Semi – Classical and WKB Approximation of Phase Shift

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الخلاصة

إن موضوع البحث الرئيسي هو استخدام التقريب شبه الكلاسيكي لكي يزود برابط يربط بين الوصف الكمي والكلاسيكي لعملية الاستطارة. لقد قمنا بتوسيع الوصف الكلاسيكي لحالتين من التصادمات الذرية حتى الطاقات الواطئة التي يكون عندها معالجة معامل الصدم قد فشلت. في هذا البحث قد بينا حساب دقيق جدا للحد شبه الكلاسيكي لمعادلة شرويدنكر والذي يمكن إن يعدل لكي يشتمل على فرق الطور. WKB هو عبارة عن طريقة تقريبية لحل معادلة شرويدنكر وان هذه الطريقة تزود بدالة الموجة التقريبية للمسائل ذات البعد الواحد. إن معادلة شرويدنكر قد حلت باستخدام تقريب WKB و شبه الكلاسيكي من اجل الحصول على فرق الطور .

ABSTRACT

A central theme is the use of semi – classical approximation to provide a link between quantum and classical description of the scattering process. We extend the semi – classical description of two state atomic collisions to low energies for which the impact parameter treatment fails. In this research, we show the rigorous computation of the semi – classical limit of the Schrodinger, can be amended to include the phase shift. WKB is an approximate method to solve the Schrodinger equation and this method provides approximate wave functions in one dimensional problems. The Schrodinger equation has been solved by using the semi – classical and WKB approximation in order to get the phase shift.

1. INTRODUCTION:-

The physical interpretation of collision theory is easier when the relative motion is described in a semi – classical approach. Many results have been obtained in a rectilinear trajectory approximation concerning various total cross sections which compare well with experimental results. All low energies, however, and in the presence of inelastic processes, small angular momenta play an important role so that trajectory effects should be considered. Then, the application of semi – classical methods may appear somewhat arbitrary since it is possible to define a single trajectory[1].

The theory of collisions between two atomic systems goes back to the early days of quantum mechanics[2, 3, 4] and the basic models of state interaction are detailed in the recent review of Nikitin[5]. Typically, the colliding atoms undergo electronic transitions and one needs to solve quantum of coupled radial Schrodinger equation. It has been noted since the early thirties that the relative motion of the heavy nuclei can be described classically[2, 6]. Semi classically,

Stueckelberg[7] first suggest the analytical continuation of the JWKB(Jeffreys – Wentzel – Kramers – Brillouin) wave function into the complex plane of the internuclear separation and a proper handling of the Stokes phenomenon. His solution of the avoided crossing time independent problem[7] shows why a description of the interference in terms of adiabatic quasiclassical phases fails if the phase difference accumulated during the adiabatic motion of the two atoms between the centre of the coupling region and the turning points is small.

Modern line shape studies, especially by non – linear spectroscopy, are a sensitive tool for the investigation of velocity – changing collisions in low pressure gases[8]. These collisions effect both the various level populations and the off – diagonal density matrix elements[9]. The usual criteria for the applicability of semi – classical treatments are, up to now, sufficient rather than necessary conditions and may well be too stringent. More quantitative criteria for the validity of semi – classical small angle scattering amplitudes for the calculation of elastic collision kernels are therefore desirable[9].

2. Semi – classical and WKB approximation:-

We are interested in an efficient numerical method to solve the linear Schrodinger equation with the high frequency initial data[10]

$$i\hbar\frac{d\psi(r)}{dt}+\frac{\hbar^2}{2}\Delta\psi(r)-V(r)\psi(r)=0$$

(1)

$$\psi(r)=A_0e^{i\delta/\hbar}$$

(2)

Where $\psi(r)$ is the wave function, and $\hbar$ is the re – scaled Plank constant.

In the semi – classical regime, where $\hbar$ is small, the wave function $\psi(r)$ and the related physical observable become oscillatory of wave length.

For a particle moving in three dimension in a spherically symmetric potential $V(r)$ the wave function $\psi(r)$ has the form[11]

$$\psi(r)=Y_{lm}(\theta,\varphi)R(r)$$

(3)

Where $Y_{lm}(\theta,\varphi)$ is spherical harmonics and $R(r)$ is the radial wave function obeying the radial equation

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}R(r)+\left[V(r)+\frac{l(l+1)\hbar^2}{2mr^2}\right]R(r)=ER(r) \qquad (4)$$

This equation can be brought to a form similar to the Schrodinger in one dimension introducing $\chi(r)$ by writing $R(r) = \chi(r)/r$ which satisfies the equation

$$-\frac{\hbar^2}{2m}\frac{d^2\chi}{dr^2} + \left[V(r) + \frac{l(l+1)\hbar^2}{2mr^2} - E\right]R(r) = 0 \qquad (5)$$

For a bound state boundary conditions satisfied by $\chi(r)$ are

$$\chi(r) \to 0 \qquad \text{as } r \to 0 \qquad (6)$$

Eq.(5) is similar to one dimensional equation but boundary conditions eq.(6) are different from those corresponding conditions for a bound state in one dimension.

For the radical wave function $\psi_l(r)$, which has the asymptotic form $\psi_l \sim \sin(kr - l\pi/2 + \delta_l)$ at large distances[12].

It should be noted that the centrifugal term appears with coefficient $(l + 1/2)^2$ instead of the usual $l(l + 1)$ and k is related to the energy E by $(2mE/\hbar^2)$.

There are three ways to evaluate the phase shifts and may be calculated from exact solution, WKB(Wentzel–Kramers – Brillouin) approximation and perturbation theory. Here we focus on the semi – classical or WKB approximation[13,14], according to which

$$\delta_l = \int_{r_1}^{r} dr\left[k^2 - \frac{\left(l+\frac{1}{2}\right)^2}{r^2} - \frac{2mV(r)}{\hbar^2}\right]^{\frac{1}{2}} - \int_{r_0}^{r} dr\left[k^2 - \frac{\left(l+\frac{1}{2}\right)^2}{r^2}\right]^{\frac{1}{2}} \qquad (7)$$

$r_0 = \frac{l+\frac{1}{2}}{k}$ is the classical turning point. In atomic unit a. u.($e = m = \hbar = 1$)

We use Newton – Raphson method to find r_1 which is defined by

$$k_l^2(r) = k^2 - \frac{\left(l+\frac{1}{2}\right)^2}{r^2} + \frac{2Z_1 e^{-r/a}}{r} \qquad (8)$$

at $r = r_1$; $k_l^2(r) = 0$ therefore,

$$k^2 - \frac{\left(l+\frac{1}{2}\right)^2}{r_1^2} + \frac{2Z_1 e^{-r_1/a}}{r_1} = 0 \qquad (9)$$

$$f(r) = k^2 - \frac{\left(l+\frac{1}{2}\right)^2}{r_1^2} + \frac{2Z_1 e^{-r_1/a}}{r_1} \qquad (10)$$

$$\frac{df}{dr_1} = f' = \frac{2\left(l+\frac{1}{2}\right)^2}{r_1^3} - (2Z_1/r_1)\left[\frac{1}{r_1} + \frac{1}{a}\right]e^{-r_1/a} \qquad (11)$$

at $r \to \infty$; $f(\infty) \approx k^2$; $f' \approx 0$

Integration goes over the intervals where the radicands are positive. The Yukawa potential which is given by the equation

$$V(r) = -\frac{Z_1 e^2}{r} e^{-r/a} \quad (12)$$

has been found to be a useful model potential, in particular for swift ions where's Bohr adiabatic radius[15]

$$a_{ad} = \frac{v}{\omega} \quad (13)$$

may be chosen[16,17] as the screening radius a. Here ω is a characteristic resonance frequency of a target atom or, if the stopping medium is an electron gas, the plasma frequency.

Where; l is the angular momentum, r is the distance, a is the screening radius, k is the wave vector, and Z_1 is the atomic number of projectile.

Figures(1, 2) show the results of phase shift which are calculated from eq.(7) as a function of angular momentum (l) at wave vector k=1, 2 and screening radius a=1 for (a) positive particle and (b) negative particle with atomic number (Z1=1, 2, 3, 5, 10, 20). From the figure, the phase shift increases with increasing the atomic number Z_1 for both positive and negative projectile charge. At l =0 the phase shifts of positive and negative particle are agreement, but $l \geq 1$ the discrepancies in phase shift are observed. The phase shift deceases with increasing the angular momentum l because the phase shift is dependent on the density of electrons n and inversely proportional with it therefore the phase shift at l=0 has the maximum values and begins to decrease when the angular momentum l increases. At low l, the difference in phase shift is apparent but at high l the values of phase shift are approaching and the difference becomes very small. For negative particle there is an inversion in phase shift at $1 \leq l \leq 2$, while there is no effect at $l > 2$.

Figure(3) shows the results of phase shift which are calculated from eq.(7) as a function of angular momentum l at wave vector k=2 and screening radius a=2 for (a) particle of positive and negative charge(Z1=+5,-5) and (b) particle of positive and negative charge(Z1=+10,-10). From the figure, the semi – classical and WKB approximation distinguish between positive and negative projectile charge because there is a difference in phase shift between positive and negative particles and the phase shift of positive particle is larger than that of negative particle especially at low values of angular momentum l but at high values of l, the difference becomes small and the values of phase shift are approaching.

Figures(4, 5) show the results of phase shift which are calculated from eq.(7) as a function of wave vector k at screening radius a=1 for (a)positive particle with atomic number (Z1=+5, +10) and (b)negative particle with atomic number(Z1= -5, -10). From the figure, the increase of wave vector k led to a strong increase in phase shift for each value of angular momentum l. In both positive and negative particle and at the angular momentum l=0, the phase shifts are agreement but at l ≥1 the phase shift increases with increasing the wave vector k and the phase shift of positive particle is larger than that of a negative particle. The phase shift decreases with increasing the angular momentum l therefore it has the maximum values at l=0 and begins to decrease with increasing the

angular momentum l.

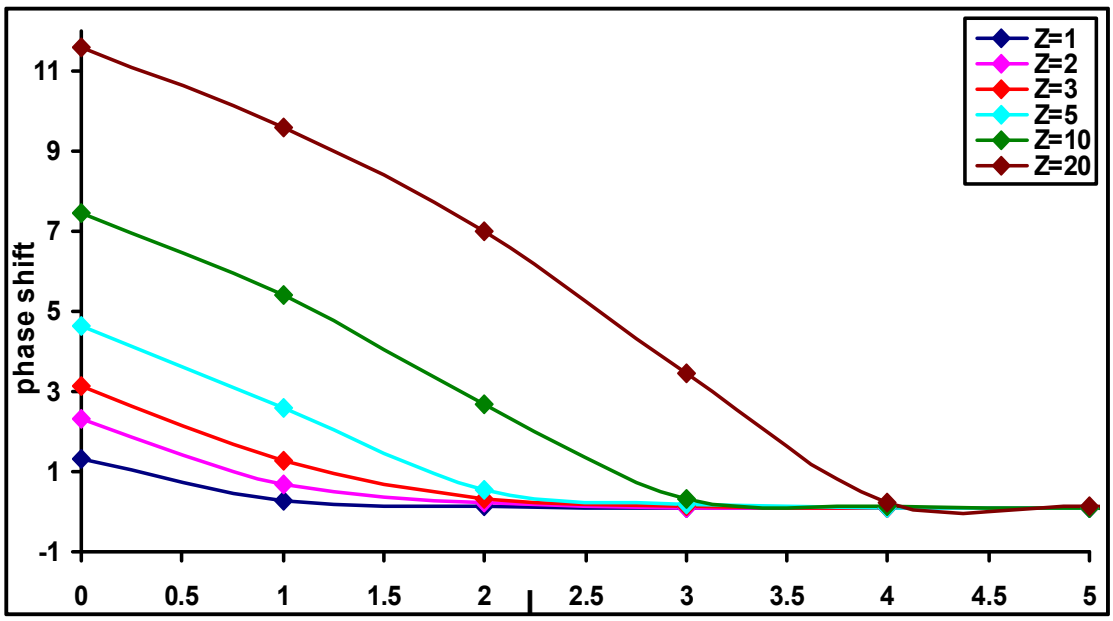

Figure-1-a: Phase Shift for Yukawa Potential with k=1 and a=1 in Atomic Unit and Positive Particle with Atomic Number (Z1=1, 2, 3, 5, 10, 20)

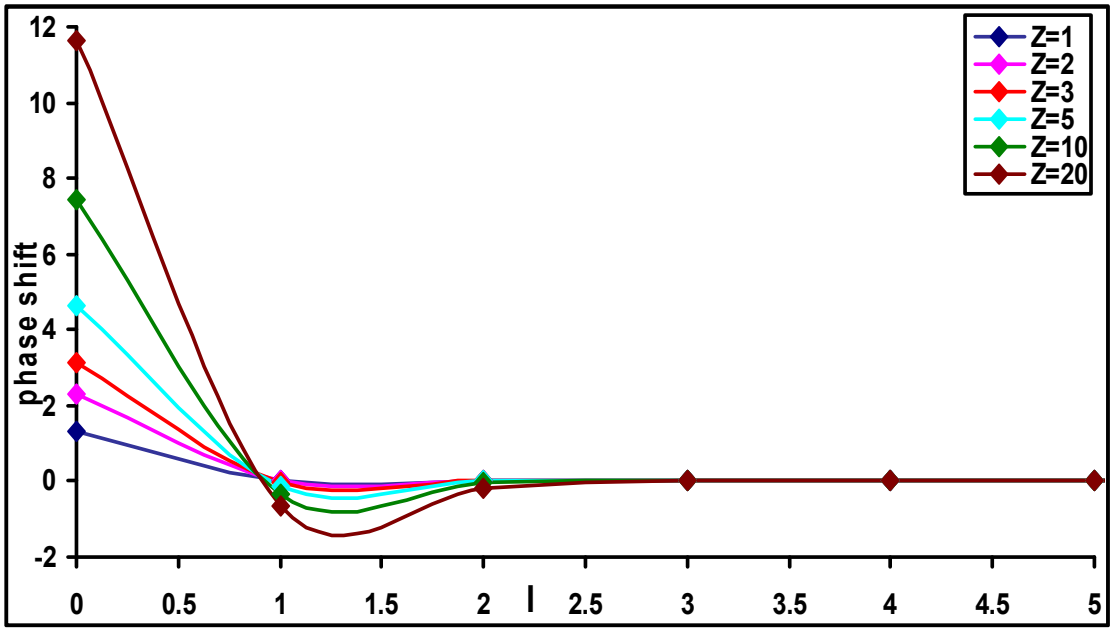

Figure-1-b: Phase Shift for Yukawa Potential with k=1 and a=1 in Atomic Unit and Negative Particle with Atomic Number (Z1= 1, 2, 3, 5, 10, 20)

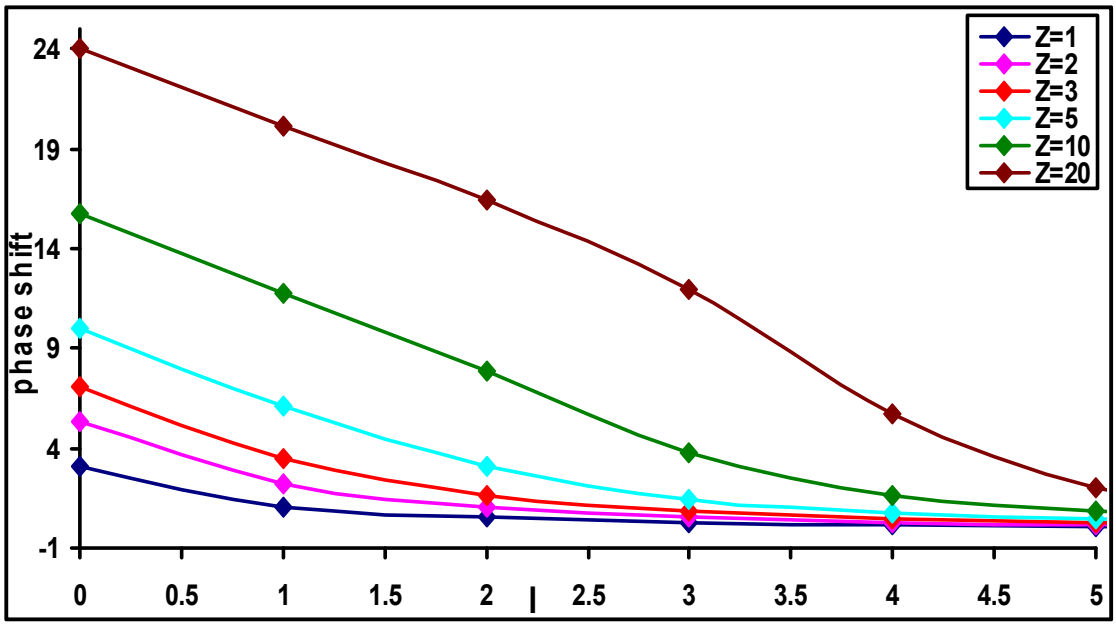

Figure-2-a: Phase Shift for Yukawa Potential with k=2 and a=1 Atomic Unit and Positive Particle with Atomic Number (Z1= 1, 2, 3, 5, 10, 20)

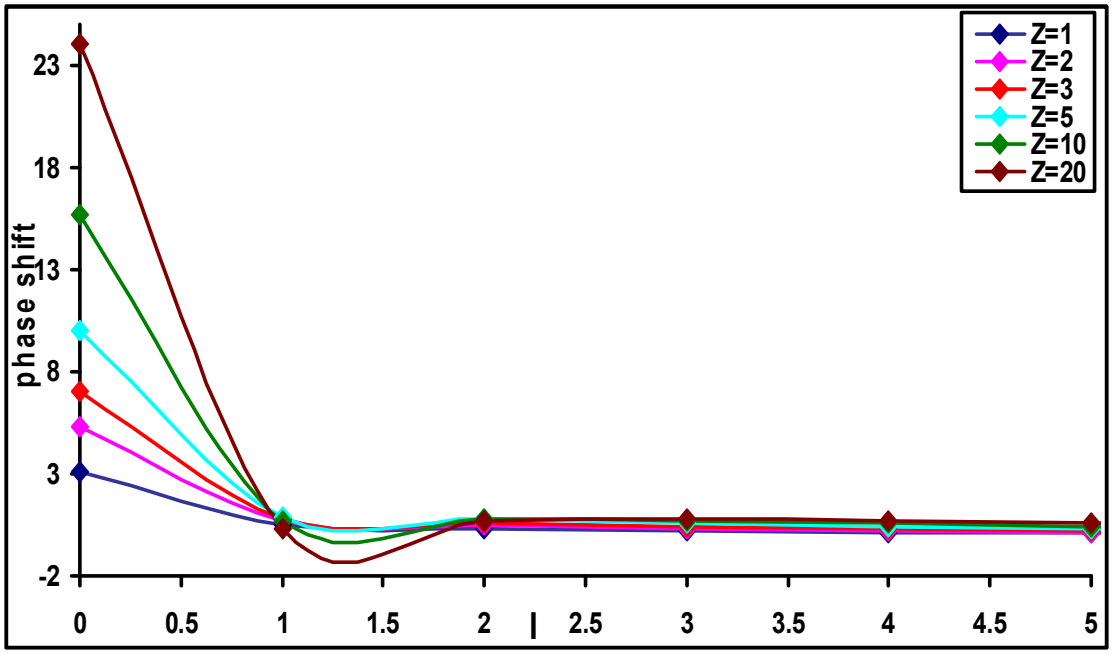

Figure-2-b: Phase Shift for Yukawa Potential with k=2 and a=1 in Atomic Unit and Negative Particle with Atomic Number (Z1= 1, 2, 3, 5, 10, 20)

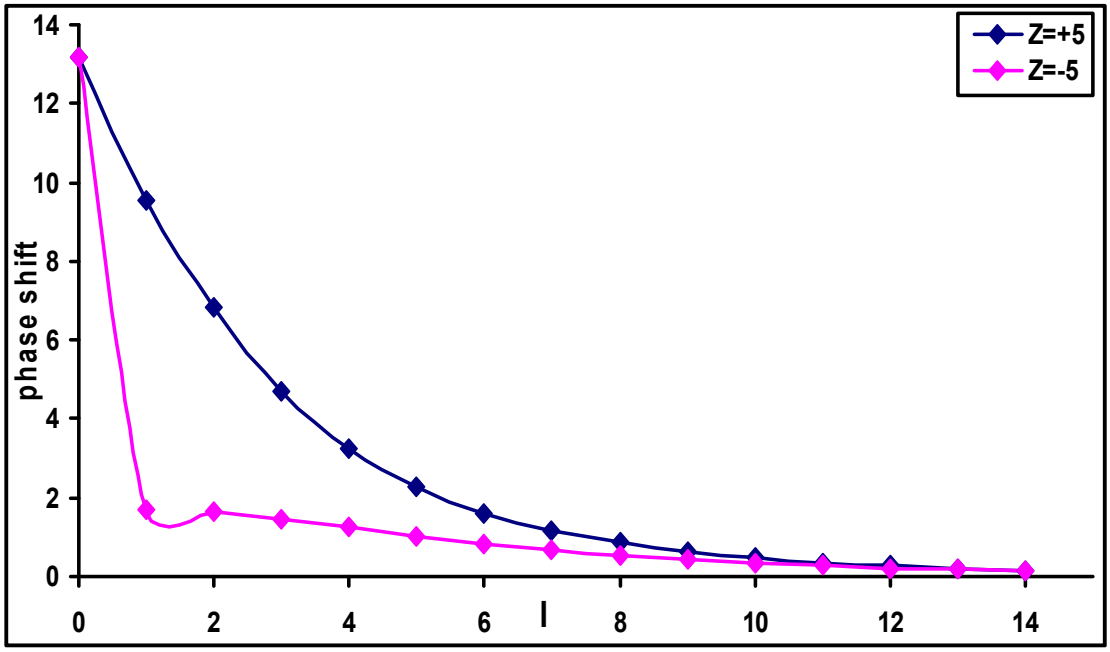

Figure-3-a: Phase Shift for Yukawa Potential with k=2 and a=2 in Atomic Unit for Positive and Negative Particle with Atomic Number (Z1= +5, -5)

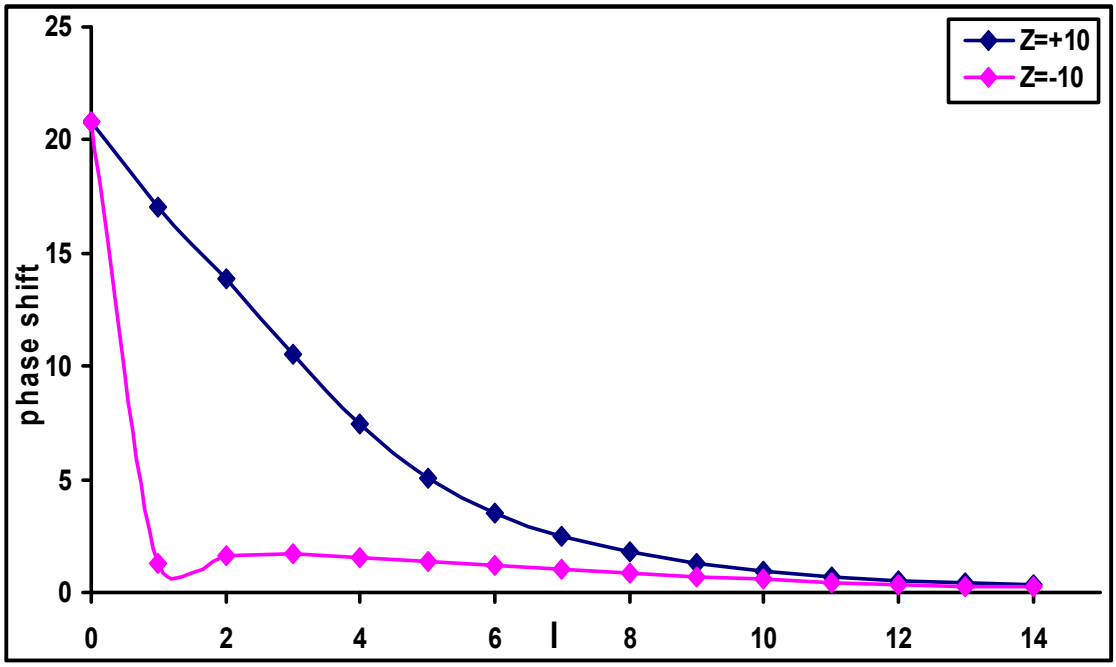

Figure-3-b: Phase Shift Yukawa Potential with k=2 and a=2 Atomic Unit for Positive and Negative Particle with Atomic Number (Z1= +10, -10)

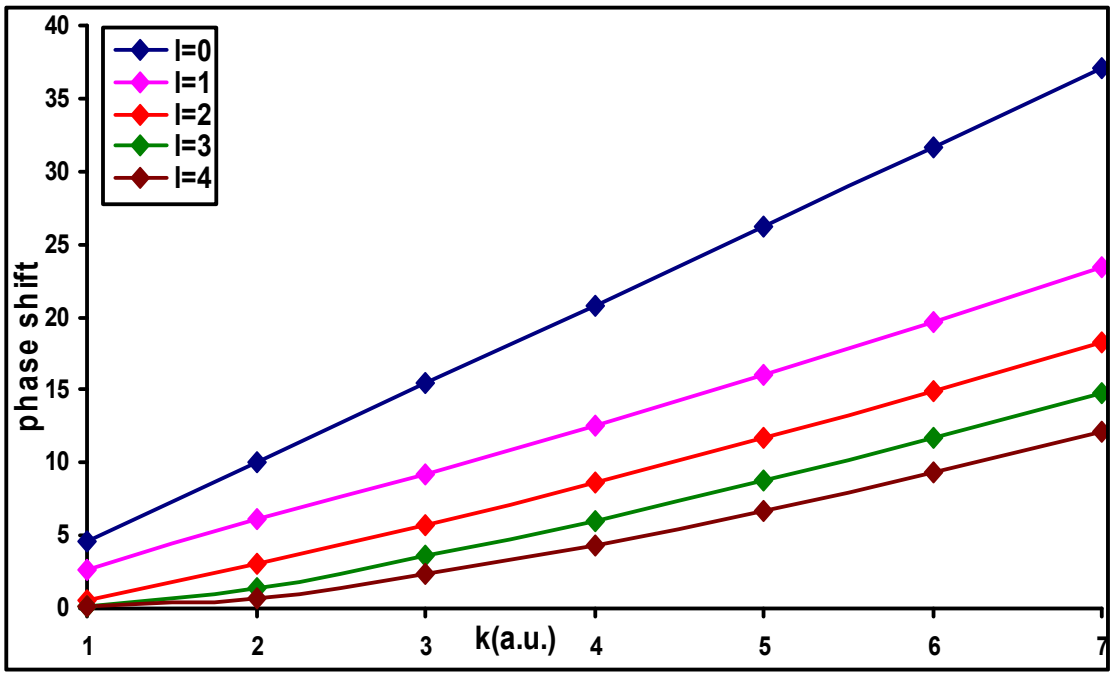

Figure-4-a: Phase Shift for Yukawa Potential with a=1 in Atomic Unit and Positive Particle with Atomic Number (Z1= +5)

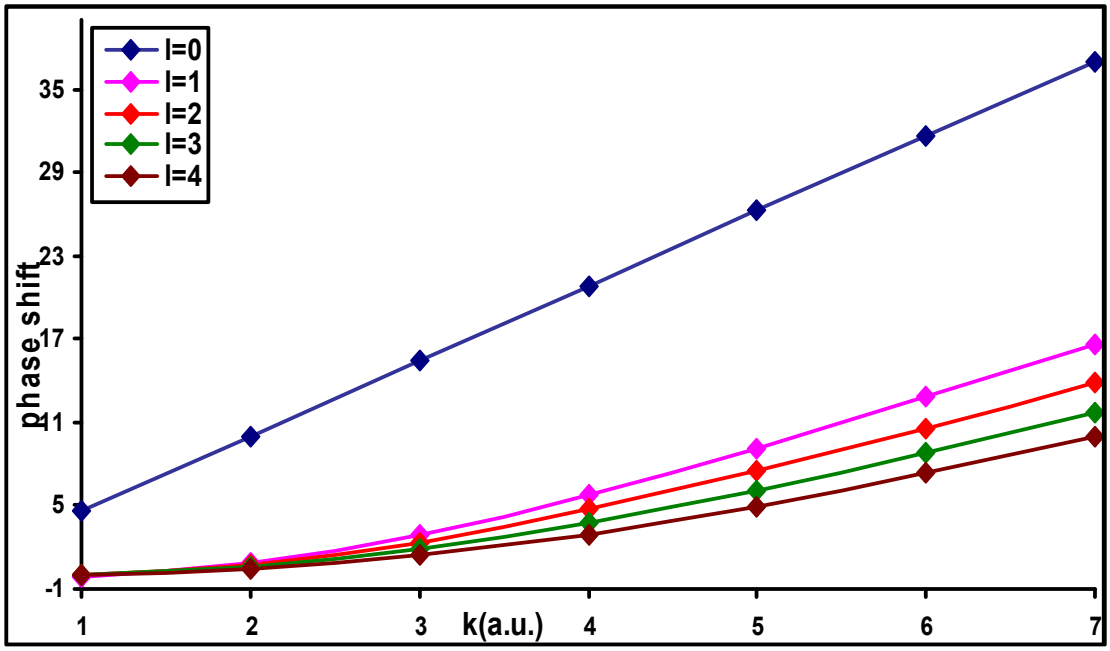

Figure-4-b: Phase Shift for Yukawa Potential with a=1 in Atomic Unit and Negative Particle with Atomic Number (Z1=-5)

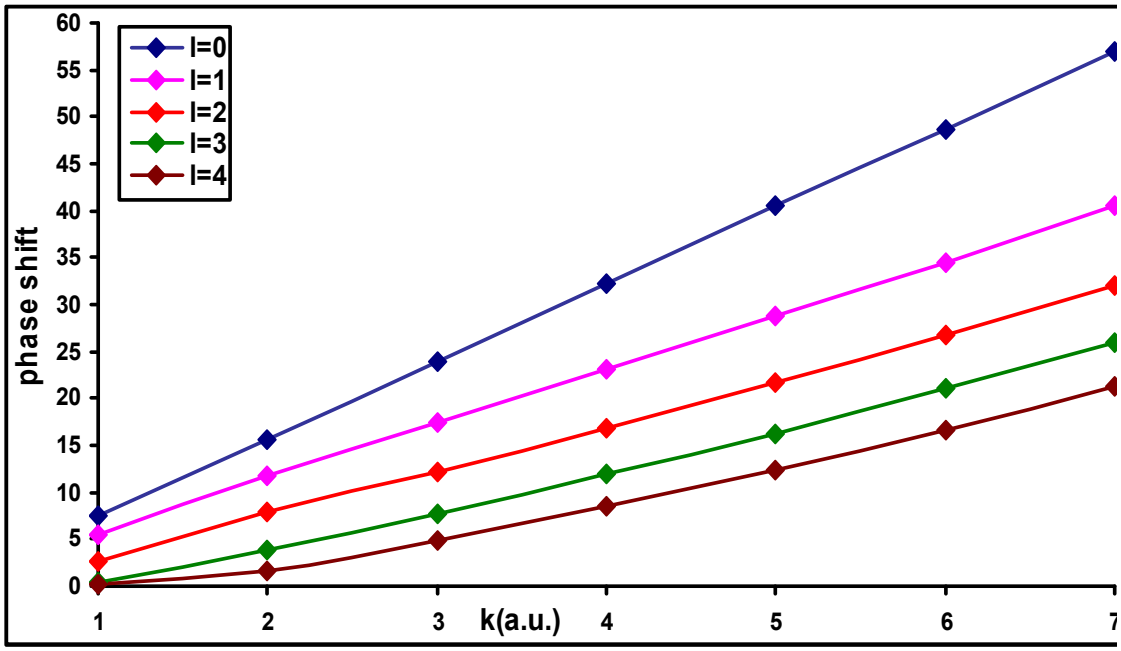

Figure-5-a: Phase Shift for Yukawa Potential with a=1 Atomic Unit and Positive Particle with Atomic Number (Z1=+10)

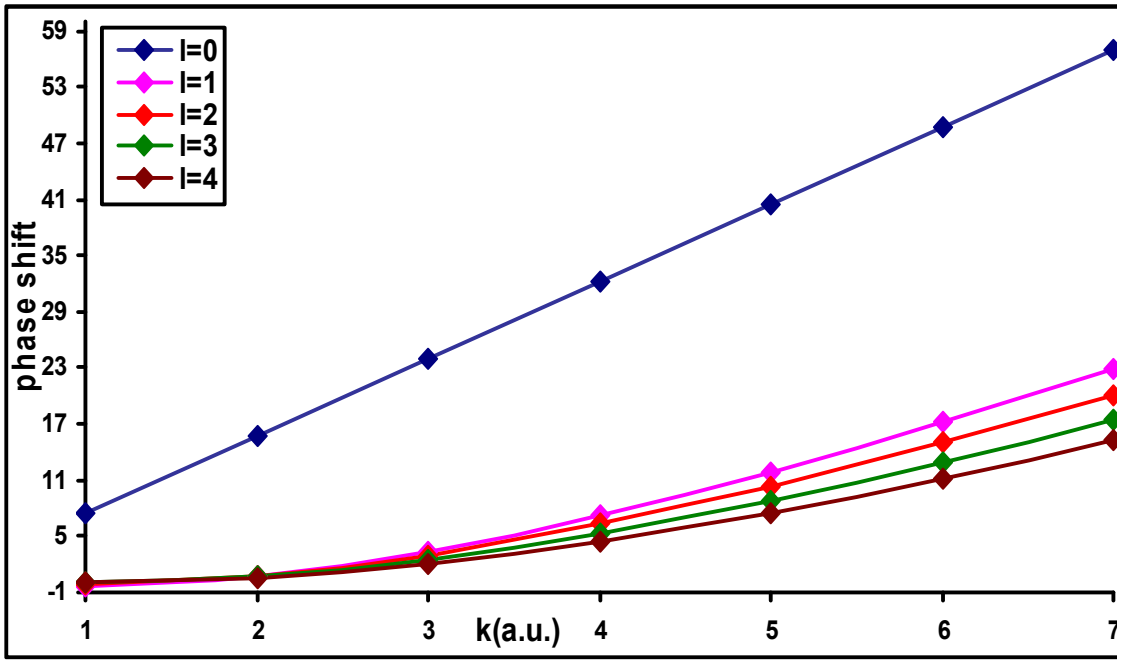

Figure-5-b: Phase Shift for Yukawa Potential with a=1 in Atomic Unit and Negative Particle with Atomic Number (z1=-10)

3. CONCLUSIONS

WKB method is one of the most useful approximations for computing the energy eign values and phase shift of the Schrodinger equation. It is important both as a practical means of approximating solutions to the Schrodinger equation, and also as a conceptual framework for understanding the classical limit of quantum mechanics.

Schrodinger equation has analytic solutions only for few selected potential energies. If the potential energy does not have a very simple form, the solution of it is generally a complicated problem. Some approximate methods to solve the Schrodinger equation are the perturbation method, the variational method and WKB approximation of great versatility which provides approximate wave function in one and three dimensional problems is a semi classical calculation in quantum mechanics in which the wave function is assumed an exponential function with amplitude λ and phase shifts δ that slowly varies compared to de Broglie wave length. The phase shift at a turning point has been found in the framework of the WKB method.

The phase shifts which are calculated from WKB method is dependent on the atomic number(Z_1) and any increase in atomic number causes a strong increase in phase shift therefore the phase shift of positive charge is larger than that of the equivalent atomic number of

negative charge. As a result, the phase shift gets larger with increasing (Z_1) and may in effect turn negative. The phase shift is parallely proportional with the wave vector(k) and it increases with increasing the wave vector and this is clear mathematically from the eq.(7)

The relative magnitude of phase shifts which are calculated from WKB approximation at constant atomic number and wave vector increases with decreasing the angular momentum l. WKB method distinguishes between positive and negative projectile charge at small values of l because the phase shift is large but at high values of l the phase shifts are approaching and become very small and at this region the perturbation method is found to be applicable.

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