Generalized JWKB two-centre Phase-shifts due to Coulomb and Yukawa potentials

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The two-centre models have their respective importance in atomic, molecular and nuclear processes. In this field A lot of work has been done by various research groups and many attempts have been made to study the scattering of a charged particles using a two-centre potential [1-3]. The scattering of an electron from two-centre Coulomb potential has been studied [3] by solving the Dirac equation and spheroidal phase-shifts are calculated by generalized JWKB approximation.

In many scattering problems, the potential consists of a mixture of long-range and short-range character. By applying the generalized JWKB method for a mixture of potentials, we have formulated the model equation in such a way that qualitatively it is similar to actual radial equation, which can be solved exactly. Using the exact solution of the model equation as basis of approximation, one can obtain an approximate wave function for the actual radial equation. Then phase-shift difference between model and actual radial equation can be determined. The total phase-shift for the mixed potential can be obtained by adding the phase-shift of long range potential to the observed difference. In this paper, we shall illustrate the method of calculation for two-centre phase-shifts applicable for the mixture of Coulomb (long range) and Yukawa (short range) potential. The correction term is included only up to the first order in present work.

The two-centre Dirac Equation (TCDE) for an electron in an electrostatic field may be written as

$$\left(\vec{\alpha}.\vec{P}+\beta+V_{TC}-E\right)\psi(\vec{r})=0 \qquad (1)$$

where $\vec{\alpha}$ and β are the usual Dirac matrices and V_{TC} is two-centre potential acting on the electron due to two-charge centres. $\vec{P}$ and E denote the electron momentum and energy, respectively. After applying the generalized Furry Sommerfeld Maue approximation [4] the electron wave function can be written in the form of radial and angular functions as

$$\psi_0(\xi,\eta,\phi)=R_{ml}(c,\xi)S_{ml}(c,\eta)\frac{e^{im\phi}}{\sqrt{2\pi}} \qquad (2)$$

where $l \geq m$ *and* $m=0,\ \pm1,\pm2.....$

The radial part of the scattering wave function after making the Langer's substitution [5] can be written as

$$\frac{d^2G_{ml}(y)}{dy^2}+\frac{q_1(y)}{\hbar^2}G_{ml}(y)=0 \qquad (3)$$

where

$$\frac{q_1(y)}{\hbar^2}=\frac{1}{\left(y^2-c^2\right)}\left(y^2+2by-\lambda_{ml}(c)-\frac{\left(m^2-1\right)c^2}{\left(y^2-c^2\right)}\right)-\frac{1}{4(y-c)^2}$$

where $G_{ml}=\left(\xi^2-1\right)^{1/2}R_{ml}(c,\xi)$ and

$$y=c\xi, \qquad b=\frac{2ZEe^2}{p},\ c=\frac{PR}{2}$$

The model equation with a combination of Coulomb and Yukawa potential can be expressed as

$$\frac{d^2F_{ml}(s)}{ds^2}+\frac{q_2(s)}{\hbar^2}F_{ml}(s)=0 \quad (4)$$

where $\frac{q_2(s)}{\hbar^2}=\frac{1}{\left(s^2-c^2\right)}\left(As^2+Bs-\lambda_{ml}-\frac{\left(m^2-1\right)c^2}{\left(s^2-c^2\right)}\right)-\frac{1}{4(s-c)^2}$

$$A=1-\frac{4Eg\mu}{P^2};\quad B=2\left(\frac{2EZ\alpha}{P}+\frac{2Eg}{P}\right)$$

The two-centre phase-shifts for the zeroth order in $\hbar^2$ is given by

$$\sigma_{ml}^0-\sigma_l=$$

$$\sqrt{A\tilde{s}^2+B\tilde{s}-\lambda_{ml}}+\sqrt{\lambda_{ml}}\left[\sin^{-1}\left(\frac{B}{\sqrt{B^2+4A\lambda_{ml}}}\right)-\sin^{-1}\left(\frac{B\tilde{s}-2\lambda_{ml}}{\tilde{s}\sqrt{B^2+4A\lambda_{ml}}}\right)\right]$$

$$-\frac{B}{2\sqrt{A}}\ln(4A)+\frac{B}{2\sqrt{A}}\ln\left(2\sqrt{A\tilde{s}^2+B\tilde{s}-\lambda_{ml}}+2A\tilde{s}+B\right)$$
$$-\sqrt{\tilde{y}^2+2b\tilde{y}-\lambda_{ml}}-\sqrt{\lambda_{ml}}\left[\sin^{-1}\left(\frac{b}{\sqrt{b^2+\lambda_{ml}}}\right)-\sin^{-1}\left(\frac{b\tilde{y}-\lambda_{ml}}{\tilde{y}\sqrt{b^2+\lambda_{ml}}}\right)\right]$$
$$-b\ln 2\left(\sqrt{\tilde{y}^2+2b\tilde{y}-\lambda_{ml}}+\tilde{y}+b\right)+\int_{y_t}^{\tilde{y}}\sqrt{q_1(y)}dy-\int_{s_t}^{\tilde{s}}\sqrt{t_1(s)}ds \quad (5)$$

In above equation y_t and s_t are the turning points and $\tilde{y}$ and $\tilde{s}$ are some suitably chosen large values of y and s respectively. The phase-shifts σ_l can be obtained by comparing the model equation with free particle radial equation and are given by

$$\sigma_l=-\left(l+1/2\right)\sin^{-1}\left(\frac{B}{\sqrt{B^2+4A\left(l+1/2\right)^2}}\right)-\frac{B}{4\sqrt{A}}\ln\sqrt{B^2+4A\left(l+1/2\right)^2} \quad (6)$$

The first order correction term to the phase-shifts, is given by

$$\sigma_{ml}^1=\frac{1}{12}\int_{y_t}^{\infty}D[\tau_1(y)]\sqrt{q_1(y)}dy-\frac{1}{12}\int_{s_t}^{\infty}D[\tau_2(s)]\sqrt{q_2(s)}ds \quad (7)$$

where $$D[\tau_i]=\frac{\tau_i'^4}{\tau_i'^2}-4\frac{\tau'''\tau_i''}{\tau_i'^3}+3\frac{\tau_i''^3}{\tau_i'^4} \quad ;$$

$\tau_1(y)=\hbar^2(y-c)^2q_1(y)$, $\tau_2(s) \ =\hbar^2(s)^2q_2(s)$

The phase shifts up to the first order correction term in $\hbar^2$ can now be written as

$$\sigma_{ml}=\sigma_{ml}^0+\sigma_{ml}^1 \quad (8)$$

Table 1, shows the results of equations (5), (6), (7) and (8**)** for b = 0.5, A = 0.99 and B = 2.02 with E = 100 MeV and c = 0.3. The parameters g and μ are taken to be 0.255 and 1.0, respectively.

The accuracy of the generalized JWKB method can be checked by comparing the numerical results of equations (6) and (8) as shown in table1. The phase-shifts calculated by this method σ_{ml} are in good agreement with the exact phase-shifts σ_l. The phase-shift difference σ_{ml}^1 decreases with the increase in l-values. In other words the first order correction term σ_{ml}^1 makes a significant contribution to the phase-shifts for small angular momenta but as l increases the contribution due to first order correction term goes on decreasing. It is also clear from the table 1 that as l increases the magnitude of the phase-shifts σ_{ml} also increases. For same partial wave, the phase-shifts with changing in m-values show a very little variation. In summary the phase-shifts calculated using generalized JWKB method are in good agreement with the exact phase-shifts and different partial phase-shifts are almost independent of m-values.

Table 1. Two-centre phase shifts σ_{ml} for Coulomb and Yukawa potential

l m	σ_{ml}^0	σ_{ml}^1	σ_l	σ_{ml}
0 0	-1.1436	.0215	-1.3823	-1.1221
1 0	-2.1602	.0518	-2.1962	-2.1084
1 1	-2.1452	.0315	-2.1962	-2.1137
2 0	-2.6912	.0156	-2.6731	-2.6756
2 1	-2.6894	.0143	-2.6731	-2.6750
2 2	-2.6840	.0107	-2.6731	-2.6733
3 0	-3.0300	.0062	-3.0022	-3.0238
3 1	-3.0297	.0060	-3.0022	-3.0236
3 2	-3.0283	.0055	-3.0022	-3.0228
3 3	-3.0263	.0047	-3.0022	-3.0216
4 0	-3.2621	.0032	-3.2522	-3.2589
4 1	-3.2617	.0031	-3.2522	-3.2586
4 2	-3.2616	.0030	-3.2522	-3.2586
4 3	-3.2605	.0028	-3.2522	-3.2577
4 4	-3.2693	.0025	-3.2522	-3.2568
5 0	-3.4564	.0019	-3.4533	-3.4545
5 1	-3.4565	.0019	-3.4533	-3.4546
5 2	-3.4576	.0018	-3.4533	-3.4558
5 3	-3.4555	.0018	-3.4533	-3.4538
5 4	-3.4569	.0017	-3.4533	-3.4552
5 5	-3.4591	.0016	-3.4533	-3.4575

References:

[1] H.K.Chauhan and P.K.Raina, J. Phys. **B29**, 5889 (1996).
[2] Y.S.Tergiman, J. Phys. **B29**, 1035 (1996).
[3] S. Mukherjee and S. S. Chandel, J. Phys. **A11**, 1257 (1978).
[4] A. Sommerfeld and A. W. Maue, Ann. Phys. Leipzing **22**, 629 (1935).
[5]R.E. Langer Phys. Rev. **51**, 669 (1937).