 | 0.1292 | 0.0947 | 0.0731 |
| | (8, 0, 0) | −0.0424 | −0.0280 | −0.0164 | −0.0122 |
| | ($\bar{8}$, 0, 0) | 0.0504 | 0.0348 | 0.0201 | −0.0036 |
| | (0, 8, 0) | −0.0424 | −0.0404 | −0.0331 | −0.0167 |
| | (0, $\bar{8}$, 0) | 0.0198 | 0.0192 | 0.0132 | 0.0052 |
| ($\bar{4}$, 4, 4) | ($\bar{4}$, 4, 4) | −1.472 | −1.646 | −1.698 | −1.736 |
| | ($\bar{4}$, 4, $\bar{4}$) | −0.2734 | −0.3336 | −0.3333 | −0.3388 |
| | ($\bar{4}$, $\bar{4}$, $\bar{4}$) | −0.1095 | −0.1026 | −0.0771 | −0.0574 |
| | (8, 0, 0) | 0.0603 | 0.0435 | 0.0372 | 0.0207 |
| | ($\bar{8}$, 0, 0) | −0.0327 | −0.0175 | −0.0032 | a |
| | (0, 8, 0) | −0.0529 | −0.0532 | −0.0459 | −0.0491 |
| | (0, $\bar{8}$, 0) | 0.0209 | 0.0178 | 0.0272 | 0.0207 |
| (8, 0, 0) | (8, 0, 0) | −0.5294 | −0.1907 | −0.0611 | −0.0235 |
| | ($\bar{8}$, 0, 0) | −0.0901 | −0.0798 | −0.0674 | −0.0601 |
| | (0, 8, 0) | 0.1126 | 0.0665 | 0.0399 | 0.0195 |
| ($\bar{8}$, 0, 0) | ($\bar{8}$, 0, 0) | −1.457 | −1.719 | −1.952 | a |
| | (0, 8, 0) | 0.1599 | 0.1492 | 0.1239 | 0.0937 |
| (0, 8, 0) | (0, 8, 0) | −0.951 | −0.866 | −0.762 | −0.5711 |
| | (0, $\bar{8}$, 0) | −0.2625 | −0.2198 | −0.2029 | −0.1630 |
| | (0, 0, 8) | 0.0388 | 0.0373 | 0.0508 | 0.0436 |

[a]Available from other terms by use of symmetry relations.

$$Q(\vec{p}+\vec{K}_t, \vec{p}+\vec{K}_s) = Q_{ts}(\vec{p}) \ . \qquad (32c)$$

Results for $\vec{p}$ along $\Gamma K$ and $\Gamma L$ directions are shown in Tables II and III, respectively.

As expected, values of $Q_{ts}(\vec{p})$ are largest (in magnitude) for the case of $\vec{K}_s = \vec{K}_t = (0, 0, 0)$. However, some other diagonal matrix elements have large values. In general, the off-diagonal elements are small. Table IV lists all the diagonal elements evaluated here. A general trend is noticed; i. e., they all have the same sign and the magnitude decreases as $|\vec{p}+\vec{K}_s|$ increases, except for some fluctuations and slight directional effects.

The dielectric matrix $\epsilon_{ts}(\vec{p})$ can now be obtained by using Eq. (20). It is well known, however, that the RPA expression [Eq. (20) here, similar to the Lindhard[18] expression for the free-electron gas] leads to some unphysical features of the pair distribution function in the range of metallic densities ($2 \le r_s \le 5$). In a classical paper on the exchange and correlation energy of a free-electron gas, Hubbard[19] proposed to replace the Lindhard expression

$$1 - \frac{1}{\epsilon(\vec{k}, \omega)} = \frac{Q^{(0)}(\vec{k}, \omega)}{1 + Q^{(0)}(\vec{k}, \omega)} \qquad (33)$$

by the more general form

$$1 - \frac{1}{\epsilon(\vec{k}, \omega)} = \frac{Q^{(0)}(\vec{k}, \omega)}{1 + [1 - G(\vec{k})] Q^{(0)}(\vec{k}, \omega)} \ , \qquad (34)$$

where $Q^{(0)}(\vec{k}, \omega)$ is the polarizability of the free-electron gas. The function $G(\vec{k})$ takes into account the exchange and correlation effects. [This is equivalent to the form given by Eq. (1) using $G(\vec{k})$ to modify the electron-electron interaction.] Hub-

TABLE II. Independent values of $Q_{ts}(\vec{p})$ for $\vec{p}$ in [110] direction.

| $\vec{K}_t$ | $\vec{K}_s$ | $\vec{p}$ (1, 1, 0) | (2, 2, 0) | (3, 3, 0) |
|---|---|---|---|---|
| (0, 0, 0) | (0, 0, 0) | −2.384 | −2.369 | −2.039 |
| | ($\bar{4}$, $\bar{4}$, 4) | −0.0796 | −0.0568 | −0.0443 |
| | (4, $\bar{4}$, 4) | −0.0904 | −0.0849 | −0.0613 |
| | ($\bar{8}$, 0, 0) | −0.0300 | −0.0003 | 0.0417 |
| | (4, 4, 4) | −0.0119 | −0.0228 | −0.0118 |
| | (0, 0, 8) | 0.0640 | 0.0893 | 0.1154 |
| | (8, 0, 0) | 0.1243 | 0.0726 | 0.0194 |
| ($\bar{4}$, $\bar{4}$, 4) | ($\bar{4}$, $\bar{4}$, 4) | −1.671 | −1.959 | −2.144 |
| | ($\bar{4}$, $\bar{4}$, $\bar{4}$) | −0.3300 | −0.4274 | −0.5512 |
| | (4, $\bar{4}$, 4) | 0.1082 | 0.0825 | 0.1186 |
| | (4, $\bar{4}$, $\bar{4}$) | 0.1461 | 0.1747 | 0.1806 |
| | ($\bar{8}$, 0, 0) | −0.0528 | −0.0365 | −0.0465 |
| | (4, 4, 4) | 0.1555 | 0.1014 | 0.0808 |
| | (4, 4, $\bar{4}$) | 0.0851 | 0.0542 | 0.0452 |
| | (0, 0, 8) | −0.0420 | −0.0800 | −0.0575 |
| | (0, 0, $\bar{8}$) | 0.0365 | 0.0185 | 0.0076 |
| | (8, 0, 0) | 0.0549 | 0.0427 | 0.0395 |
| (4, $\bar{4}$, 4) | (4, $\bar{4}$, 4) | −1.281 | −1.181 | −0.950 |
| | (4, $\bar{4}$, $\bar{4}$) | −0.2215 | −0.2049 | −0.1299 |
| | ($\bar{4}$, 4, 4) | −0.0050 | 0.0071 | 0.0458 |
| | ($\bar{4}$, 4, $\bar{4}$) | 0.0897 | 0.0621 | 0.0724 |
| | ($\bar{8}$, 0, 0) | 0.0530 | 0.0526 | 0.0513 |
| | (0, $\bar{8}$, 0) | −0.0253 | −0.0184 | −0.0207 |
| | (4, 4, 4) | 0.1454 | 0.1086 | 0.0456 |
| | (4, 4, $\bar{4}$) | 0.1244 | 0.0971 | 0.0492 |
| | (0, 0, 8) | −0.0505 | −0.0423 | −0.0389 |
| | (0, 0, $\bar{8}$) | 0.0283 | 0.0243 | 0.0171 |
| | (8, 0, 0) | −0.0369 | −0.0144 | −0.0125 |
| | (0, 8, 0) | 0.0386 | 0.0224 | 0.0208 |
| ($\bar{8}$, 0, 0) | ($\bar{8}$, 0, 0) | −1.380 | −1.585 | −1.705 |
| | (0, $\bar{8}$, 0) | 0.0313 | 0.0212 | 0.0246 |
| | (4, 4, 4) | 0.0390 | 0.0250 | 0.0233 |
| | (0, 0, 8) | 0.1621 | 0.1499 | 0.1088 |
| | (8, 0, 0) | −0.0830 | −0.0711 | −0.0526 |
| | (0, 8, 0) | 0.0414 | 0.0339 | 0.0502 |
| (4, 4, 4) | (4, 4, 4) | −0.960 | −0.4570 | −0.1309 |
| | (4, 4, $\bar{4}$) | −0.1573 | −0.0610 | −0.0274 |
| | (0, 0, 8) | −0.0732 | −0.0344 | −0.0131 |
| | (0, 0, $\bar{8}$) | 0.0116 | 0.0063 | 0.0009 |
| | (8, 0, 0) | −0.0475 | −0.0260 | −0.0165 |
| (0, 0, 8) | (0, 0, 8) | −0.922 | −0.7858 | −0.5343 |
| | (0, 0, $\bar{8}$) | −0.2281 | −0.2004 | −0.1362 |
| | (8, 0, 0) | 0.1027 | 0.0589 | 0.0235 |
| (8, 0, 0) | (8, 0, 0) | −0.5117 | −0.1638 | −0.0425 |
| | (0, 8, 0) | 0.0112 | −0.0137 | −0.0019 |

TABLE III. Independent values of $Q_{ts}(\vec{p})$ for p in [111] direction.

| $\vec{K}_t$ | $\vec{K}_s$ | $\vec{p}$ (1,1,1) | $\vec{p}$ (2,2,2) |
|---|---|---|---|
| (0,0,0) | (0,0,0) | −2.464 | −2.340 |
| | $(\bar{4},\bar{4},\bar{4})$ | 0.0178 | −0.1730 |
| | $(\bar{4},\bar{4},4)$ | −0.0711 | −0.0262 |
| | $(\bar{8},0,0)$ | 0.0011 | −0.1136 |
| | $(4,4,\bar{4})$ | −0.0658 | −0.0563 |
| | (4,4,4) | −0.0197 | −0.0354 |
| | (8,0,0) | 0.1151 | 0.0668 |
| $(\bar{4},\bar{4},\bar{4})$ | $(\bar{4},\bar{4},\bar{4})$ | −1.890 | a |
| | $(\bar{4},\bar{4},4)$ | −0.0943 | a |
| | $(\bar{8},0,0)$ | −0.0365 | a |
| | $(4,4,\bar{4})$ | 0.0581 | 0.0348 |
| | (4,4,4) | 0.0937 | 0.0821 |
| | (8,0,0) | 0.0058 | 0.0210 |
| $(\bar{4},\bar{4},4)$ | $(\bar{4},\bar{4},4)$ | −1.481 | −1.450 |
| | $(\bar{4},4,\bar{4})$ | 0.0170 | 0.0010 |
| | $(\bar{8},0,0)$ | −0.0361 | −0.0203 |
| | $(0,0,\bar{8})$ | 0.0473 | −0.0183 |
| | $(4,4,\bar{4})$ | 0.0285 | 0.0152 |
| | $(4,\bar{4},4)$ | 0.0953 | 0.1202 |
| | (4,4,4) | 0.1406 | 0.0859 |
| | (8,0,0) | 0.0527 | 0.0385 |
| | (0,0,8) | −0.0357 | −0.0120 |
| $(\bar{8},0,0)$ | $(\bar{8},0,0)$ | −1.345 | a |
| | $(0,\bar{8},0)$ | 0.0345 | a |
| | $(4,4,\bar{4})$ | 0.0443 | 0.0121 |
| | $(\bar{4},4,4)$ | −0.0264 | 0.0217 |
| | (4,4,4) | 0.0392 | 0.0115 |
| | (8,0,0) | −0.0806 | −0.0246 |
| | (0,8,0) | 0.0412 | 0.0526 |
| $(4,4,\bar{4})$ | $(4,4,\bar{4})$ | −1.121 | −0.724 |
| | $(4,\bar{4},4)$ | 0.0294 | 0.0527 |
| | (4,4,4) | 0.1614 | 0.0482 |
| | (8,0,0) | −0.0281 | −0.0097 |
| | (0,0,8) | 0.0375 | 0.0185 |
| (4,4,4) | (4,4,4) | −0.814 | −0.1893 |
| | (8,0,0) | −0.0411 | −0.0201 |
| (8,0,0) | (8,0,0) | −0.4800 | −0.1410 |
| | (0,8,0) | 0.0039 | −0.0089 |

[a]Available from other terms by use of symmetry relations.

bard proposed the simple form

$$G(\vec{k}) = \frac{1}{2}\frac{k^2}{k^2+k_F^2}\ , \tag{35}$$

where $\vec{k}_F$ is the Fermi momentum. Singwi *et al.*[20] arrived at an expression similar to that in (34) by an equation-of-motion method relating $G(\vec{k}), S(\vec{k})$ (the static form factor), and $\epsilon(\vec{k},\omega)$ self-consistently. Of the many forms proposed[5,21–25] for $G(\vec{k})$, we have decided to use the numerical values given by Toigo and Woodruff.

The dielectric matrix, corrected for exchange and correlation effects [modifying the electron-electron interaction $4\pi e^2/\Omega(\vec{p}+\vec{K}_t)^2$ in Eq. (20) by Eq. (2)], is now given by

$$\epsilon_{tt}(\vec{p}) = 1 + \frac{Q^{(0)}(\vec{p}+\vec{K}_t)}{1-G(\vec{p}+\vec{K}_t)Q^{(0)}(\vec{p}+\vec{K}_t)} \tag{36a}$$

and

TABLE IV. Diagonal terms $Q_{tt}(\vec{p})$ for all $\vec{p}+\vec{K}_t$ values involved. Also shown are the values of $\epsilon_{tt}(\vec{p})$ in the RPA and including exchange and correlation correction (Toigo and Woodruff factor). Last column gives the corresponding value for the free-electron model (including Lindhard factor and the TW correction). Units for $\vec{p}+\vec{K}_t$, $|\vec{p}+\vec{K}_t|^2$, and $Q_{tt}(\vec{p})$ are $\pi/2a$, $(\pi/2a)^2$, and $\mathrm{Ry}^{-1}$, respectively.

| $\vec{p}+\vec{K}_t$ | $\lvert p+K_t\rvert^2$ | $Q_{tt}(p)$ | $\epsilon_{\mathrm{RPA}}$ | $\epsilon_{\mathrm{corr}}$ | $\epsilon_{\mathrm{FE}}$ |
|---|---|---|---|---|---|
| (1,0,0) | 1 | −2.321 | 25.77 | 33.76 | 41.90 |
| (1,1,0) | 2 | −2.384 | 13.72 | 18.83 | 22.57 |
| (1,1,1) | 3 | −2.464 | 9.77 | 14.32 | 16.43 |
| (2,0,0) | 4 | −2.499 | 7.67 | 11.07 | 12.31 |
| (2,2,0) | 8 | −2.369 | 4.16 | 5.68 | 6.54 |
| (3,0,0) | 9 | −2.444 | 3.90 | 5.40 | 5.94 |
| (2,2,2) | 12 | −2.340 | 3.08 | 4.09 | 4.63 |
| (4,0,0) | 16 | −2.234 | 2.49 | 3.15 | 3.61 |
| (3,3,0) | 18 | −2.039 | 2.21 | 2.69 | 3.30 |
| $(\bar{1},\bar{1},4)$ | 18 | −2.144 | 2.27 | 2.81 | 3.30 |
| $(\bar{2},\bar{2},4)$ | 24 | −1.959 | 1.871 | 2.19 | 2.63 |
| $(\bar{5},0,0)$ | 25 | −1.952 | 1.833 | 2.14 | 2.56 |
| $(\bar{3},\bar{3},\bar{3})$ | 27 | −1.890 | 1.747 | 2.01 | 2.42 |
| (0,4,4) | 32 | −1.736 | 1.579 | 1.762 | 2.14 |
| $(\bar{1},4,4)$ | 33 | −1.698 | 1.549 | 1.716 | 2.10 |
| $(\bar{5},3,0)$ | 34 | −1.705 | 1.535 | 1.699 | 2.05 |
| $(\bar{3},\bar{3},4)$ | 34 | −1.671 | 1.525 | 1.681 | 2.05 |
| $(\bar{2},4,4)$ | 36 | −1.646 | 1.488 | 1.631 | 1.975 |
| $(\bar{6},0,0)$ | 36 | −1.719 | 1.510 | 1.667 | 1.975 |
| $(\bar{6},2,0)$ | 40 | −1.585 | 1.423 | 1.540 | 1.841 |
| $(\bar{3},4,4)$ | 41 | −1.472 | 1.383 | 1.479 | 1.812 |
| $(\bar{3},\bar{3},5)$ | 43 | −1.481 | 1.368 | 1.460 | 1.757 |
| $(\bar{2},\bar{2},6)$ | 44 | −1.450 | 1.352 | 1.438 | 1.732 |
| $(\bar{7},0,0)$ | 49 | −1.457 | 1.317 | 1.394 | 1.618 |
| $(5,\bar{3},4)$ | 50 | −1.281 | 1.273 | 1.330 | 1.599 |
| $(\bar{7},1,0)$ | 50 | −1.380 | 1.295 | 1.362 | 1.599 |
| $(\bar{7},1,1)$ | 51 | −1.345 | 1.281 | 1.343 | 1.580 |
| $(6,\bar{2},4)$ | 56 | −1.181 | 1.225 | 1.267 | 1.495 |
| (5,4,4) | 57 | −1.154 | 1.216 | 1.255 | 1.478 |
| $(5,5,\bar{3})$ | 59 | −1.121 | 1.203 | 1.238 | 1.447 |
| (1,8,0) | 65 | −0.951 | 1.156 | 1.178 | 1.368 |
| (5,5,4) | 66 | −0.960 | 1.155 | 1.177 | 1.355 |
| (1,1,8) | 66 | −0.922 | 1.149 | 1.169 | 1.355 |
| $(7,\bar{1},4)$ | 66 | −0.950 | 1.154 | 1.175 | 1.355 |
| (2,8,0) | 68 | −0.866 | 1.136 | 1.152 | 1.330 |
| (6,4,4) | 68 | −0.928 | 1.146 | 1.165 | 1.330 |
| (2,2,8) | 72 | −0.7858 | 1.116 | 1.129 | 1.285 |
| (3,8,0) | 73 | −0.7620 | 1.111 | 1.122 | 1.273 |
| (5,5,5) | 75 | −0.8140 | 1.116 | 1.128 | 1.250 |
| $(6,6,\bar{2})$ | 76 | −0.7240 | 1.102 | 1.111 | 1.238 |
| (4,8,0) | 80 | −0.5711 | 1.076 | 1.081 | 1.191 |
| (9,0,0) | 81 | −0.5294 | 1.070 | 1.074 | 1.183 |
| (7,4,4) | 81 | −0.6070 | 1.080 | 1.085 | 1.183 |
| (9,1,0) | 82 | −0.5117 | 1.067 | 1.070 | 1.176 |
| (3,3,8) | 82 | −0.5343 | 1.070 | 1.073 | 1.176 |
| (9,1,1) | 83 | −0.4800 | 1.062 | 1.065 | 1.169 |
| (6,6,4) | 88 | −0.4570 | 1.055 | 1.058 | 1.142 |
| (8,4,4) | 96 | −0.2871 | 1.032 | 1.033 | 1.112 |
| (10,0,0) | 100 | −0.1907 | 1.020 | 1.021 | 1.101 |
| (10,2,0) | 104 | −0.1638 | 1.017 | 1.017 | 1.091 |
| (6,6,6) | 108 | −0.1893 | 1.019 | 1.019 | 1.083 |
| (10,2,2) | 108 | −0.1410 | 1.014 | 1.014 | 1.083 |
| (7,7,4) | 114 | −0.1309 | 1.012 | 1.012 | 1.073 |
| (11,0,0) | 121 | −0.0611 | 1.0054 | 1.0054 | 1.064 |
| (11,3,0) | 130 | −0.0425 | 1.0035 | 1.0035 | 1.054 |
| (12,0,0) | 144 | −0.0235 | 1.0017 | 1.0017 | 1.043 |

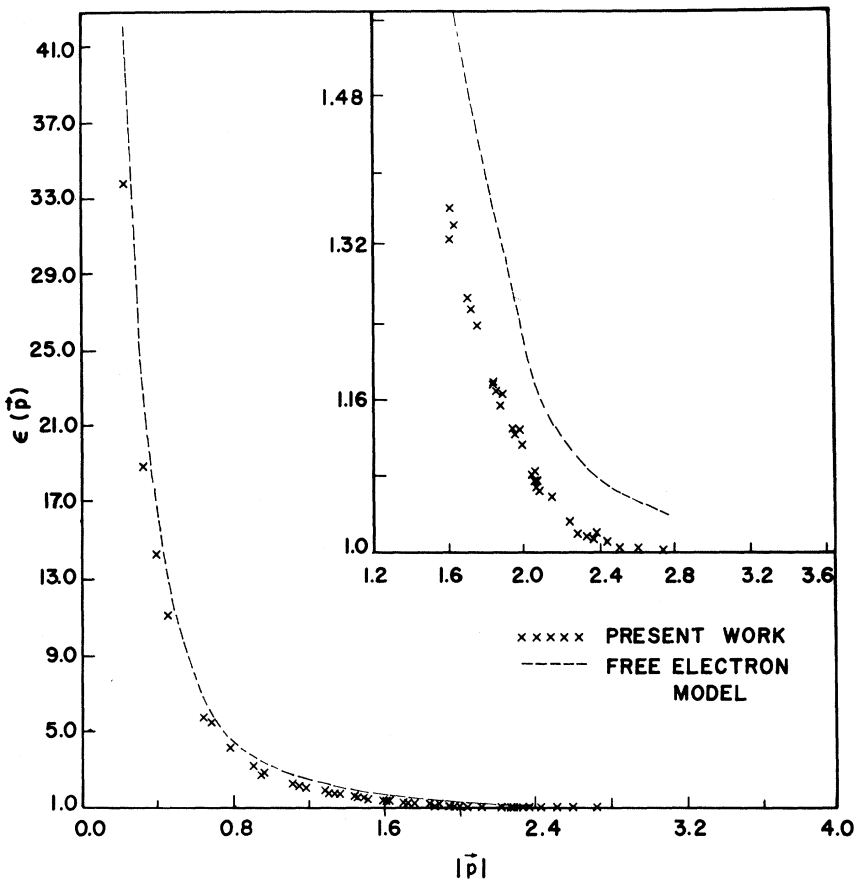


FIG. 2. Plot of $\epsilon(\vec{p})$ vs $|\vec{p}|$ (measured in units of $k_F = 1.097 \times 2\pi/a$). Dashed line is the corresponding result for the free-electron model. Insert shows the details when $\epsilon(\vec{p})$ approaches its asymptotic value.

$$\epsilon_{ts}(\vec{p}) = [\epsilon_{tt}(\vec{p}) - 1]\frac{Q_{ts}(\vec{p})}{Q_{tt}(\vec{p})}, \quad t \neq S \tag{36b}$$

where

$$Q^{(0)}(\vec{p}+\vec{K}_t) = -\frac{4\pi e^2}{\Omega(\vec{p}+\vec{K}_t)^2}[2Q_{tt}(\vec{p})] \ . \tag{36c}$$

Equation (36c) includes an extra factor of 2 to account for both spins. Table IV shows the values of $\epsilon(\vec{p})$, for all the diagonal cases calculated here, both with and without the exchange and correlation correction. The last column in Table IV shows the result for a free-electron (FE) model corrected for the exchange and correlation effects, using the Lindhard expression

$$Q^{(0)}_{FE}(\vec{q}) = -\frac{4\pi e^2}{\Omega q^2}\frac{3Z}{2E_F}\left(\tfrac{1}{2} + \frac{4k_F^2 - q^2}{8k_F q}\ln\left|\frac{2k_F + q}{2k_F - q}\right|\right) \ . \tag{37}$$

Figure 2 shows a plot of the diagonal terms in $\epsilon(\vec{p})$ (plotted against $|\vec{p}|$) for the actual aluminum band structure and the free-electron model. The apparent scatter in the data results from small directional variations of $\epsilon(\vec{p})$. The results differ from the free-electron case only slightly, confirming the view that aluminum is a nearly-free-electron metal.

Table V shows the complete matrix for $\vec{p} = (\pi/2a)(1, 0, 0)$ evaluated from (36). In general the off-diagonal terms are small. However, elements in the first row are not so small, owing to the large value of the interaction potential, $1/(\vec{p}+\vec{K}_t)^2$, for $\vec{p}+\vec{K}_t = (\pi/2a)(1, 0, 0)$. This may cause a slow convergence for some expressions using $\epsilon^{-1}$ and may require the evaluation of $\epsilon_{ts}(\vec{p})$ for $\vec{K}_s$ going beyond the $(2\pi/a)(2, 0, 0)$ used here. A look at the other cases shows that such a problem exists only for the small values of $\vec{p}$.

## ACKNOWLEDGMENT

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## APPENDIX

The band structure is obtained self-consistently only for $\vec{k}$ values in the irreducible subzone ($k_x \geq k_y \geq k_z \geq 0$). However, to evaluate the dielectric matrix [and the matrices $m(\vec{p}, \vec{q})$] we need the wave functions for all points in the FBZ. To obtain these wave functions, we investigate the rotation properties of the quantities involved.

First we define a rotation matrix, $\mathfrak{D}(\beta)$, for the Gaussian orbitals by

TABLE V. Complete matrix $\epsilon_{ts}(\vec{p})$ for $\vec{p}=(\pi/2a)$ (1, 0, 0); $K_s$ and $K_t$ are in units of $\pi/2a$.

| $K_t$ \ $K_s$ | (0, 0, 0) | $(\bar{4}, 4, 4)$ | $(\bar{4}, 4, 4)$ | $(\bar{4}, \bar{4}, 4)$ | $(\bar{8}, 0, 0)$ | (4, 4, 4) | $(4, 4, \bar{4})$ | $(4, \bar{4}, 4)$ | $(4, \bar{4}, \bar{4})$ | (0, 8, 0) | $(0, \bar{8}, 0)$ | (0, 0, 8) | $(0, 0, \bar{8})$ | (8, 0, 0) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| (0, 0, 0) | 33.76 | 1.371 | 1.371 | 1.371 | 0.930 | 0.930 | 0.367 | 0.367 | 0.367 | −0.407 | −0.407 | −0.407 | −0.407 | −2.078 |
| $(\bar{4}, 4, 4)$ | 0.0316 | 1.4794 | 0.0890 | 0.0357 | 0.0106 | −0.0427 | −0.0481 | −0.0513 | 0.0172 | 0.0068 | −0.0068 | 0.0172 | −0.0068 | −0.0196 |
| $(\bar{4}, 4, \bar{4})$ | 0.0316 | 0.0890 | 1.4794 | 0.0357 | 0.0106 | −0.0481 | −0.0427 | −0.0513 | 0.0172 | −0.0068 | 0.0068 | −0.0068 | 0.0172 | −0.0196 |
| $(\bar{4}, \bar{4}, 4)$ | 0.0316 | 0.0890 | 0.0357 | 1.4794 | 0.0106 | −0.0481 | −0.0513 | −0.0427 | −0.0481 | −0.0068 | 0.0172 | 0.0172 | −0.0068 | −0.0196 |
| $(\bar{4}, \bar{4}, \bar{4})$ | 0.0316 | 0.0357 | 0.0890 | 1.4794 | 0.0106 | −0.0513 | −0.0481 | −0.0481 | −0.0427 | −0.0068 | 0.0172 | −0.0068 | 0.0172 | −0.0196 |
| $(\bar{8}, 0, 0)$ | 0.0178 | 0.0089 | 0.0089 | 0.0089 | 1.3944 | −0.0136 | −0.0136 | −0.0136 | −0.0136 | −0.0433 | −0.0433 | −0.0433 | −0.0433 | 0.0244 |
| (4, 4, 4) | 0.0057 | −0.0290 | −0.0327 | −0.0348 | −0.0111 | 1.2551 | 0.0421 | 0.0094 | 0.0421 | 0.0094 | −0.0044 | 0.0094 | −0.0044 | 0.0094 |
| $(4, 4, \bar{4})$ | 0.0057 | −0.0327 | −0.0290 | −0.0348 | −0.0111 | 0.0421 | 1.2551 | 0.0421 | 0.0094 | 0.0044 | −0.0094 | −0.0044 | 0.0094 | 0.0094 |
| $(4, \bar{4}, 4)$ | 0.0057 | −0.0327 | −0.0327 | −0.0290 | −0.0111 | 0.0421 | 0.0094 | 1.2551 | 0.0421 | −0.0044 | 0.0094 | 0.0094 | −0.0044 | 0.0094 |
| $(4, \bar{4}, \bar{4})$ | 0.0057 | −0.0348 | −0.0327 | −0.0327 | −0.0111 | 0.0094 | 0.0421 | 1.2551 | −0.0044 | 0.0094 | −0.0044 | −0.0044 | 0.0094 | 0.0094 |
| $(0, 8, 0)$ | −0.0054 | 0.0099 | 0.0099 | −0.0039 | −0.0299 | 0.0079 | −0.0037 | −0.0037 | 1.1778 | 0.0491 | −0.0073 | −0.0073 | −0.0073 | −0.0210 |
| $(0, \bar{8}, 0)$ | −0.0054 | −0.0039 | −0.0039 | 0.0099 | −0.0299 | −0.0037 | 0.0079 | −0.0037 | 1.1778 | −0.0073 | 0.0491 | −0.0073 | −0.0073 | −0.0210 |
| $(0, 0, 8)$ | −0.0054 | −0.0039 | 0.0099 | −0.0039 | −0.0299 | 0.0079 | −0.0037 | 0.0079 | −0.0073 | −0.0073 | −0.0073 | 1.1778 | 0.0491 | −0.0210 |
| $(0, 0, \bar{8})$ | −0.0054 | 0.0099 | −0.0039 | 0.0099 | −0.0299 | −0.0037 | 0.0079 | −0.0037 | 0.0079 | 0.0073 | −0.0073 | 0.0491 | 1.1778 | −0.0210 |
| (8, 0, 0) | −0.0205 | −0.0084 | −0.0084 | −0.0084 | 0.0125 | 0.0059 | 0.0059 | 0.0059 | 0.0059 | −0.0157 | −0.0157 | −0.0157 | −0.0157 | 1.0736 |

$$u_i(\beta\vec{r}) = \sum_j \mathfrak{D}_{ij}(\beta) u_j(\vec{r}) \quad . \tag{A1}$$

This matrix $\mathfrak{D}$ must be diagonal in block form,

$$\mathfrak{D}(\beta) = \begin{array}{c} \\ d \\ s \\ p \end{array} \begin{array}{c} \begin{array}{ccc} d & s & p \end{array} \\ \begin{pmatrix} \times & 0 & 0 \\ 0 & \times & 0 \\ 0 & 0 & \times \end{pmatrix} \end{array}, \tag{A2}$$

where the three sections indicate the division of the Gaussian orbitals in the three sets of $d$, $s$, and $p$ types, respectively.

Combining the transformation given by (A1) with the Bloch theorem, we find

$$a_{nj}(\beta\vec{k}) = e^{i\phi_n(\beta)} \sum_i a_{ni}(\vec{k}) \mathfrak{D}_{ij}(\beta^{-1}) \quad , \tag{A3}$$

where $e^{i\phi_n(\beta)}$ is the phase factor (of value $\pm 1$). In matrix form, we have

$$A_{jn}(\beta\vec{k}) = e^{i\phi_n(\beta)} [\mathfrak{D}^T(\beta^{-1}) A(\vec{k})]_{jn} \tag{A4a}$$

and the corresponding form

$$A^\dagger_{li}(\beta\vec{k}) = e^{-i\phi_l(\beta)} [A^\dagger(\vec{k}) \mathfrak{D}^*(\beta^{-1})]_{li} \quad . \tag{A4b}$$

Now let us consider the $P$ matrix. From the definition

$$P_{ij}(\vec{p}, \vec{q}) = \sum_\mu e^{-i\vec{q}\cdot\vec{R}_\mu} \langle u_i(\vec{r} - \vec{R}_\mu) | e^{i\vec{p}\cdot\vec{r}} | u_j(\vec{r}) \rangle \tag{A5}$$

we can write

$$\begin{aligned} P_{ij}(\vec{p}, \beta\vec{q}) &= \sum_\mu e^{-i\beta\vec{q}\cdot\vec{R}_\mu} \langle u_i(\vec{r} - \vec{R}_\mu) | e^{i\vec{p}\cdot\vec{r}} | u_j(\vec{r}) \rangle \\ &= \sum_\nu e^{-i\vec{q}\cdot\vec{R}_\nu} \langle u_i(\beta(\vec{r}' - \vec{R}_\nu)) | e^{i\beta^{-1}\vec{p}\cdot\vec{r}'} | u_j(\beta\vec{r}') \rangle \quad , \end{aligned}$$

where

$$\beta^{-1}\vec{R}_\mu = \vec{R}_\nu \quad \text{and} \quad \beta^{-1}\vec{r} = \vec{r}' \quad .$$

Now we use the transformation (A1) to give

$$\begin{aligned} P_{ij}(\vec{p}, \beta\vec{q}) &= \sum_{\nu, i', j'} e^{-i\vec{q}\cdot\vec{R}_\nu} \mathfrak{D}^*_{ii'}(\beta) \langle u_{i'}(\vec{r}' - \vec{R}_\nu) \\ &\quad \times | e^{i\beta^{-1}\vec{p}\cdot\vec{r}'} | u_{j'}(\vec{r}') \rangle \mathfrak{D}_{jj'}(\beta) \\ &= [\mathfrak{D}^*(\beta) P(\beta^{-1}\vec{p}, \vec{q}) \mathfrak{D}^T(\beta)]_{ij} \quad . \end{aligned}$$

Thus we have the matrix transformation

$$P(\vec{p}, \beta\vec{q}) = \mathfrak{D}^*(\beta) P(\beta^{-1}\vec{p}, \vec{q}) \mathfrak{D}^T(\beta) \quad . \tag{A6}$$

Finally the transformation for the matrix $m$ is obtained by

$$\begin{aligned} m_{ln}(\vec{p} + \vec{K}_s, \beta\vec{q}) &= \sum_{ij} a^*_{li}(\beta\vec{q}) P_{ij}(\vec{p} + \vec{K}_s, \beta\vec{q}) a_{nj}((\beta\vec{q} - \vec{p})_R) \\ &= [A^\dagger(\beta\vec{q}) P(\vec{p} + \vec{K}_s, \beta\vec{q}) A((\beta\vec{q} - \vec{p})_R)]_{ln} \\ &= e^{-i\phi_l(\beta) + i\phi_n(\beta)} m_{ln}(\beta^{-1}(\vec{p} + \vec{K}_s), \vec{q}) . \end{aligned} \tag{A7}$$

A substantial saving in the evaluation of the matrix elements $m_{ln}$ can be achieved by the use of (A7) in combination with Eq. (23). For a given value of $\vec{p}+\vec{K}_s$, it would seem that we need to evaluate $m_{ln}$ for all $\vec{q}$ points in the Brillouin zone. However, a first reduction is obvious in the fact that if an operator leaves $\vec{q}$ unchanged, $m_{ln}$ would not change. A similar saving is achieved when the operator leaves $\vec{p}+\vec{K}_s$ unchanged, i.e.,

$$m_{ln}(\vec{p}+\vec{K}_s, \beta\vec{q}) = m_{ln}(\vec{p}+\vec{K}_s, \vec{q}) \quad \text{if} \quad \beta\vec{q}=\vec{q} \ , \tag{A8}$$

and

$$m_{ln}(\vec{p}+\vec{K}_s, \gamma_s\vec{q}) = e^{-i\phi_l(\gamma_s)+i\phi_n(\gamma_s)} m_{ln}(\vec{p}+\vec{K}_s, \vec{q}) \ , \tag{A9}$$

where

$$\gamma_s(\vec{p}+\vec{K}_s) = \vec{p}+\vec{K}_s \ .$$

Thus we need only those values of $\vec{q}$ that are distinct members of the star and not connected by an operator $\gamma_s \in G(\vec{p}+\vec{K}_s)$, where $G(\vec{k})$ is the group of operators that leaves $\vec{k}$ unchanged. Similarly, when a given $\vec{p}+\vec{K}_s$ is connected by an operator to another $\vec{p}+\vec{K}_s$, we do not need to reevaluate the matrix elements. Consider the case

$$\Gamma_s(\vec{p}+\vec{K}_s) = \vec{p}'+\vec{K}'_s \ . \tag{A10}$$

Using (A7), we find the result

$$\begin{aligned} m_{ln}(\vec{p}+\vec{K}_s, \beta\vec{q}) &= m_{ln}(\Gamma_s^{-1}(\vec{p}'+\vec{K}'_s), \beta\vec{q}) \\ &= e^{i\phi_l(\Gamma_s)-i\phi_n(\Gamma_s)} m_{ln}(\vec{p}'+\vec{K}'_s, \Gamma_s\beta\vec{q}). \end{aligned} \tag{A11}$$

Since all independent vectors $\vec{q}$ have been used for evaluating the $\vec{p}'+\vec{K}'_s$ case, all cases for $\vec{p}+\vec{K}_s$ are available from (A11). This reduces the number of $\vec{p}+\vec{K}_s$ values to be used for $m_{ln}$ and as a bonus, we find that the phase factors need not be evaluated. We define a new set of matrix elements $(m'_{ln})$ that are exactly the same as $m_{ln}$ except that we ignore all phase factors that are not basically inherent in its definition, i.e., those due to the wave functions in the $\frac{1}{48}$ zone. Using the notation that $\vec{q}$ is a vector in this restricted subzone and that all other $\vec{q}$ vectors will have a $\beta$-type operator attached to it, we can write

$$\begin{aligned} m_{ln}(\vec{p}+\vec{K}_s, \vec{q}) &= [A^\dagger(\vec{q})P(\vec{p}+\vec{K}_s, \vec{q})A((\vec{q}-\vec{p})_R)]_{ln} \\ &= [A^\dagger(\vec{q})P(\vec{p}+\vec{K}_s, \vec{q})\mathfrak{D}^T(\beta'^{-1})A(\vec{q}')]_{ln} e^{i\phi_n(\beta')} \\ &= e^{i\phi_n(\beta')} m'_{ln}(\vec{p}+\vec{K}_s, \vec{q}) \ , \end{aligned} \tag{A12}$$

where

$$(\vec{q}-\vec{p})_R = \beta'\vec{q}'$$

and

$$m'_{ln}(\vec{p}+\vec{K}_s, \vec{q}) = [A^\dagger(\vec{q})P(\vec{p}+\vec{K}_s, \vec{q})\mathfrak{D}^T(\beta'^{-1})A(\vec{q}')]_{ln} \ .$$

The expression in Eq. (23) involving the sum of the product of matrix elements over the operators that leave $\vec{p}$ unchanged [$G(\vec{p})$ as distinguished from $\gamma_s \in G(\vec{p}+\vec{K}_s)$, etc.] can now be rewritten in various other convenient forms:

$$S = \sum_\gamma m_{ln}(\alpha^{-1}\gamma^{-1}(\vec{p}+\vec{K}_s), \vec{q}) m^*_{ln}(\alpha^{-1}\gamma^{-1}(\vec{p}+\vec{K}_t), \vec{q}) \ . \tag{A13}$$

Using the definition of $m'_{ln}$ and the fact that the phase factors are multiplicative for a product of operators, we find

$$S = \sum_\gamma m'_{ln}(\vec{p}+\vec{K}_s, \gamma_s\gamma\alpha\vec{q}) m'^*_{ln}(\vec{p}+\vec{K}_t, \gamma_t\gamma\alpha\vec{q}) \ , \tag{A14}$$

where $\gamma_s$ and $\gamma_t$ belong to the group of $\vec{p}+\vec{K}_s$ and $\vec{p}+\vec{K}_t$, respectively. Finally, another similar expression, containing (A14) as a special case, can be written:

$$S = \sum_\gamma m'_{ln}(\vec{p}'+\vec{K}'_s, \gamma'_s\Gamma_s\gamma\alpha\vec{q}) m'^*_{ln}(\vec{p}'+\vec{K}'_t, \ \gamma'_t\Gamma'_t\gamma\alpha\vec{q}) \tag{A15}$$

where

$$\Gamma_s(\vec{p}+\vec{K}_s) = \vec{p}'+\vec{K}'_s \ ,$$

$$\Gamma_t(\vec{p}+\vec{K}_t) = \vec{p}'+\vec{K}'_t \ ,$$

and $\gamma'_s$ and $\gamma'_t$ belong to the group of $\vec{p}'+\vec{K}'_s$ and $\vec{p}'+\vec{K}'_t$, respectively.

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