THE PHASE SHIFTS FOR THE THOMAS-FERMI POTENTIAL CORRECTED FOR THE SELF-INTERACTION OF THE ELECTRON

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In this paper using the approximate Rozental solution for the Thomas-Fermi function for free neutral atoms we derive a formula for the phase shifts for the Thomas-Fermi potential, which does not include the electrostatic self-interaction of the electron. The derivation of this formula for the considered phase shift is similar to the Born method, and the difference consists only in the fact that instead of Bessel functions we take hydrogenic functions.

As known a number of modifications in the Thomas-Fermi potential have been suggested [1], one of them is the Thomas-Fermi potential corrected for the self-interaction of the electron which may be expressed by the following formula:

$$V(r) = -[(Z-1)\,e^2\,\Phi(r/\mu) + e^2]/r\,, \tag{1}$$

where $\Phi(r/\mu)$ is the universal Thomas-Fermi function for free neutral atoms of atomic number Z and $\mu = 0.88534\ a_0/Z^{1/3}$. In the last formula for $\bar{\mu}$; a_0 is the Bohr radius. In the present paper we derive an analytical formula for the phase shifts using the potential given by equation (1). First we write the Schrödinger equation for this potential:

$$\frac{d^2R_l}{dr^2} + \left[\frac{2m}{\hbar^2}\left(E + \frac{(Z-1)}{r}\,e^2\,\Phi(r/\mu) + \frac{e^2}{r^2}\right) - \frac{l(l+1)}{r^2}\right]R_l = 0\,. \tag{2}$$

Since the Thomas-Fermi function $\Phi(r/\mu)$ vanishes more rapidly than the term e^2/r, the Schrödinger equation (2) turns for a sufficient large r into the following Schrödinger equation

$$\frac{d^2\,{}_0R_l}{dr^2} + \left[\frac{2m}{\hbar^2}\left(E + \frac{e^2}{r}\right) - \frac{l(l+1)}{r^2}\right]{}_0R_l = 0\,. \tag{3}$$

Using the following notations

$$\frac{2m}{\hbar^2}E = k^2 \quad \text{and} \quad -\eta = \frac{me^2}{\hbar^2 k} \tag{4}$$

we can write the bounded solution ${}_0R_l$ of the Schrödinger equation (3), as known [2], in the following form:

$$
\begin{aligned}
{}_0R_l(kr) = \frac{1}{2} e^{-\pi\eta/2} \frac{|\Gamma(l+1+i\eta)|}{\Gamma(2l+2)} (2kr)^{l+1} e^{-ikr} \\
{}_1F_1(l+1-i\eta, 2l+2, 2ikr) .
\end{aligned}
\tag{5}
$$

The properties of the bounded solution ${}_0R_l$ have been studied extensively by BREIT and his collaborators. They have shown that this solution has for large kr the following asymptotic behaviour:

$${}_0R_l(kr) \to \sin\left(kr - \eta \ln 2kr - \frac{l\pi}{2} + \delta_{l,c}\right), \tag{6}$$

where the symbol $\delta_{l,c}$ denotes the Coulomb phase shifts

$$\delta_{l,c} = \arg \Gamma(l+1+i\eta). \tag{7}$$

The bounded solution R_l of the Schrödinger equation given by equation (5) has for large kr according to the theory of the phase shifts the following asymptotic behaviour:

$$R_l(kr) \to \sin\left(kr - \eta \ln 2kr - \frac{l\pi}{2} + \delta_{l,c} + \delta_l\right), \tag{8}$$

where δ_l is the phase shift caused by the term of the Schrödinger equation (2) which includes the Thomas-Fermi function. Multiplying the Schrödinger equation (3) by ${}_0R_l$ and the Schrödinger equation (2) by R_l and subtracting we obtain an expression which after integration, bearing in mind the asymptotic behaviours of ${}_0R_l$ and R_l given by formulas (6) and (8), gives us for the phase shift δ_l the following expression:

$$\sin \delta_l = \frac{2m}{\hbar^2 k} (Z-1) e^2 \int_0^\infty dr\, \Phi(r/\mu)\, {}_0R_l(kr)\, R_l(kr)\, r^{-1} . \tag{9}$$

Using the notation $\varrho = kr$ and substituting for the unknown bounded solution R_l the known solution ${}_0R_l$ we obtain for larger quantum numbers l the following approximate expression for the phase shift δ_l:

$$\delta_l = \frac{2m}{\hbar^2 k} (Z-1) e^2 \int_0^\infty d\varrho\, \Phi(\varrho/\mu k)\, {}_0R_l^2(\varrho)\, \varrho^{-1} . \tag{10}$$

In order to obtain an analytical expression for δ_l we must admit such approximate solutions for the Thomas-Fermi function Φ appearing in equation (10) which allows calculating the integral occurring in equation (10).

A convenient form is the approximate solution of the Thomas-Fermi function for free neutral atoms given by ROZENTAL [3],

$$\Phi(r/\mu) = \sum_{i=1}^{3} a_i e^{-b_i r/\mu}, \tag{11}$$

where the constants a_i and b_i are given by $a_1 = 0{,}255$, $a_2 = 0{,}581$,

$$a_3 = 0{,}164\,, \qquad b_1 = 0{,}246\,, \qquad b_2 = 0{,}947\,, \qquad b_3 = 4{,}356\,.$$

Substituting equation (11) into equation (10) we obtain for the phase shift the following formula [4] :

$$\delta_l = \frac{2m}{\hbar^2 k}(Z-1)e^2 \sum_{i=1}^{3} \frac{a_i}{2} M_l\left(1 + \frac{b_i^2}{2k^2\mu^2}\right), \tag{12}$$

where the symbol $M_l\,(1 + 2z^{-2})$ is given by

$$M_l(1+2z^{-2}) = \frac{1}{2} e^{-\pi\eta}\left(\frac{z^2}{1+z^2}\right)^{l+1}\left(\frac{1-iz}{1+iz}\right)^{i\eta} \cdot \left|\frac{\Gamma(l+1+i\eta)}{\Gamma(2l+2)}\right|^2 {}_2F_1\left(l+1+i\eta;\quad l+1-i\eta;\quad 2l+2;\quad \frac{z^2}{1+z^2}\right). \tag{13}$$

In the last formula for M_l the symbol ${}_2F_1$ denotes the hypergeometric function. The formula for the phase shifts δ_l for the Thomas-Fermi potential which is corrected for the self-interaction of the electron is not simple for practical calculations. If we adopt for the Thomas-Fermi potential

$$V(r) = -Ze^2\Phi(r/\mu)/r \tag{14}$$

it means that the potential of equation (14) includes the electrostatic self-interaction of the electron ; in this case in the BORN approximation we obtain for the phase shifts in atomic units the following formula [5] for the ROZENTAL approximate solution for η_l (BORN) :

$$\eta_l(\text{BORN}) = \frac{Z}{\sqrt{E}} \sum_{i=1}^{3} a_i Q_l\left(1 + \frac{1}{2}\left(\frac{b_i}{\mu\sqrt{E}}\right)^2\right). \tag{15}$$

The symbol Q_l denotes the Legendre functions of second kind. In Table I we have a comparison of η_l (BORN) with the numerical values for the phase shift given by HENNEBERG [6] for $Z = 80$ and $E = Z^2$.

Table I

A comparison of the phase shifts according to formula (15) with the numerical values of HENNEBERG

l	Numerical values for η_l HENNEBERG	η_l (BORN) eq. (15)
0	203°	208°40′
1	157°	152°11′
2	129°50′	124°48′
3	111°30′	107°04′
4	98°	94°15′
5	87°50′	84°18′

For the constants a_l and b_l were taken the values of ROZENTAL. Table I shows that for larger l the phase shifts η_l (BORN) give good results. Since the formula (12) for δ_l was carried out in the same mode as is required by the BORN approximation we may expect that δ_l will give also good results. It is necessary to stress that the solution ${}_0R_l$ fits the exact solution R_l better, than the Bessel function of half integral fits the exact solution of the Schrödinger equation for the potential given by eq. (14).

REFERENCES

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СДВИГИ ФАЗ ДЛЯ ПОТЕНЦИАЛА ТОМАСА—ФЕРМИ, СКОРРЕКТИРОВАННОГО СОБСТВЕННЫМ ВЗАИМОДЕЙСТВИЕМ ЭЛЕКТРОНОВ

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Резюме

В настоящей работе с помощью приближенного решения Розенталя функции Томаса—Ферми для нейтрального атома выводим такую формулу для сдвигов фаз потенциала Томаса—Ферми, которая не содержит электростатического собственного взаимодействия электрона. Вывод формулы аналогичен методу Борна, с той разницей,что мы пользуемся водородными функциями вместо Бесселевых функций.