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MODIFICATION OF RUTHERFORD'S fORMULA

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ABSTRACT:
In the paper, in the scattering problem for the valence electron model potential a self-adjoint extension is performed and Rutherford formula is modified formula. Is also discussed the changes caused by the self-adjoint extension in the differential and integral cross-sections

Key words: self-adjoint extension, Schrodinger equation, additional solutions, scattering amplitude, valence electron model

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I . Intoduction

The inverse squared r^{-2} potential has received widespread attention in various problems of quantum mechanics [1-6]. These problems are interesting not only from an academic standpoint. A number of physically significant quantum mechanical problems manifest in such a behavior.

A detailed consideration of papers devoted to problems concerning this potential put in doubt the motivations for neglecting so-called additional (singular) solutions, which are based on mathematical sets of quantum mechanics, without invoking specific physical ideas.

The aim of this study is to consider the singular solution by using a well-known procedure of self-adjoint extension (SAE), in particular, a “pragmatic approach” [7], which is much simpler than the general Weil method but is applied only to Hamiltonians.

In [8-9] we studied the self-adjoint extension procedure for bound states in the Schrödinger equation for several analytically solvable examples (inverse-squared, valence electron and singular oscillator potentials). At the same time, it becomes necessary to carry out an analogous procedure in scattering problems, which we carried out for the inverse-squared potential in [10-11]. In this paper, a self-adjoint extension is carried out in the scattering problem for the valence electron model potential and the Rutherford formula is modified. The main results of the paper are briefly summarized in the conclusion.

II. Modification of Rutherford's formula

Consider the scattering problem in the valence electron model

$$V = -\frac{V_0}{r^2} - \frac{\alpha}{r} \quad ; \quad (V_0, \alpha > 0) \tag{2.1}$$

Note that this potential appears “naturally” in the Klein-Gordon equation for the Coulomb potential. If we follow the formalism of [12], in the scattering case we obtain the following general solution of the Schrödinger equation

$$R(r) = C_1 \rho^{-1/2+P} e^{-\frac{\rho}{2}} {}_1F_1(1/2+P-\lambda, 1+2P; \rho) + C_2 \rho^{-1/2-P} e^{-\frac{\rho}{2}} {}_1F_1(1/2-P-\lambda, 1-2P; \rho)$$

(2.2)

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$$P = \sqrt{(l+1/2)^2 - 2mV_0} > 0$$

(2.3) and

$$\rho = 2ikr;\ \lambda = -i\frac{m\alpha}{k} = -i\eta;\ k = \sqrt{2mE};\ E > 0; \qquad \eta = \frac{m\alpha}{k}$$

(2.4)

From the behavior of the (2.2) wave function at small distances and the definition of the self-adjoint extension τ_S parameter, we obtain [10-11]

$$\tau_S = \frac{C_2(k)}{C_1(k)}(2ik)^{-2P} \qquad (2.5)$$

To find the scattering amplitude, we write the representation of the (2.2) radial function at large distances. If we use the asymptotics of ${}_1F_1(kr)$ confluent hypergeometric functions [13]

$${}_1F_1(a,c,z) \underset{z\to\infty}{\approx} e^{-i\pi a}\frac{\Gamma(c)}{\Gamma(c-a)}z^{-a} + \frac{\Gamma(c)}{\Gamma(a)}e^z z^{a-c};\ c \neq -n,\ \ n = 0,1,2... \qquad (2.6)$$

and the definition of the Coulomb standard scattering amplitude [14]

$$e^{2i\delta^{st}_{Coulomb}} = \frac{\Gamma\left(\frac{1}{2}+P+\lambda\right)}{\Gamma\left(\frac{1}{2}+P-\lambda\right)}$$

(2.7)

We obtain

$$\underset{r\to\infty}{R} \approx e^{-\frac{\pi}{2}\eta}\frac{1}{r}e^{ikr}\left[C_1\frac{\Gamma(1+2P)}{\left|\Gamma\left(\frac{1}{2}+P+\lambda\right)\right|}e^{i\left(P+\frac{1}{2}\right)\frac{\pi}{2}}e^{i\left(X_+ + \delta^{st}_{Coulomb}\right)} + C_2\frac{\Gamma(1-2P)}{\left|\Gamma\left(\frac{1}{2}-P+\lambda\right)\right|}e^{-i\left(P-\frac{1}{2}\right)\frac{\pi}{2}}e^{i\left(X_- + \delta^{add}_{Coulomb}\right)}\right] +$$

$$+ e^{-\frac{\pi}{2}\eta}\frac{1}{r}e^{-ikr}\left[C_1\frac{\Gamma(1+2P)}{\left|\Gamma\left(\frac{1}{2}+P+\lambda\right)\right|}e^{i\left(P+\frac{1}{2}\right)\frac{\pi}{2}}e^{-i\left(X_+ + \delta^{st}_{Coulomb}\right)} + C_2\frac{\Gamma(1-2P)}{\left|\Gamma\left(\frac{1}{2}-P+\lambda\right)\right|}e^{i\left(\frac{1}{2}-P\right)\frac{\pi}{2}}e^{-i\left(X_- + \delta^{add}_{Coulomb}\right)}\right]$$

(2.8)

where the following notations are introduced:

$$X_+ = \eta\ln 2kr - (1/2+P)\frac{\pi}{2};\ \ X_- = \eta\ln 2kr - (1/2-P)\frac{\pi}{2}$$

(2.9)

And, respectively, $\delta^{st}_{Coulomb}$ and $\delta^{add}_{Coulomb}$ are the Coulomb scattering amplitudes of the first (standard) and second (additional) terms of the solution to (2.1):

$$\delta^{st}_{Coulomb} = \arg\Gamma\left(\frac{1}{2}+P+\lambda\right);\quad \delta^{add}_{Coulomb} = \arg\Gamma\left(\frac{1}{2}-P+\lambda\right)$$

(2.10)

On the other hand, the behavior of the R radial wave function at infinity through the scattering δ_l phase shift

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$$\underset{r\to\infty}{R} \approx \frac{2}{r}\sin\left(kr-\frac{l\pi}{2}+\eta\ln 2kr+\delta_l\right)$$

(2.11)

(here $\eta\ln 2kr$ is the well-known term due to the slow decay of the Coulomb potential at infinity [14]), we can write as

$$\underset{r\to\infty}{R} \approx \frac{1}{ir}\left\{e^{ikr}e^{i\left(\eta\ln 2kr-\frac{\pi}{2}l+\delta_l\right)}-e^{-ikr}e^{-i\left(\eta\ln 2kr-\frac{\pi}{2}l+\delta_l\right)}\right\}$$

(2.12)

And comparing (2.8) and (2.12) gives us

$$\left[C_1\frac{\Gamma(1+2P)}{\left|\Gamma\left(\frac{1}{2}+P+\lambda\right)\right|}e^{i\left(P+\frac{1}{2}\right)\frac{\pi}{2}}e^{i\left(-\left(\frac{1}{2}+P\right)\frac{\pi}{2}+\delta_{Coulomb}^{st}\right)}+C_2\frac{\Gamma(1-2P)}{\left|\Gamma\left(\frac{1}{2}-P+\lambda\right)\right|}e^{-i\left(P-\frac{1}{2}\right)\frac{\pi}{2}}e^{i\left(-\left(\frac{1}{2}+P\right)\frac{\pi}{2}+\delta_{Coulomb}^{add}\right)}\right]=$$

$$=\frac{1}{i}e^{i\left(\delta_l-\frac{\pi}{2}l+\frac{\pi}{2}\eta\right)}$$

(2.13)

$$\left[C_1\frac{\Gamma(1+2P)}{\left|\Gamma\left(\frac{1}{2}+P+\lambda\right)\right|}e^{i\left(P+\frac{1}{2}\right)\frac{\pi}{2}}e^{-i\left(-\left(\frac{1}{2}+P\right)\frac{\pi}{2}+\delta_{Coulomb}^{st}\right)}+C_2\frac{\Gamma(1-2P)}{\left|\Gamma\left(\frac{1}{2}-P+\lambda\right)\right|}e^{i\left(P-\frac{1}{2}\right)\frac{\pi}{2}}e^{-i\left(-\left(\frac{1}{2}+P\right)\frac{\pi}{2}+\delta_{Coulomb}^{add}\right)}\right]=$$

$$=-\frac{1}{i}e^{-i\left(\delta_l-\frac{\pi}{2}l+\frac{\pi}{2}\eta\right)}$$

(2.14)

From which, by dividing (2.13) by (2.14) and taking into account the definition of (2.5), we obtain the S_{VE} partial scattering amplitude

$$S_{VE}=e^{2i\left[l+\frac{1}{2}-P\right]\frac{\pi}{2}+2i\delta_{Coulomb}^{st}}\frac{1+\tau_S(2ik)^{2P}We^{i\left(\delta_{Coulomb}^{add}-\delta_{Coulomb}^{st}\right)}}{1+\tau_S(2ik)^{2P}We^{-2i\pi P}e^{i\left(\delta_{Coulomb}^{add}-\delta_{Coulomb}^{st}\right)}}$$

(2.15)

where the index VE indicates that the scattering occurs at the valence electron potential (2.1) and

$$W=\frac{\Gamma(1-2P)}{\Gamma(1+2P)}\frac{\left|\Gamma\left(\frac{1}{2}+P+\lambda\right)\right|}{\left|\Gamma\left(\frac{1}{2}-P+\lambda\right)\right|}$$

(2.16)

Note that in expression (2.16), the term represented by the fraction is a new term and is obtained because this time we have kept the second term in expression (2 .2) and so we have performed the SAE.

(2.15) gives the correct physical results. In particular, when $\tau_S=0$ i.e $C_2=0$, (2.15) gives us the standard result [17]

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$$S_{VE}^{st} = e^{2i\left[l+\frac{1}{2}-P\right]\frac{\pi}{2}+2i\delta_{Coulomb}^{st}}$$

(2.17)

and for $\tau_S = \pm\infty$ i.e. $C_2 = 0$, from (2.16) we obtain an additional partial amplitude

$$S_{VE}^{st} = e^{2i\left[l+\frac{1}{2}+P\right]\frac{\pi}{2}+2i\delta_{Coulomb}^{add}}$$

(2.18)

It is necessary to note that in our work [10] we obtained the following transcendental equation for the energies of the bound states of the (2.1) potential

$$\frac{\Gamma(1/2-\lambda-P)}{\Gamma(1/2-\lambda+P)} = -\tau(-8mE)^P \frac{\Gamma(1-2P)}{\Gamma(1+2P)}$$

(2.19)

Now let us take equation (2.19) as the pole of the scattering amplitude (2.15). Here a slightly more detailed analysis is required. In particular, let us consider 3 cases.

a) $\tau_S = 0$. Standard solutions. In this case, the standard amplitude (2.17) is written using equation (2.7) as

$$S_l^{st} = e^{2i\left[l+\frac{1}{2}-P\right]\frac{\pi}{2}} \frac{\Gamma\left(\frac{1}{2}+P+\lambda\right)}{\Gamma\left(\frac{1}{2}+P-\lambda\right)}$$

(2.20)

whose poles coincide with the poles of $\Gamma(\frac{1}{2}+\lambda+P)$

$$\frac{1}{2}-\lambda+P = -n_r; \qquad n_r = 0,1,2...$$

(2.21)

and condition (2.21), taking into account the notations (2.4), give us the standard levels obtained in the work [8]

$$E_{st} = -\frac{m\alpha^2}{2[1/2+n_r+P]^2} = -\frac{m\alpha^2}{2\left[1/2+n_r+\sqrt{(l+1/2)^2-2mV_0}\right]^2}$$

(2.22)

ბ) $\tau_S = \pm\infty$ Additional solutions. In this case, analogously to the above arguments, the poles of (2.18) will give us the E_{add} additional levels obtained in [8] work.

$$E_{add} = -\frac{m\alpha^2}{2[1/2+n_r-P]^2} = -\frac{m\alpha^2}{2\left[1/2+n_r-\sqrt{(l+1/2)^2-2mV_0}\right]^2}$$

(2.23)

3) $\tau \neq 0,\ \pm\infty$. In this case (2.15) has a pole at the point

$$\tau_S (2ik)^{2P} We^{-2i\pi P} e^{i\left(\delta_{Coulomb}^{add}-\delta_{Coulomb}^{st}\right)} = -1$$

(2.24)

If we follow the usual procedure, i.e., we take the link to move to the states $k = i\mu$ i.e.

$$k^2 = -\mu^2 = 2mE; \quad (E<0)$$

(2.25)

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Then, taking into account (2.4), (2.16) and the following equations

$$\Gamma\left(\frac{1}{2}+P+\lambda\right)=\left|\Gamma\left(\frac{1}{2}+P+\lambda\right)\right|e^{i\delta^{st}_{Coulomb}};\qquad \Gamma\left(\frac{1}{2}-P+\lambda\right)=\left|\Gamma\left(\frac{1}{2}-P+\lambda\right)\right|e^{i\delta^{add}_{Coulomb}}$$

(2.26)

We obtain the formula (2.19) for the energies of the bound states.

To write the scattering phase, we use the formula[14]

$$e^{2i\tan^{-1}z}=\frac{1+iz}{1-iz} \tag{2.27}$$

And then (2.15) can be written as

$$S_{VE}=e^{2i\delta_{VE}}$$

(2.28)

Where

$$\delta_{VE}=\delta^{st}_{l}+\delta^{st}_{Coulomb}+arctgZ$$

(2.29)

The third term in the expression (2.29)

$$\delta_{SAE}=arctgZ;\qquad Z=\frac{\tau_S(2k)^{2P}W\sin\left(\pi P+\delta^{add}_{Coulomb}-\delta^{st}_{Coulomb}\right)}{1+\tau_S(2k)^{2P}W\cos\left(\pi P+\delta^{add}_{Coulomb}-\delta^{st}_{Coulomb}\right)}$$

(2.30)

is a new term caused by the expansion of the self-consistent expansion, and is given by the formula (2.16).

Let us now see what changes the self-extension procedure will make to Rutherford's well-known formula. As shown in [11] the elastic scattering amplitude may be rewritten as

$$f(\theta)=\frac{1}{2ik}\left\{\sum_{l=0}^{l_0-1}(2l+1)\mathscr{P}_l(\cos\theta)\left[S_{l,fall}-1\right]+(2l_0+1)\mathscr{P}_{l_0}(\cos\theta)\right\}\left[e^{2i\left(\delta_{VE}+\tan^{-1}X_{l_0}\right)}-1\right]+$$

$$+\frac{1}{2ik}\sum_{l=l_0+1}^{\infty}(2l+1)\mathscr{P}_l(\cos\theta)\left[e^{2i\delta^{st}_l}-1\right]\equiv f^{st}_1(\theta)+f^{SAE}_{l_0}(\theta)+f^{st}_2(\theta)$$

(2.31)

In this case, for the “fall” on the center, in the first term of (2.31), we can calculate it by our method, as was shown in [11] for the potential

$$V=-\frac{V_0}{r^2};\ V_0>0$$

(2.32)

However, below we do not need this term, because we consider $l=0$ case. In the second term of (2.31), the power of the exponent is given by (2.29).

Consider the case of small V_0-s, where we need to keep only the $l=0$ member and by using following identity.

$$e^{2i(x+y)}-1=e^{2ix}-1+e^{2ix}\left(e^{2iy}-1\right) \tag{2.33}$$

the scattering amplitude(2.31) is written as

$$f(\theta)=\frac{1}{2ik}\left\{e^{2i\left\{\left[\frac{1}{2}-P\right]\frac{\pi}{2}+\delta^{st}_{0,Coulomb}\right\}}\left[e^{2iarctgZ}-1\right]+\sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta)\left[e^{2i\left\{\left[l+\frac{1}{2}-P\right]\frac{\pi}{2}+\delta^{st}_{l,Coulomb}\right\}}-1\right]\right\}$$

(2.34)

The second term of (2.34) is the standard scattering amplitude of the potential (2.1) and it is calculated in the case of small V_0-s in the monograph [15], but there the scattering on the Coulomb potential is considered for the Klein-Gordon equation, but as we mentioned at the beginning of this

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chapter, the potential (2.1) appears “naturally” in the Klein-Gordon equation for the Coulomb potential. Therefore, the results of the monograph [15] coincide with ours with the accuracy of the notations in (2.4) and so the second term of (2.34) will be

$$f_{VE}^{0}(\theta)= f_{Coulomb}(\theta)\left\{1-\pi V_0 k\sin\frac{\theta}{2}e^{2i[\sigma_{-1/2}-\sigma_0]}\right\}$$

(2.35)

where the $f_{Coulomb}(\theta)$ Rutherford scattering amplitude is [14]

$$f_{Coulomb}(\theta)=-\frac{\eta}{2k\sin^2\frac{\theta}{2}}e^{\left\{-i\eta\ln\left(\sin^2\frac{\theta}{2}\right)+2i\sigma_0\right\}}$$

(2.36)

and

$$e^{2i\sigma_0}=\frac{\Gamma(1+i\eta)}{\Gamma(1-i\eta)};\qquad e^{2i\sigma_{-1/2}}=\frac{\Gamma(1/2+i\eta)}{\Gamma(1/2-i\eta)}$$

(2.37)

Therefore, finally (2.34) the scattering amplitude for the potential (2.1) will be

$$f(\theta)=-\frac{\eta}{2k\sin^2\frac{\theta}{2}}e^{\left\{-i\eta\ln\left(\sin^2\frac{\theta}{2}\right)+2i\sigma_0\right\}}\left\{1-\pi V_0 k\sin\frac{\theta}{2}e^{2i[\sigma_{-1/2}-\sigma_0]}\right\}+$$
$$+\frac{1}{k}e^{2i\left\{\left[\frac{1}{2}-P\right]\frac{\pi}{2}+\delta_{0,Coulomb}^{st}\right\}}e^{iarctgZ}\sin arctgZ$$

(2.38)

Here the second term, due to the self-coupled broadening, does not depend on the θ scattering angle and for large scattering angles it becomes more pronounced when the Rutherford term itself is small; but if we take into account the terms $l\neq 0$ as well, it already becomes θ angle-dependent.

The differential scattering cross section will be

$$\frac{d\sigma}{d\Omega}=\frac{\eta^2}{4k^2\sin^2\frac{\theta}{2}}\left\{1+(\pi V_0 k)^2\sin^2\frac{\theta}{2}-2\pi V_0 k\sin\frac{\theta}{2}\cos 2\left(\sigma_{-\frac{1}{2}}-\sigma_0\right)\right\}+\frac{1}{k^2}\sin^2 Z-$$
$$-\frac{\eta\sin arctgZ}{k^2\sin^2\frac{\theta}{2}}\left\{\begin{array}{l}\cos\left[\left(\frac{1}{2}-P\right)\pi+2\delta_{0,Coulomb}^{st}+\eta\ln\sin^2\frac{\theta}{2}-2\sigma_0+arctgZ\right]-\\ -\pi V_0 k\sin\frac{\theta}{2}\cos\left[\left(\frac{1}{2}-P\right)\pi+2\delta_{0,Coulomb}^{st}+\eta\ln\sin^2\frac{\theta}{2}-2\sigma_{-\frac{1}{2}}+arctgZ\right]\end{array}\right\}$$

(2.39)

The last two terms in (2.39) were formed due to the self-adjoint extension procedure. The last term is especially interesting, since it depends on the sign of the parameter Z SAE defined by the formula (2.30) and therefore increases or decreases the $\frac{d\sigma_{st}}{d\Omega}$ standard cross section (when $Z=0$) of the potential (2.1) and which may be observed in the experiment. This effect can be observed during the scattering of slow particles on the potential of the type (2.1), since at this time it is most important $l=0$ and the situation formally resembles the inclusion of short-acting forces in the discussion.

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IV. CONCLUSIONS

In the paper, in the scattering problem for the valence electron model potential a self-adjoint extension is performed and Rutherford formula is modified formula. In particular, it is shown that in the differential scattering cross-section formula, due to the SAE procedure, two new terms arise, which depend on the sign of the self-adjoint extension parameter and by this reason increases or decreases the $\frac{d\sigma_{st}}{d\Omega}$ standard cross section of the potential (2.1) and which may be observed in the experiment.The changes caused by the self-adjoint extension in the representations of the differential and integral scattering cross-sections are studied.

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