Improved WKB Approximation for Nuclear Fusion Reactions

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Abstract. In this study, we have developed a mathematical approach to enhance the calculation of the probability of the WKB approximation in the semiclassical approach. This enhanced method was applied to study the total cross section of fusion reaction $\sigma_{\text{fus}}$, the barrier distribution of fusion $D_{\text{fus}}$ and the probability of fusion $P_{\text{fus}}$ for the light systems $^6\text{Li}^+^{64}\text{Zn}$, $^{13}\text{C}^+^{48}\text{Ti}$ and $^{16}\text{O}^+^{46}\text{Ti}$. A quantum coupled-channel calculation is conducted using CC code with all order coupling to compare it with the calculations of the semiclassical method before and after improvement of the WKB probability. The improved approach used with WKB enhances the semiclassical calculations and more closer our theoretical results to the measured data to be in more agreement with the treatment of quantum mechanics which agrees with the measured data for the total reaction cross section $\sigma_{\text{fus}}$, the distribution of fusion barrier $D_{\text{fus}}$ and the probability of fusion $P_{\text{fus}}$.

1. Introduction
Fusion is a reaction that combines two separate nuclei to form a compound nucleus. The relative movement of the colliding nuclei must overcome the obstacle created by the long-range repulsive Coulomb and the attractive, short-range nuclear force known as the Coulomb barrier [1]. At energies below this barrier, which is known as a classically forbidden region, fusion reaction can occur through the tunnelling phenomenon [1,2]. To evaluate the tunnelling probability, must approximate solution of the Schrodinger equation in this forbidden region, which is accomplished by WKB method [1,3]. In collisions of weakly bound nuclei, two types of fusion processes can distinguish between them, complete fusion (CF), where all projectile-target nucleons merge into the compound nucleus, and incomplete fusion (ICF), when some fragments of the projectile drifting away from interaction region. The total fusion cross section represents the sum of (CF) and (ICF) cross sections, which is measured in most experiments[4, 5-8]. The effect of the breakup channel on systems with weakly-bound projectiles was investigated by the coupling to the continuum [2]. The continuum according to the discretized continuum of the coupling channels (CDCC) is approximated by the finite set of states [9-11]. This procedure has been applied to fusion interactions [12-14]. The alternative method is the semiclassical treatment of Alder and Winther (AW) [10], where applied by [5,15]. Since this method is enhancements the theoretical calculations of fusion reactions [7, 16-20], therefore it is adopted in current work for testing the improved method in the semiclassical calculation with the code (Imp-SCF) to calculate the cross section of fusion $\sigma_{\text{fus}}$, the distribution barrier of the fusion $D_{\text{fus}}$ and the probability of the fusion
$P_{fus}$ by comparing the results of this code with traditional calculations of semiclassical method with (SCF) code, (CC) code for quantum mechanical calculations and the measured data for the systems $^6\text{Li}+^{64}\text{Zn}$, $^{13}\text{C}+^{48}\text{Ti}$ and $^{16}\text{O}+^{46}\text{Ti}$.

2. Theoretical framework

2.1. Fusion cross section

In the semiclassical approach, the $\sigma_{fus}$ calculation is a very good fit with experimental data as we indicated above, by adopting the coupled channels model. In this model, the potential between the colliding nuclei is not dependent on the relative distance between them, but also on the internal degrees of freedom[21,22]. The system Hamiltonian is

$$H = h_0(\xi) + V(\vec{r}, \xi)$$

(1)

where $h_0(\xi)$ is the Hamiltonian intrinsic motion, and $V(\vec{r}, \xi)$ represent the interaction between the projectile and the target potential [23-25]. The eigenvectors of $h_0(\xi)$ is

$$H_0|\psi_\alpha\rangle = \epsilon_\alpha |\psi_\alpha\rangle$$

(2)

$\epsilon_\alpha$ is internal motion energy. With CDCC method based on Alder and Winther (AW) [2,12,26,27]. The solution of Schrodinger equation with coupling interaction implemented as time dependent interaction, where $V(t, \xi) \equiv V(\vec{r}(t), \xi)$. According to the Schrodinger equation

$$H\Psi(\xi, t) = i\hbar \frac{\partial \Psi(\xi, t)}{\partial t}$$

Expanding $\Psi(\xi, t)$ in the basis of intrinsic eigenstates

$$\Psi(\xi, t) = \sum_{\alpha} a_\alpha(\ell, t) \psi_\alpha(\xi) e^{-i\epsilon_\alpha t/\hbar}$$

(4)

Substituting (4) in (3) we get a set of coupled channel equations

$$i\hbar \dot{a}_\alpha(\ell, t) = \sum_{\beta} \alpha_\beta(\ell, t) \langle \psi_\alpha | V(\xi, t) | \psi_\beta \rangle e^{i(\epsilon_\alpha - \epsilon_\beta)t/\hbar}$$

(5)

The initial conditions were used to solve the above equations, $\alpha(\ell, t \rightarrow -\infty) = \delta_{\beta_0}$. i.e., the projectile is found in the ground state at $(t \rightarrow -\infty)$ before the collision. The final population of channel $\beta$ in reaction with angular momentum $\ell$ is $P_\ell^{(\alpha\beta)}$ = $|a_\beta(\ell, t \rightarrow +\infty)|^2$ and the $\sigma_\beta$ is[24,26].

$$\sigma_\beta = \frac{\pi}{k^2} \sum_\ell (2\ell + 1) P_\ell^{(\beta)}$$

(6)

The fusion cross section is the sum of all channels, using partial wave expansions, we get

$$\sigma_F = \frac{\pi}{k^2} \sum_\ell (2\ell + 1) P_\ell^{(\beta)}$$

(7)

with the channels probability $P_\ell^{(\beta)}$

$$P_\ell^{(\beta)} = \frac{4k}{\pi} \int W_\ell^{(\beta)}(r) |u_\ell(k, r)|^2 dr$$

(8)

where $u_\ell(k, r)$ is wave equation of a radial part, for the $\ell$ th partial wave in channel $\beta$ and $W_\ell^{(\beta)}$ is the imaginary part of the optical potential associated to fusion in this channel, by using the approximation [1,25].

$$P_\ell^{(\beta)} = |\tilde{T}_\ell^{(\beta)}(E_\beta)|^2$$

(9)

where $T_\ell^{(\beta)}$ is the tunneling probability. For particle with reduced mass $\mu_\beta = \frac{m_{A_\beta}A_T}{A_{p+}A_T}$ and energy $E_\beta = E - \epsilon_\beta$ and $P_\ell^{(\beta)}$ is the probability of the system in channel $\beta$ when the classical trajectory is closest. The elastic channel is combined with the breakup-channel. This connection has an important impact on $\sigma_F$.

To evaluate the complete fusion cross section, we represent the breakup channel by a single channel using semiclassical theory [1,12,24].

$$P_\ell^{(\beta)} = |\alpha_\ell(\ell, t_{ca})|^2$$

(10)

$P_\ell^{(\beta)}$ is called survival probability. Therefore,

$$\sigma_{CF} = \frac{\pi}{k^2} \sum (2\ell + 1) P_\ell^{(\beta)} T_\ell^{(\beta)}$$

(11)

2.2. Fusion barrier distribution
The fusion barrier distribution $D_{\text{ fus}}$ is an important function to probe the reaction dynamics of the system around Coulomb barrier [27,28]. At low energies the breakup or breakup like processes, such as, transfer followed by breakup strongly vies with fusion reaction. The barrier distribution can be obtained by[28,29].

$$D_{\text{ fus}} = \frac{1}{\pi R_b^2} \frac{d^2 (\sigma)}{dE^2}$$

which was found theoretically from $\sigma$ by three point difference method, and The second derivative statistical error is given as [28]

$$\delta_c \cong \frac{E}{\Delta E} \sqrt{\rho_1^2 + 4 \rho_2^2 + \rho_3^2}$$

where $\rho$ is the absolute cross section uncertainties. While the experimental data of $D_{\text{ fus}}$ can be found by fitting data of $\sigma$ using approximate Wong formula [29].

$$\sigma^{\text{Wong}} = R_b^2 \frac{h \omega}{2E} \ln[1 + \exp\left(\frac{2\pi(E-V)}{h \omega}\right)]$$

3. Results and discussion

The semiclassical approach with coupled channels results for the cross section of fusion reaction $\sigma_{\text{ fus}}$, the distribution of fusion barrier $D_{\text{ fus}}$ and the probability of fusion $P_{\text{ fus}}$ for the systems $^6\text{Li}+^{64}\text{Zn}$, $^{13}\text{C}+^{48}\text{Ti}$ and $^{16}\text{O}+^{46}\text{Ti}$, were conducted using (SCF) code and (Imp-SCF) codes, and the calculations of quantum mechanics were performed by using (CC) code. The Wood-Saxon potential parameters for above systems are fitted to the experimental barrier height and are listed in table 1.

| System     | $V_c$ (MeV) | $r_c$ (fm) | $a_c$ (fm) | $W_c$ (MeV) | $r_l$ (fm) | $a_l$ (fm) |
|------------|-------------|------------|------------|-------------|------------|------------|
| $^{6}\text{Li}+^{64}\text{Zn}$ | 54.5        | 1.25       | 0.63       | 18.2        | 0.927      | 0.784      |
| $^{13}\text{C}+^{48}\text{Ti}$ | 50.6        | 1.091      | 0.781      | 16.9        | 0.951      | 0.769      |
| $^{1e}\text{O}+^{46}\text{Ti}$ | 39          | 1.102      | 0.895      | 13          | 0.959      | 0.764      |

3.1. $^{6}\text{Li} + ^{64}\text{Zn}$ system

The $\sigma_{\text{ fus}}$, $D_{\text{ fus}}$ and $P_{\text{ fus}}$ results are shown in figure 1, panels (a), (b) and (c), respectively. The measured data (green circles) is taken for this system are from [30]. Below the Coulomb barrier $V_b$, as indicated by the (magenta arrow on the E$_{c.m.}$ axis) the calculations of quantum mechanics (the red curve) for $\sigma_{\text{ fus}}$, performed by (CC) are in better agreement with measured data, as shown in figure 1, panel (a). The improved SCF calculations (blue curve) below $V_b$ are lower than the calculations of the traditional SCF (dashed blue curve) and the quantum mechanical calculations. Above $V_b$, the improved semiclassical calculations of $\sigma_{\text{ fus}}$ coincide with calculations of quantum mechanics and the measured data are more consistent than traditional semiclassical calculations. In this range of energy, whenever closest to the energy limit, these three curves are matching the experimental data. This behavior is caused by the probability of fusion above the barrier approaches to unity, as shown in figure 1, panel (c), while the probability below the barrier is smaller than above the barrier, because at low energy region many processes different from CF such us ICF, direct cluster transfers and transfer of single nucleon can be take place [32].

The mechanical quantum estimates best match the measured data as shown in panel (c) under the barrier. The fusion barrier distribution figure 1, panel (b) shows that the quantum mechanical
calculations as close as to experimental data, while the traditional semiclassical calculations far from these points.

Figure 1. (a) The cross section of fusion, (b) the distribution of fusion barrier and (c) the probability of fusion for the system $^6\text{Li}+^{64}\text{Zn}$ (red curve represent the quantum mechanical calculations, dashed and solid blue curves represent the semiclassical and improved semiclassical calculations respectively, solid green circles are experimental data [32], the barrier position indicated by magenta arrow on the E$_{\text{c.m.}}$ axis).

3.2. $^{13}\text{C}+^{48}\text{Ti}$ system
The results of $\sigma_{\text{fus}}$, $D_{\text{fus}}$ and $P_{\text{fus}}$ for this system illustrated in figure 2, panels (a), (b) and (c) respectively. The experimental data obtained from [31]. The comparison between semiclassical (dashed blue curve), improved semiclassical (blue curve) and quantum mechanical (red curve) calculations for $\sigma_{\text{fus}}$ with experimental data (green circles) below the $V_b$ (magenta arrow on the E$_{\text{c.m.}}$ axis) as shown in figure 2, panel (a) which refers to the calculations of quantum mechanics with (CC) code in the best fit with data (although there is one data point in this energy region), while above the barrier the improved method is matching the experimental data.

Figure 2. (a) The cross section of fusion, (b) the distribution of fusion barrier and (c) the probability of fusion for the system $^{13}\text{C}+^{48}\text{Ti}$ (red curve represents the quantum mechanical calculations, dashed and solid blue curves represent the semiclassical and improved semiclassical calculations respectively, solid green circles are experimental data [33], the barrier position indicated by the magenta arrow on the E$_{\text{c.m.}}$ axis. The data point after 29 MeV are deleted in panel (b) because it is don’t effect on the behavior of $D_{\text{fus}}$).

In general, above the barrier at high energy region the $\sigma_{\text{fus}}$ is increases due to increase the $P_{\text{fus}}$ at this region as shown in panel (c) in figure 2 which represent the probability of fusion for this system.
The fusion barrier distribution with (Imp-SCF) code in best agreement with measured data near and below the height of the Coulomb barrier $V_b$.

3.3. $^{16}O+^{46}Ti$ system

Figure 3, panels (a), (b) and (c) represent the results of $\sigma_{fus}$, $D_{fus}$ and $P_{fus}$ calculations respectively, for this system. The measured data (green circles) are obtained from[32]. The semiclassical calculations with (SCF) code (dashed blue curve) under the barrier (magenta arrow on the $E_{cm}$ axis) is a better result comparing with data as shown in figure 3, panel (a), whilst, the quantum mechanical calculations (red curve) with (CC) code underestimation the data. On the contrary, above the barrier, the (CC) calculations are in best match with the data, which corresponding the $P_{fus}$ calculations in figure 3, panel (c).

The fusion barrier distributions figure 3, panel (b), quantum calculations below the barrier in better agreement with experimental data, while above $V_b$, the (Imp-SCF) code calculations closest to the experimental data.

![Figure 3](image-url)

**Figure 3.** (a) The cross section of fusion, (b) the distribution of fusion barrier and (c) the probability of fusion for the system $^{16}O+^{46}Ti$. (red curve represents the quantum mechanical calculations, dashed and solid blue curves represent the semiclassical and improved semiclassical calculations respectively, solid green circles are experimental data [34], the barrier position indicated by magenta arrow on the $E_{cm}$ axis)

4. Conclusions

In the present study an improved WKB method was adopted to study the coupled channel calculations for the systems $^6Li+^{64}Zn$, $^{13}C+^{48}Ti$ and $^{16}O+^{46}Ti$. These calculations were compared with the semiclassical calculations using the standard WKB method before improvement and with the full quantum mechanical calculations. The improved WKB approach proved to be very successful in reproducing the data for the cross-section of fusion $\sigma_{fus}$, the distribution of fusion barrier $D_{fus}$ and the probability of fusion $P_{fus}$. The choice of the Woods-Saxon parameters from fitting is very adequate to perform the conclusions. This work can be extended to study light-medium, medium-medium and medium-heavy systems to sustain its success or shortfall in describing the measured data.

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