Partial-Wave Scattering by Non-Spherically-Symmetric Potentials. I. General Theory of Elastic Scattering

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A general method is developed to obtain the elastic-scattering cross section of an asymmetric potential $V(\mathbf{r})=\sum_l v_l(r)P_l(\hat{\Omega}_l\cdot\hat{r})$ where we have expanded the potential as a sum of multipoles and $\hat{\Omega}_l$ is a unit vector along the $2l$-pole axis. We assume that $v_l(r)$ is effectively zero beyond a cutoff radius R and we solve the resulting set of coupled differential equations in terms of a scattering matrix $\mathbf{S}$. A general expression for the scattering amplitude $f(\mathbf{k},\mathbf{k}')$ is derived in terms of the elements of $\mathbf{S}$ and $3j$ symbols. Finally, as an example, we apply the method to the problem of calculating the total and momentum-transfer cross sections for a randomly orientated set of axially symmetric centers.

I. INTRODUCTION

MUCH attention has, in the past, been devoted to the problem of elastic scattering of an electron by a spherically symmetric point charge. In this case it is a relatively straightforward matter to calculate the cross section of the interaction using either a Born approximation or a phase-shift analysis.

However, in many solids, defects in the form of ionized impurities can be associated with each other to form tightly or loosely coupled complexes. An example of the former is acceptor-donor dipoles in semiconductors,[1,2] while an example of the latter is ion-vacancy pair formation in metals.[3,4] The distinction in terms of coupling depends quite naturally on the effectiveness of the electron gas inside the solid in screening one impurity from another. Similarly, the scattering of electrons by polar molecules[5] involves a study of dipole and higher-pole potentials.

The Born approximation is inadequate to describe the scattering of slow electrons, and in this paper we develop a general formalism, analogous to the phase-shift analysis used for spherically symmetric centers, for the elastic scattering cross section of a particle by an asymmetric potential $V(\mathbf{r})$. We write, for convenience, $V(\mathbf{r})$ as the general multipole expansion[6]

$$V(\mathbf{r})=\sum_l v_l(r)P_l(\hat{\Omega}_l\cdot\hat{r}), \tag{1}$$

where $\hat{\Omega}_l$ is the unit vector denoting the direction of the $2l$-pole axis.

In Sec. II we derive the radial wave equation for this problem and it takes the form of a set of coupled differential equations. Section III contains general expressions for the scattering amplitude. Finally, in Sec. IV, we derive scattering cross sections relevant to a randomly orientated array of axially symmetric centers.

II. THE RADIAL WAVE EQUATION

We envisage a scattering event in which a particle of energy $\hbar^2k^2/2m$, mass m and momentum $\hbar\mathbf{k}$ is elastically scattered without change of spin into a state $\hbar\mathbf{k}'$. If $V(\mathbf{r})$ is the potential energy of this particle, in the field of the scattering complex, then its wave function $\psi_{\mathbf{k}}(\mathbf{r})$ satisfies the Schrödinger equation

$$[-(\hbar^2/2m)\nabla^2+V(\mathbf{r})]\psi_{\mathbf{k}}(\mathbf{r})=E(\mathbf{k})\psi_{\mathbf{k}}(\mathbf{r}). \tag{2}$$

A partial-wave expansion of $\psi_{\mathbf{k}}(\mathbf{r})$ enables us to define a set of radial wave functions $g_{l\lambda}(r)$ as follows:

$$\psi(\mathbf{r})=\sum_{l=0}^{\infty}\sum_{\lambda=-l}^{l}\frac{g_{l\lambda}(r)}{r}Y_l^{\lambda}(\hat{r}), \tag{3}$$

where we have dropped the subscript $\mathbf{k}$ for ease of notation.

If we substitute (3) into (2), premultiply the resulting equation by the complex-conjugate harmonic $Y_{l'}^{*\lambda'}(\hat{r})$, and integrate over the solid angle $d\Omega_{\mathbf{r}}$ we obtain the set of radial equations

$$\left(\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}+k^2\right)g_{l\lambda}(r)=\frac{2m}{\hbar^2}\sum_{l'\lambda'}g_{l'\lambda'}(r)\int Y_l^{*\lambda}(\hat{r})V(\mathbf{r})Y_{l'}^{\lambda'}(\hat{r})d\Omega_{\mathbf{r}}. \tag{4}$$

The potential function given by Eq. (1) can also be

[1] A. D. Boardman, Proc. Phys. Soc. (London) **85**, 141 (1965).
[2] A. D. Boardman, Phys. Rev. **147**, 532 (1966).
[3] C. P. Flynn, Phys. Rev. **126**, 533 (1962).
[4] J. M. Keller, J. Phys. Chem. Solids **24**, 1121 (1963).
[5] M. H. Mittleman and R. E. von Holdt, Phys. Rev. **140**, A726 (1965).
[6] This view was recently adopted in a paper by L. C. R. Alfred [Phys. Rev. **152**, 693 (1966)] which appeared while this paper was in preparation.

written as

$$V(\mathbf{r})=4\pi\sum_{L\Lambda}\frac{v_L(r)}{2L+1}Y_L^{*\Lambda}(\hat{\Omega}_L)Y_L^{\Lambda}(\hat{r}), \tag{5}$$

where we have used the familiar spherical-harmonic addition theorem.

The substitution of (5) into the right-hand side of (4) gives

$$\left(\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}+k^2\right)g_{l\lambda}(r)=\frac{8m\pi}{\hbar^2}\sum_{\substack{l'\lambda'\\L\Lambda}}\frac{v_L(r)}{2L+1}Y_L^{*\Lambda}(\hat{\Omega}_L)$$
$$\times g_{l'\lambda'}(r)\int Y_L^{\Lambda}(\hat{r})Y_l^{*\lambda}(\hat{r})Y_{l'}^{\lambda'}(\hat{r})d\Omega_r. \tag{6}$$

The integration over the solid-angle $d\Omega_r$ can be immediately performed, using the result[7]

$$\int Y_L^{\Lambda}(\hat{r})Y_l^{*\lambda}(\hat{r})Y_{l'}^{\lambda'}(\hat{r})d\Omega_r$$
$$=(-1)^{\lambda}\left\{\frac{(2L+1)(2l+1)(2l'+1)}{4\pi}\right\}^{1/2} \tag{7}$$
$$\times\begin{pmatrix}l & l' & L\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l & l' & L\\ \lambda & -\lambda' & \lambda'-\lambda\end{pmatrix}\delta_{\Lambda,\lambda-\lambda'}.$$

The $3j$ vector coupling coefficient

$$\begin{pmatrix}a & b & c\\ \alpha & \beta & \gamma\end{pmatrix}$$

is defined by Edmonds,[7] who gives tables and formulas for some specific cases. A useful property of the $3j$ symbols is that

$$\begin{pmatrix}l & l' & L\\ 0 & 0 & 0\end{pmatrix}=0, \quad \text{if} \quad l+l'+L \quad \text{is odd.} \tag{8}$$

Equation (6) now becomes

$$\left(\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}+k^2\right)g_{l\lambda}(r)=\sum_{l'\lambda'}W_{l\lambda,l'\lambda'}(r)g_{l'\lambda'}(r), \tag{9}$$

where

$$W_{l\lambda,l'\lambda'}(r)=\frac{2m}{\hbar^2}\sum_L(-1)^{\lambda'}\left\{\frac{4\pi(2l+1)(2l'+1)}{2L+1}\right\}^{1/2}$$
$$\times\begin{pmatrix}l & l' & L\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l & l' & L\\ \lambda & -\lambda & \lambda'-\lambda\end{pmatrix}v_L(r)Y_L^{\lambda'-\lambda}(\hat{\Omega}_L). \tag{10}$$

We have therefore arrived at a set of coupled differential equations for the functions $g_{l\lambda}(r)$, which we will, in practice, cut off at the value of l beyond which the solutions no longer make a significant contribution to the scattering cross section.

It is interesting to note, at this stage, the following properties of the coupling function $W_{l\lambda,l'\lambda'}(r)$:

$$\begin{aligned}W_{l'\lambda',l\lambda}^{*}(r)&=W_{l\lambda,l'\lambda'}(r),\\ W_{l-\lambda,l'-\lambda'}^{*}(r)&=(-1)^{\lambda'-\lambda}W_{l\lambda,l'\lambda'}(r).\end{aligned} \tag{11}$$

If the scattering potential happens to possess an axis of symmetry (for example a dipole potential), we can always choose it as our z axis, i.e., we can set $\hat{\Omega}_L=0$ in the harmonic $Y_L^{\lambda'-\lambda}(\hat{\Omega}_L)$, which then becomes

$$Y_L^{\lambda'-\lambda}(\hat{\Omega}_L)=((2L+1)/4\pi)^{1/2}\delta_{\lambda\lambda'}. \tag{12}$$

The substitution of (12) into Eqs. (9) and (10) gives, respectively,

$$\left(\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}+k^2\right)g_{l\lambda}(r)=\sum_{l'}W_{ll'\lambda}(r)g_{l'\lambda}(r) \tag{13}$$

and

$$W_{ll'\lambda}(r)=\frac{2m}{\hbar^2}\sum_L(-1)^{\lambda}(2l+1)^{1/2}(2l'+1)^{1/2}$$
$$\times v_L(r)\begin{pmatrix}l & l' & L\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l & l' & L\\ \lambda & -\lambda & 0\end{pmatrix}, \tag{14}$$

where $W_{ll'\lambda}(r)$ is real and

$$W_{ll'-\lambda}(r)=W_{ll'\lambda}(r). \tag{15}$$

Equation (13) no longer has a coupling term connecting different values of λ. In this case we need only to solve the coupled set of equations (13) for positive values of λ.

III. THE SCATTERING AMPLITUDE

In the problem of elastic scattering by spherically symmetric potentials, the phase shift δ_l, which the lth partial wave possesses in the asymptotic region, removed from the scatterer, contains all the information needed to define the scattering cross section.

In practice the wave function becomes

$$\psi_{\mathbf{k}}(\mathbf{r})\rightarrow e^{i\mathbf{k}\cdot\mathbf{r}}+f(\mathbf{k},\mathbf{k}')e^{ikr}/r \tag{16}$$

and the differential cross section is defined as

$$\sigma(\mathbf{k},\mathbf{k}')=|f(\mathbf{k},\mathbf{k}')|^2. \tag{17}$$

We return to the problem at hand and note that if, in practice, the potential terms $v_L(r)$ vanish beyond some radius R, Eq. (13) becomes

$$(d^2/dr^2-l(l+1)/r^2+k^2)g_{l\lambda}(r)=0, \tag{18}$$

the solutions of which can be written in the form

$$g_{l\lambda}(r)=i^lA_{l\lambda}[rj_l(kr)+rS_{l\lambda}h_l^{+}(kr)], \tag{19}$$

[7] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, New Jersey, 1957), p. 31.

where $j_l(kr)$ is the usual spherical Bessel function and the asymptotic form of h_l^+ is

$$h_l^+(kr) = -ie^{i(kr-l\pi/2)}/kr. \tag{20}$$

The coefficient $A_{l\lambda}$ is fixed by requiring the asymptotic form of the total wave function to be

$$\psi(r) \sim e^{i\mathbf{k}\cdot\mathbf{r}} + \sum_{l\lambda} A_{l\lambda} S_{l\lambda} Y_l^{\lambda}(\hat{k}') \frac{e^{ikr}}{kr}. \tag{21}$$

The expansion of $e^{i\mathbf{k}\cdot\mathbf{r}}$ into spherical harmonics gives

$$e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi \sum_{l\lambda} i^l Y_l^{*\lambda}(\hat{k}) Y_l^{\lambda}(\hat{k}') j_l(kr), \tag{22}$$

which immediately shows that

$$A_{l\lambda} = 4\pi Y_l^{*\lambda}(\hat{k}). \tag{23}$$

It is interesting to note at this stage that for a spherically symmetric center we have

$$f(\mathbf{k},\mathbf{k}') = 4\pi \sum_{l\lambda} i^l Y_l^{*\lambda}(\hat{k}) Y_l^{\lambda}(\hat{k}') S_l = \sum_l i^l (2l+1) P_l(\cos\chi) S_l, \tag{24}$$

where x is the scattering angle. Equation (24) shows that

$$S_l = e^{i\delta_l} \sin\delta_l, \tag{25}$$

where δ_l is the usual phase shift.

The general expression for the scattering amplitude is therefore

$$f(\mathbf{k},\mathbf{k}') = \frac{4\pi}{k} \sum_{l\lambda} S_{l\lambda} Y_l^{*\lambda}(\hat{k}) Y_l^{\lambda}(\hat{k}'). \tag{26}$$

However, it is inconvenient to express $f(\mathbf{k},\mathbf{k}')$ in this form because, although we dropped the suffix $\mathbf{k}$ on the wave function at an earlier point in the text, we must note that $S_{l\lambda}$ depends on $\mathbf{k}$, the direction of the incident beam. We therefore write

$$S_{l\lambda,\mathbf{k}} Y_l^{*\lambda}(\hat{k}) = \sum_{l'\lambda'} S_{l'\lambda',l\lambda} Y_{l'}^{*\lambda'}(\hat{k}). \tag{27}$$

The scattering amplitude then becomes[8]

$$f(\mathbf{k},\mathbf{k}') = \frac{4\pi}{k} \sum_{l\lambda} \sum_{l'\lambda'} S_{l\lambda,l'\lambda'} Y_{l'}^{*\lambda'}(\hat{k}) Y_l^{\lambda}(\hat{k}'). \tag{28}$$

Equation (28) is still not in its most useful form, because the coordinate frame is fixed in the scattering center. We therefore rotate the coordinate frame, through $-\mathbf{k}$, to a new frame in which $\mathbf{k}$ lies along the z axis, and write

$$Y_{l'}^{*\lambda'}(\hat{k}) Y_l^{\lambda}(\hat{k}') = \sum_{\lambda''} D_{l'\lambda''\lambda'}(-\hat{k}) Y_{l'}^{\lambda''}(0) \times \sum_{\lambda'''} D_{l\lambda\lambda'''}(-\hat{k}) Y_l^{\lambda'''}(\chi), \tag{29}$$

where $D_{\alpha\beta\gamma}$ are the matrix elements of the rotation operator.[7]

It is obvious that

$$Y_{l'}^{\lambda''}(0) = ((2l+1)/4\pi)^{1/2}, \quad \lambda''=0; \qquad = 0, \quad \lambda''\neq 0 \tag{30}$$

and this results in the first summation of (29) becoming

$$((2l+1)/4\pi)^{1/2} D_{l'0\lambda'}(-\hat{k}) = Y_{l'}^{\lambda'}(-\hat{k}). \tag{31}$$

The final expression for the scattering amplitude is thus

$$f(\chi,\omega) = \frac{4\pi}{k} \sum_{l\lambda} \sum_{l'\lambda'} \sum_{\lambda'''} S_{l\lambda,l'\lambda'} D_{\lambda\lambda'''}{}^{l} \times (-\hat{k}) Y_{l'}^{\lambda'}(-\hat{k}) Y_l^{\lambda'''}(\chi), \tag{32}$$

where the scattering amplitude is now only a function of the scattering angle χ and the angle ω of an axis fixed in the scattering center, relative to the new frame.

IV. AXIALLY SYMMETRIC SCATTERING

The majority of physical applications of our theory will involve potentials with an axis of symmetry.[1,2,5] We will therefore for simplicity develop below the total cross section for a randomly oriented set of axially symmetric centers.[9]

The general differential cross section is

$$\sigma(x,\omega) = |f(x,\omega)|^2, \tag{33}$$

giving a total cross section of

$$\sigma(\omega) = \int \sigma(x,\omega) d\Omega_x \tag{34}$$

and a momentum-transfer cross section

$$\sigma(\omega) = \int \sigma(x,\omega)(1-\cos x) d\Omega_x. \tag{35}$$

The result for random orientation of the centers is obtained by a simple classical average over ω.[1,2] We therefore obtain for the total cross section

$$\sigma = \frac{4\pi}{k^2} \sum_{ll'\lambda} |S_{ll'\lambda}|^2. \tag{36}$$

In order to determine (35), after averaging over ω, it is only necessary to begin with Eq. (28), which for a

[8] The method of solution in terms of $S_{l'\lambda',l\lambda}$ is discussed in the Appendix.

[9] A discussion of a partially oriented set of scatterers, based on Eqs. (34) and (35), will be the subject of a forthcoming paper.

potential possessing an axis of symmetry becomes

$$f(\mathbf{k},\mathbf{k}')=\frac{4\pi}{k}\sum_{l\lambda l'} S_{ll'\lambda}Y_{l'}{}^{*\lambda}(\hat{k})Y_l{}^{\lambda}(\hat{k}'). \tag{37}$$

We write

$$\cos\chi\equiv\cos(\hat{k}\cdot\hat{k}')=\frac{4\pi}{3}\sum_m Y_1{}^{*m}(\hat{k})Y_1{}^{m}(\hat{k}'), \tag{38}$$

and we find that the integral involving $\cos\chi$ becomes

$$I=\frac{4\pi}{3}\left(\frac{4\pi}{k}\right)^2\sum_{ll'\lambda}\sum_{LL'\Lambda}\sum_m S_{LL'\Lambda}{}^{*}S_{ll'\lambda}\int\int Y_{L'}{}^{\Lambda}(\hat{k})Y_{l'}{}^{*\lambda}(\hat{k})\times Y_1{}^{*m}(\hat{k}')Y_l{}^{\lambda}(\hat{k}')Y_1{}^{m}(\hat{k}')d\Omega_{\mathbf{k}}d\Omega_{\mathbf{k}'}, \tag{39}$$

which on using

$$\int Y_l{}^{*\lambda}Y_{l'}{}^{\lambda'}d\Omega=\delta_{ll'}\delta_{\lambda\lambda'},$$

$$\int Y_l{}^{\lambda}Y_1{}^{m}Y_L{}^{*\Lambda}d\Omega=\left[\frac{3(2l+1)(2L+1)}{4\pi}\right]^{1/2}\times\begin{pmatrix} l & L & 1\\ 0 & 0 & 1\end{pmatrix}\begin{pmatrix} l & L & 1\\ \lambda & -\Lambda & m\end{pmatrix}, \tag{40}$$

finally becomes

$$I=\left(\frac{4\pi}{k}\right)^2\sum_{ll'\lambda}\sum_{LL'\Lambda}\sum_m S_{ll'\lambda}S_{LL'\Lambda}{}^{*}\times[(2l+1)(2L+1)(2l'+1)(2L'+1)]^{1/2}\begin{pmatrix} l & L & 1\\ 0 & 0 & 1\end{pmatrix}\times\begin{pmatrix} l & L & 1\\ \lambda & \Lambda & m\end{pmatrix}\begin{pmatrix} l' & L' & 1\\ 0 & 0 & 1\end{pmatrix}\begin{pmatrix} l' & L' & 1\\ \lambda & -\Lambda & m\end{pmatrix}. \tag{41}$$

Equations (41) and (36) give us the result we desire.

V. CONCLUSION

We have developed a method of solving the problem of elastic scattering of particles by an asymmetric, point potential in a very general fashion. However, we should like to emphasize that the work can be used to attack a number of well-defined physical problems. The first problem of interest is the scattering of electrons by screened dipoles in semiconductors.[1,2] Other problems include the analogous problem of scattering of slow electrons by polar molecules such as ammonia and scattering by molecular hydrogen where a quadrupole term will have to be considered.

The problems mentioned are being investigated by the authors and detailed numerical solutions will appear as sequels to the present paper.

APPENDIX

Let us suppose that we generate N linearly independent solutions of our set of coupled differential equations by using N different initial conditions. If this set is $g_l{}^{(i)}(r)$ (where we drop the λ suffices for convenience) then the true solution must be a linear combination:

$$g_l(r)=\sum_i B_i g_l{}^{(i)}(r). \tag{A1}$$

We determine B_i by matching solutions (A1) to the asymptotic solution (19), i.e.,

$$\sum_i \frac{B_i g_l{}^{(i)}(R)}{R}=i^l[A_l j_l(kR)+A_l S_l h_l{}^{+}(kR)], \tag{A2}$$

and by matching the derivatives, i.e.,

$$\sum_i \frac{\frac{d}{dR}\left(\frac{g_l{}^{(i)}(R)}{R}\right)}{i^l k j_l'(kR)}B_i-\frac{h_l{}^{+\prime}(kR)}{i^l j_l'(kR)}A_l S_l=A_l. \tag{A3}$$

Equations (A2) and (A3) can be written in the matrix form

$$\mathbf{Cx}=\mathbf{d}, \tag{A4}$$

where

$$\mathbf{C}=\begin{pmatrix} G & H\\ G' & H'\end{pmatrix};\quad \mathbf{x}=\begin{pmatrix} B_i\\ A_l S_l\end{pmatrix};\quad \mathbf{d}=\begin{pmatrix} A_l\\ A_l\end{pmatrix}; \tag{A5}$$

and

$$G=\frac{g_l{}^{(i)}(R)}{i^l R j_l(kR)};\qquad H=-\frac{h_l{}^{+}(kR)}{i^l j_l(kR)};$$
$$G'=\frac{\frac{d}{dR}\left(\frac{g^{(i)}(R)}{R}\right)}{i^l k j_l'(kR)};\qquad H'=-\frac{h_l{}^{+\prime}(kR)}{i^l j_l'(kR)}. \tag{A6}$$

If we now invert $\mathbf{C}$ and write

$$\mathbf{x}=\mathbf{C}^{-1}\mathbf{d}, \tag{A7}$$

where

$$\mathbf{C}^{-1}=\begin{pmatrix} \hat{G} & \hat{H}\\ \hat{G}' & \hat{H}'\end{pmatrix}, \tag{A8}$$

then we obtain

$$A_l S_l=\sum_{l'}(\hat{G}_{ll'}+\hat{H}_{ll'})A_{l'}\equiv\sum_{l'} S_{ll'}A_{l'}, \tag{A9}$$

which essentially is the result used in Eq. (27) provided that one includes the generalization to a dependence on λ and λ'.