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Elastic electron scattering from a multicentred potential

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The amplitude and the cross-section of elastic electron scattering from a multicentred system are obtained as a result of an exact solution of the scattering problem in the case of one Coulomb potential and any number of short-range potentials.

1. The aim of the present paper is to calculate the amplitude and the cross-section of elastic electron scattering from the system in which one Coulomb potential and any number of short-range potentials are included. Within this calculation the zero-radius potential (ZRP) model [1–4] will be used as multicentred pseudopotential. Our interest in this system was stimulated by the problem of the interpretation of the electron-scattering experiments for complex molecular ions, ionized gases and low-ionized plasma [5,6], on the one hand; and on the other hand, by the problem of generalisation and developing of theories of scattering from a single Coulomb center with a short-range potential well [7–9] and from a superposition of ZRPs [10–17] separately. The ZRP model for the pseudopotential has been used in view of successful applications of the ZRP in numerical calculations of electron scattering from a hydrogen molecule [18] and, also, because of the possibility of an exact solution of the problem in this case.

2. Consider elastic scattering of a monochromatic electron beam with energy E from a multicentred target which includes a single Coulomb and N short-range potentials where the latter describe a superposition of ZRPs. Let us assume that the target particles are structureless and also can be considered as being at rest during the elementary act of scattering. Putting the origin **O** of the coordinate system in the centre of the Coulomb potential and following the general theory of ZRPs [1–4] we write the stationary Schrödinger equation for the whole system: electron plus target, in the following dimensionless form,

$$\left(-\tfrac{1}{2}\Delta_r+\frac{s}{r}-E+2\pi\sum_{j=1}^{N} l_j\delta(r-R_j)\frac{\partial}{\partial\tau_j}\tau_j\right)\Psi(r,\{R\})=0\,, \tag{1}$$

where $\Delta_r\equiv\partial^2/\partial r^2$, $\tau_j=|r-R_j|$, l_j is the scattering length for the jth ZRP, $s=-1$ for attractive and $+1$ for repulsive Coulomb potentials, respectively, $\Psi(r,\{R\})$ is the wave function of the whole system, which includes the dependence on all coordinates of the target particles, $\{R\}=R_1,\ldots,R_N$, as parameters. In (1) and below will be used a Coulomb system of units in which $\hbar^2/m_e e^2 Z$ and $m_e e^4 Z^2/\hbar^2$ are the length and energy scales respectively; $\delta(\ )$ is the Dirac delta function.

Equation (1) is not a closed equation due to the inclusion, along with $\Psi(r,\{R\})$, of N unknown functions $\{\Psi(R_j,\{R\})\}$. Taking into account the physical properties of the wave functions, eq. (1) will be considered with a typical boundary condition in the following form,

$$\frac{1}{\tau_j \Psi}\frac{\partial}{\partial \tau_j}(\tau_j \Psi)\bigg|_{\tau_j \to 0} = -\frac{1}{l_j} \equiv -\kappa_j, \qquad j=1, 2, ..., N. \tag{2}$$

3. Introducing the Green function for the Schrödinger equation with a Coulomb potential unperturbed by short-range potentials in closed form, which was first obtained by Hostler and Pratt [4,19–21],

$$G(\boldsymbol{r}, \boldsymbol{r}') = \frac{\Gamma(1-\eta)}{2\pi|\boldsymbol{r}-\boldsymbol{r}'|}\left(\frac{\partial}{\partial(\mathrm{i}kx)} - \frac{\partial}{\partial(\mathrm{i}ky)}\right) W_{\eta,1/2}(-\mathrm{i}kx) M_{\eta,1/2}(-\mathrm{i}ky), \qquad k=\sqrt{2E}, \tag{3}$$

we can write down an exact solution of (1), namely

$$\Psi(\boldsymbol{r}, \{\boldsymbol{R}\}) = \psi^+(\boldsymbol{r}) + \sum_{j=1}^{N} \bar{\Psi}(\boldsymbol{R}_j, \{\boldsymbol{R}\}) G(\boldsymbol{r}, \boldsymbol{R}_j), \tag{4}$$

where

$$\psi^+(\boldsymbol{r}) = \exp(-s\pi/2k)\Gamma(1+\mathrm{i}s/k)\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}) F(-\mathrm{i}s/k, 1, \mathrm{i}(kr-\boldsymbol{k}\cdot\boldsymbol{r})) \tag{5}$$

is the Coulomb wave function for the continuous spectrum, $x=r+r'+|\boldsymbol{r}-\boldsymbol{r}'|$, $y=r+r'-|\boldsymbol{r}-\boldsymbol{r}'|$, $\Gamma(z)$ is the gamma-function, $W_{\eta,1/2}(z)$ and $M_{\eta,1/2}(z)$ are Whittaker functions, $F(\alpha, \beta, z)$ is the confluent hypergeometric function, $\eta=\mathrm{i}s/k$.

The set of coefficients $\{\bar{\Psi}(\boldsymbol{R}_j, \{\boldsymbol{R}\})\}$ can be determined as a result of solving a system of algebraic equations which follows from (2) and (4). We just represent here the final result of this calculation, namely

$$\bar{\Psi}(\boldsymbol{R}_j, \{\boldsymbol{R}\}) = \frac{\Delta_j}{\Delta}, \tag{6}$$

where

$$\Delta = \begin{Vmatrix} \xi(\boldsymbol{R}_1)+\kappa_1 & 2\pi G(\boldsymbol{R}_1, \boldsymbol{R}_2) & \dots & 2\pi G(\boldsymbol{R}_1, \boldsymbol{R}_N) \\ 2\pi G(\boldsymbol{R}_2, \boldsymbol{R}_1) & \xi(\boldsymbol{R}_2)+\kappa_2 & & 2\pi G(\boldsymbol{R}_2, \boldsymbol{R}_N) \\ \vdots & & & \\ 2\pi G(\boldsymbol{R}_N, \boldsymbol{R}_1) & 2\pi G(\boldsymbol{R}_N, \boldsymbol{R}_2) & \dots & \xi(\boldsymbol{R}_N)+\kappa_N \end{Vmatrix},$$

$$\Delta_j = \begin{Vmatrix} \xi(\boldsymbol{R}_1)+\kappa_1 & \dots & -2\pi\psi^+(\boldsymbol{R}_1) & \dots & 2\pi G(\boldsymbol{R}_1, \boldsymbol{R}_N) \\ 2\pi G(\boldsymbol{R}_2, \boldsymbol{R}_1) & & -2\pi\psi^+(\boldsymbol{R}_2) & & 2\pi G(\boldsymbol{R}_2, \boldsymbol{R}_N) \\ \vdots & & \vdots & & \vdots \\ 2\pi G(\boldsymbol{R}_N, \boldsymbol{R}_1) & \dots & -2\pi\psi^+(\boldsymbol{R}_N) & \dots & \xi(\boldsymbol{R}_N)+\kappa_N \end{Vmatrix}, \tag{7}$$

and

$$\xi(\boldsymbol{R}_j) = 2\pi \frac{\partial}{\partial \tau_j} \tau_j G(\boldsymbol{r}, \boldsymbol{R}_j)\bigg|_{\tau_j \to 0}. \tag{8}$$

We emphasize that expressions (4), (6) and (7) are obtained without any additional approximations and thus represent an exact solution.

4. Using the known asymptotic properties of $\psi^+(\boldsymbol{r})$, $W_{\eta,1/2}(z)$ and $M_{\eta,1/2}(z)$ [22,23], with the help of (4), (6) and (7) we obtain an expression for the wave function of the scattered electron Ψ_{sc} in the following form,

$$\Psi_{sc}(r, \{R\}) = [f_C(\vartheta) + f_{C,1,\ldots,N}] \frac{[\exp(ikr - (i/k)\ln(2kr)]}{r}, \tag{9}$$

where

$$f_C(\vartheta) = -\frac{1}{2k^2 \sin^2(\vartheta/2)} \frac{\Gamma(1+i/k)}{\Gamma(1-i/k)} \exp\left(-\frac{2i}{k} \ln \sin(\vartheta/2)\right) \tag{10}$$

is the Coulomb amplitude and ϑ is the angle of scattering.

Thus, from (9) it follows that the expression

$$f_{C,1,\ldots,N} = \frac{1}{2\pi} \exp(-\pi/2k)\Gamma(1+i/k) \sum_{j=1}^{N} \tilde{\Psi}(R_j, \{R\})\Xi(R_j, \omega_j) \tag{11}$$

can be considered as the amplitude of scattering from the multicentred short-range pseudopotential in the Coulomb field. Note that in (11)

$$\Xi(R_j, \omega_j) = M'_{-i/k,1/2}(ikR_j(1+\cos\omega_j)) + \tfrac{1}{2} M_{-i/k,1/2}(ikR_j(1+\cos\omega_j)), \tag{12}$$

and ω_j is the angle between the vectors r and R_j. Also note, that for the definition, we put here that the Coulomb potential is repulsive,

$$M'_{-i/k,1/2}(z) \equiv \frac{d}{dz} M_{-i/k,1/2}(z).$$

As follows from (9)–(11) the amplitude $f_{C,1,\ldots,N}$ is not the same as the known Coulomb or ZRP amplitudes, separately. At the same time, because the $\{\tilde{\Psi}(R_j, \{R\})\}$ are determined for the whole set $\{R\}$, $f_{C,1\ldots,N}$ cannot be considered as a pair-additive function which includes the contributions from pair-wise complexes of the type: Coulomb centre plus ZRP, only. We emphasise the factorisation of the amplitudes $f_{C,1,\ldots,N}$ as functions of all angular arguments.

5. As follows from (6)–(12), for the case of complexes of the type: Coulomb plus ZRP, which are shifted one from another by a vector R, in the limit, when $R \to \infty$ we have the known result [1–4]

$$f_{C,1} = -\frac{1}{\kappa - 1/\eta} - \frac{f_C(\vartheta)}{\kappa - 1/\eta} \frac{1}{R} \to -\frac{1}{\kappa - 1/\eta} = f_1. \tag{13}$$

The using the asymptotic properties of Whittaker functions [22,23] for the complexes of the type: Coulomb and two ZRP which are centred at the points R_1 and R_2, in the limit $R_1 \to \infty$, $R_2 \to \infty$ and $|R_1 - R_2| = R$ kept fixed, we obtain

$$f_{C,1,2} = -\frac{(\kappa_1 - 1/\eta) + (\kappa_2 - 1/\eta) - (1/2\pi)\exp(ikR)/R}{(\kappa_1 - 1/\eta)(\kappa_2 - 1/\eta) - (1/4\pi^2)\exp(2ikR)/R^2}. \tag{14}$$

When $\kappa_1 = \kappa_2$ expression (14) is exactly the same as the known result which is usually called the Brueckner formula [1–4],

$$f_{C,1,2} = -\frac{2}{\kappa - 1/\eta + (1/2\pi)\exp(ikR)/R}. \tag{15}$$

For complexes of the type: Coulomb centre and ZRP at the point R, when $R \to 0$, from (11) follows the famous Landau and Smorodynsky formula which can be reproduced here in the following form,

$$f_{C=1} = -\frac{2\pi}{k}\frac{\Gamma(1+\mathrm{i}/k)}{\Gamma(1-\mathrm{i}/k)}\frac{1}{1-\exp(2\pi/k)}\frac{1}{\kappa-\Gamma(1+\mathrm{i}/k)[(\partial/\partial R)W_{-\mathrm{i}/k,1/2}(-2\mathrm{i}kR)]_{R\to 0}}. \tag{16}$$

As the next step we represent here the amplitude of scattering from complexes of the type: Coulomb centre plus ZRP at the common point and the next ZRP at $\boldsymbol{R}$, which can be considered as a generalisation of the Brueckner and Landau and Smorodynsky results, namely

$$\begin{aligned} f_{C=1,2} &= -\exp(-\pi/2k)\Gamma(1+\mathrm{i}/k) \\ &\times\{\exp(-\pi/2k)\Gamma(1+\mathrm{i}/k)[\kappa_2+\xi(\boldsymbol{R})-\Xi(R,\omega)G(0,\boldsymbol{R})] \\ &+\psi^{+}(\boldsymbol{R})(\Xi(R,\omega)\{\kappa_1-\Gamma(1+\mathrm{i}/k)[(\partial/\partial r)W_{-\mathrm{i}/k,1/2}(-2\mathrm{i}kr)]_{r\to 0}\}-G(0,\boldsymbol{R}))\} \\ &\times\{\kappa_1-\Gamma(1+\mathrm{i}/k)[(\partial/\partial r)W_{-\mathrm{i}/k,1/2}(-2\mathrm{i}kr)]_{r\to 0}[\kappa_2+\xi(\boldsymbol{R})]-(2\pi)^3G^2(0,\boldsymbol{R})\}^{-1} \\ G(0,\boldsymbol{R}) &= \frac{W_{-\mathrm{i}/k,1/2}(-2\mathrm{i}kR)}{R}. \end{aligned} \tag{17}$$

In the limit $R\to\infty$ expression (17) becomes $f_{C=1,2}\to f_{C=1}+f_2$, which includes results (14)–(16). Without any difficulties this scheme can be extrapolated to higher order complexes.

6. The differential cross section of scattering which is given by the following formula,

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left| f_{C,1,\ldots,N} + f_C \right|^2, \tag{18}$$

must be correctly averaged over all configurations $\{\boldsymbol{R}\}$. In particular, following refs. [24,25] this averaging can be realised with the help of the correlational expansion of $\overline{\mathrm{d}\sigma/\mathrm{d}\Omega}$ in a doubly irreducible series, every pth fragment of which represents an averaged contribution to $\overline{\mathrm{d}\sigma/\mathrm{d}\omega}$ due to scattering from the $p+1$ particle complexes which include one Coulomb and p ZRP centres, namely

$$\begin{aligned} \overline{\mathrm{d}\sigma/\mathrm{d}\Omega} &= |f_C|^2 + \sum_{p=1}^{N}\frac{N(N-1)\ldots(N-p+1)}{p!V^p}\int\ldots\int\left\{\left|\sum_{j=1}f_{C,j}\right|^2-\left|\sum_{j=1}^{p}f_j\right|^2\right. \\ &\left.+2\,\mathrm{Re}\left[f_C\left(\sum_{j=1}^{p}f_{C,j}-\sum_{j=1}^{p}f_j\right)^{*}\right]\right\}H_p^{(C,1,\ldots,p)}(\boldsymbol{R}_1,\ldots,\boldsymbol{R}_p)\,\mathrm{d}\boldsymbol{R}_1,\ldots,\mathrm{d}\boldsymbol{R}_p, \end{aligned} \tag{19}$$

where the set of the density-particle functions $\{H_p^{(C,1,\ldots,p)}(\boldsymbol{R}_1,\ldots,\boldsymbol{R}_p)\}$ (form factors of the particle complexes) must be determined from alternative sources [24,25].

The effects of backscattering and the statistical analysis of the cross-section will be discussed separately.

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