明治大学教養論集　通巻266号（1994・3）pp. 1—7

Coulomb Scattering of a Spherical Wave

Koichi NAKAMURA

In our paper[1] on the point source electron microscope, we solved the scattering problem with a spherical incident wave to simulate the holographic image. There the scattering potential has been assumed to be a short range one, so that we can not apply the result we obtained to the case that an object contains ions, because of the slow decrease of the Coulomb potential. To treat such an object, we need to extend our argument to one with long range potentials. In this note, we will discuss the simplest case where the object consists of only one ion.

Our problem is to find a solution of the Schrödinger equation with the Coulomb potential,

$$\left(-\Delta+\frac{ZZ'e^2}{r}\right)\psi(\vec{r})=k^2\psi(\vec{r}) \tag{1}$$

such that

$$\psi(\vec{r})=\frac{e^{ik|\vec{r}-\vec{R}|}}{|\vec{r}-\vec{R}|}+\phi(\vec{r}), \tag{2}$$

where $\phi(\vec{r})$ contains only outgoing wave component. Here we take the origin at the center of the potential and $\vec{R}$ is the position vector of the source of the incident spherical wave.

We expand $\psi(\vec{r})$ into partial waves,

$$\psi(\vec{r})=\frac{1}{r}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}u_{lm}(r)\,Y_l^m(\theta,\phi),\tag{3}$$

then the spherical function $u_{lm}(r)$ satisfies the equation

$$\left(\frac{d^2}{dr^2}-\frac{2kn}{r}-\frac{l(l+1)}{r^2}+k^2\right)u_{lm}(r)=0,\tag{4}$$

with $n=ZZ'e^2/2k$.

We also have the expansion

$$\frac{e^{ik|\vec{r}-\vec{R}|}}{|\vec{r}-\vec{R}|}=\frac{1}{r}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}u_{lm}^{(0)}(r)\,Y_l^m(\theta,\phi),\tag{5}$$

where

$$u_{lm}^{(0)}(r)=4\pi ikrj_l(kr_-)\,h_l^{(1)}(kr_+)\,Y_l^{m*}(\Theta,\Phi),\tag{6}$$

with $r_-=\min(r,R)$, $r_+=\max(r,R)$. Here j_l and $h_l^{(1)}$ are the spherical Bessel function and the spherical Hankel function respectively and Θ and Φ denote the polar and azimuth angles of the vector $\vec{R}$ respectively.

We note that $u_{lm}^{(0)}(r)$ given by (6) satisfies

$$\left(\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}+k^2\right)u_{lm}^{(0)}(r)=0.\tag{7}$$

Now we consider the Green's function $\mathcal{G}_l^{(+)}(r,r')$ of eq.(4) with outgoing wave boundary condition which is described as satisfying the equation

$$\left(\frac{d^2}{dr^2}-\frac{2kn}{r}-\frac{l(l+1)}{r^2}+k^2\right)\mathcal{G}_l^{(+)}(r,r')=\delta(r-r').\tag{8}$$

This Green's function is found to be (cf. eq.(14.50) in Newton's book[2])

$$\mathcal{G}_l^{(+)}(r,r')=i(-1)^l(4k^2rr')^{l+1}e^{ik(r+r')}\frac{\Gamma(l+1+in)}{2k(2l+1)!}$$
$$\times\Phi(l+1+in,2l+2;-2ikr_<)\,\Psi(l+1+in,2l+2;-2ikr_>),\tag{9}$$

where $r_<=\min(r,r')$, $r_>=\max(r,r')$. $\Phi(a,b;x)$ is the confluent hypergeometric function,

$$\Phi(a, b; x)=\sum_{s=0}^{\infty}\frac{\Gamma(a+s)\Gamma(b)x^s}{\Gamma(b+s)\Gamma(a)s!}, \tag{10}$$

and $\Psi(a, b; x)$ is the irregular cofluent hypergeometric function defined by

$$\Psi(a, b; x)=\frac{\Gamma(1-b)}{\Gamma(a-b+1)}\Phi(a, b; x)+\frac{\Gamma(b-1)}{\Gamma(a)}x^{1-b}\Phi(a-b+1, 2-b; x). \tag{11}$$

By using the above Green's function, the solution of eq. (4), $u_{lm}(r)$, is written as

$$u_{lm}(r)=u_{lm}^{(0)}(r)+2kn\int_0^{\infty}dr'\mathcal{G}_l^{(+)}(r, r')\frac{1}{r'}u_{lm}^{(0)}(r'). \tag{12}$$

We can see that the above $u_{lm}(r)$ satisfies eq. (4) by making use of eqs. (7) and (8).

Substituting (12) into eq. (3), we obtain the solution of eq. (1), $\psi(\vec{r})$. Eq. (5) shows that the first term of (12) leads to the first term of (2) and hence the scattered wave function $\phi(\vec{r})$ is written as

$$\phi(\vec{r})=-n\frac{e^{ikr}}{r}\sum_{l=0}^{\infty}(2l+1)(2kr)^{l+1}\frac{\Gamma(l+1+in)}{\Gamma(2l+2)}P_l\left(-\frac{\vec{r}\cdot\vec{R}}{rR}\right)$$

$$\times k\int_0^{\infty}dr'(2kr')^{l+1}e^{ikr'}j_l(kr'_-)h_l^{(1)}(kr'_+)$$

$$\times\Phi(l+1+in, 2l+2; -2ikr'_<)\Psi(l+1+in, 2l+2; -2ikr'_>). \tag{13}$$

The integral with respect to r' is devided into three parts:

$$k\int_0^{\infty}dr'\cdots=k\int_0^{R}dr'\cdots+k\int_R^{r}dr'\cdots+k\int_r^{\infty}dr'\cdots. \tag{14}$$

By the definitions of r_-, r_+, $r_<$ and $r_>$, the third part takes the form as

$$k\int_r^{\infty}dr'\cdots=j_l(kR)\Phi(l+1+in, 2l+2; -2ikr)$$

$$\times k\int_r^\infty dr'(2kr')^{l+1}e^{ikr'}\Psi(l+1+i\eta,2l+2;-2ikr')h_l^{(1)}(kr'). \tag{15}$$

Since the configuration which we are interested in is $1 \ll kR \ll kr$, we can use the asymptotic form of Ψ and $h_l^{(1)}$ for large kr' in the integrand:

$$\Psi(l+1+i\eta,2l+2;-2ikr')\sim\frac{1}{(-2ikr')^{l+1+i\eta}}, \tag{16}$$

$$h_l^{(1)}(kr')\sim(-i)^{l+1}\frac{e^{ikr'}}{kr'}. \tag{17}$$

Then the integral in (15) reads

$$k\int_r^\infty dr'\cdots\sim\int_{kr}^\infty dx\frac{e^{2ix}}{x}\frac{1}{(-2ix)^{i\eta}}\sim O\left(\frac{1}{kr}\right). \tag{18}$$

Therefore we can neglect the third term of (14).

Simlarly the second part of (14) is written as

$$k\int_R^r dr'\cdots=j_l(kR)\Psi(l+1+i\eta,2l+2;-2ikr)$$

$$\times k\int_R^r dr'(2kr')^{l+1}e^{ikr'}\Phi(l+1+i\eta,2l+2;-2ikr')h_l^{(1)}(kr'). \tag{19}$$

Here we can also use the asymptotic form of Φ and $h_l^{(1)}$ in the integrand, that is,

$$\Phi(l+1+i\eta,2l+2;-2ikr')\sim\frac{\Gamma(2l+2)}{\Gamma(l+1-i\eta)}\frac{1}{(2ikr')^{l+1+i\eta}}$$

$$+\frac{\Gamma(2l+2)}{\Gamma(l+1+i\eta)}e^{-2ikr'}\frac{1}{(-2ikr')^{l+1-i\eta}} \tag{20}$$

and eq. (14) for $h_l^{(1)}$. Then the integral in (19) becomes

$$\frac{\Gamma(2l+2)}{\Gamma(l+1+in)}\int_{kR}^{kr} dx \frac{1}{x}\frac{1}{(-2ix)^{in}}+\frac{\Gamma(2l+2)}{\Gamma(l+1-in)}(-1)^{l+1}\int_{kR}^{kr} dx \frac{e^{2ix}}{x}\frac{1}{(2ix)^{in}}. \tag{21}$$

The contribution of the second term is $O(1/kR)$ as (18), so that we can neglect this. And the first term yields

$$\frac{\Gamma(2l+2)}{\Gamma(l+1+in)} e^{(\pi/2)n} \frac{1}{in} (2kr)^{in} \left[1-\left(\frac{R}{r}\right)^{in}\right]. \tag{22}$$

Therefore, for the second part of (14), we have

$$k\int_R^r dr' \cdots \sim \frac{1}{in}\frac{\Gamma(2l+2)}{\Gamma(l+1+in)} j_l(kR) \frac{1}{(-2ikr)^{l+1}}\left[1-\left(\frac{R}{r}\right)^{in}\right], \tag{23}$$

here we make use of the asymptotic form (16).

For the first part of (14), we have

$$k\int_0^R dr' \cdots = h_l^{(1)}(kR)\,\Psi(l+1+in,\, 2l+2;\, -2ikr)$$

$$\times k\int_0^R dr' (2kr')^{l+1} e^{ikr'} \Phi(l+1+in,\, 2l+2;\, -2ikr') j_l(kr')$$

$$\sim (-i)^{l+1}\frac{e^{ikR}}{kR}\frac{1}{(-2ikr)^{l+1+in}}$$

$$\times k\int_0^R dr' (2kr')^{l+1} e^{ikr'} \Phi(l+1+in,\, 2l+2;\, -2ikr') j_l(kr'). \tag{24}$$

To get the last expression, we use the asymptotic form of Ψ and $h_l^{(1)}$, (16) and (17).

Adding (23) to (24), we have the integral (14) and hence the expression for the scattered wave function $\phi(\vec{r})$:

$$\phi(\vec{r}) \sim -\frac{e^{ikr}}{r} e^{-ik\vec{r}\cdot\vec{R}/r}\left[1-\left(\frac{R}{r}\right)^{in}\right]$$

$$+\frac{e^{kR}}{R}\frac{e^{kr}}{r}(2kr)^{-in}\sum_{l=0}^{\infty}(2l+1)I_l(R)P_l\left(-\frac{\vec{r}\cdot\vec{R}}{rR}\right). \tag{25}$$

Here $I_l(R)$ is given by

$$I_l(R)=-2n\int_0^R dr'\psi_l^{(c)(+)}(kr')j_l(kr'), \tag{26}$$

where we use the Newton's notation (eq. (14.46) in Newton's book[2]),

$$\psi_l^{(c)(+)}(kr)-\frac{1}{2}(2kr)^{l+1}i^{in}\frac{\Gamma(l+1+in)}{\Gamma(2l+2)}e^{ikr}\Phi(l+1+in,2l+2;-2ikr). \tag{27}$$

To obtain the first term of (25), the following expansion is made use of,

$$e^{-ik\vec{r}\cdot\vec{R}/r}=\sum_{l=0}^{\infty}(2l+1)i^l j_l(kR)P_l\left(-\frac{\vec{r}\cdot\vec{R}}{rR}\right). \tag{28}$$

In the previous paper [1], we wrote the wave equation by taking the origin at the source of the incident spherical wave. Therefore, in order to compare the wave function which we obtained in this note with the corresponding one in the paper [1], we rewrite eq. (25) in terms of the vectors $\vec{\xi}=\vec{r}-\vec{R}$ and $\vec{\rho}=-\vec{R}$ to yield

$$\phi(\vec{\xi})\sim\frac{e^{ik\xi}}{\xi}\left[1-\left(\frac{\rho}{\xi}\right)^{in}\right]+\frac{e^{k\rho}}{\rho}e^{-ik\vec{\xi}\cdot\vec{\rho}/\xi}\frac{e^{k\xi}}{\xi}(2k\xi)^{-in}\sum_l(2l+1)I_l(\rho)P_l\left(\frac{\vec{\xi}\cdot\vec{\rho}}{\xi\rho}\right) \tag{29}$$

where we assume $\rho/\xi\ll 1$ (note that $\vec{\xi}$ is the vector from the source of the incident wave to the observation point and $\vec{\rho}$ is one from the source to the position of the ion).

The complete wave function including the incident wave reads

$$\psi(\vec{r})\sim\frac{e^{ikr}}{r}e^{-in\{\log(2kr)-\log(2kR)\}}\left[1+e^{-ik\vec{r}\cdot\vec{R}/r}\frac{e^{ikR}}{R}\sum_{l=0}^{\infty}(2l+1)\hat{I}_l(R)P_l\left(\frac{\vec{r}\cdot\vec{R}}{rR}\right)\right] \tag{30}$$

where $I_l(R)$ is given by

$$\hat{I}_l(R) = e^{-in\log(2kR)} I_l(R). \tag{31}$$

with $I_l(R)$ defined by eq.(26). Here we put the notations $\vec{\xi}$ and $\vec{\rho}$ back to $\vec{r}$ and $\vec{R}$ respectively.

In the case of the short range potential, the wave function corresponding to eq.(30) is expressed as (cf. eq.(21) in [1])

$$\psi(\vec{r}) \sim \frac{e^{ikr}}{r}\left[1+e^{-ik\vec{r}\cdot\vec{R}/r}\frac{e^{ikR}}{R}\sum_{l=0}^{\infty}(2l+1)\tau_l P_l\left(\frac{\vec{r}\cdot\vec{R}}{rR}\right)\right] \tag{32}$$

where $\tau_l = k^{-1}e^{i\delta_l}\,sin\,\delta_l$ with δ_l, the phase shift of l-th partial wave.

In conclusion, comparing (30) with (32), we find that the long range property of the Coulomb potential gives the extra phase factor $e^{-in\{\log(2kr)-\log(2kR)\}}$ and that the partial wave scattering amplitude τ_l is given by $\hat{I}_l(R)$ in (31).

This work was done while I was a visitor at the Department of Physics, Dalhousie University, Halifax, Nova Scotia, Canada. I would like to thank Professor H. J. Kreuzer for helpful discussions and for warm hospitality.

Reference

[1] H. J. Kreuzer, K. Nakamura, A. Wierzbicki, H.-W. Fink and H. Schmid, Ultramicroscopy **45** (1992) 381–403.

[2] Roger G. Newton, *Scattering Theory of Waves and Particles* (Springer-Verlag, 1982).