Description of coupled-channel in Semiclassical treatment of heavy ion fusion reactions

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Abstract. Fusion cross sections were measured for the systems $^{40}$Ar+$^{144}$Sm, $^{40}$Ar+$^{148}$Sm and $^{40}$Ar+$^{154}$Sm above and under Coulomb barrier to understand the role of coupled channels effects involved in barriers fusion. The fusion barriers distributions and fusion probabilities were analyzed using the semiclassical mechanical code which called Sequential Complete Fusion (SCF) as well as Full Coupled Channel code (CCFULL). These calculations show that the observed fusion cross sections fusion barrier distribution and fusion probabilities for these systems are reproduced clearly in the semiclassical mechanical for all excitation states above and under Coulomb barrier.

1. Introduction
Reactions of two nucleus fusion have been researched to understand fundamental features of the fusion processes for several years and synthesis of particular compound nuclei by establish optimum conditions, such as, exotic nuclei far from β stability or create super-heavy nuclei. An effective central potential is resultant from the complex interactions between composite nuclei [1,2]. In describing the phenomena which may occur during a collision which is general problem in many sciences of physics and chemistry, is influence of internal degrees of freedom on this potential and its fundamental importance. the fusion of heavy nuclei presents good a way to study the quantum tunnelling below the Coulomb barrier of many-body systems, the relative motion is coupled with internal degrees of freedom happens a splitting in energy of the uncoupled fusion barrier and called the single-barrier penetration model (BPM) within the (WKB) approximation method, which modify the single Coulomb barriers, producing a distribution of barriers [3,4]. However, by using the semiclassical method of Alder-Winther (AW) for heavier systems dramatic enhancements beyond the BPM were observed in the fusion probability below the barrier [5]. The Coulomb excitations of collective states was studied by this method which was originally proposed to this study and it was latter generalized to include the excitations of the breakup channel in other nuclear reactions [6,7]. More recently, sophisticated quantum Coupled-channels calculations approximate the continuum by a discrete set of states, according to the Continuum Discretized Coupled-Channels method (CDCC) [8]. In Ref. [9] F. A. Majeed is used semiclassical method in study light and weakly bound nuclei fusion reaction with Ref. [10] had performed medium and heavy systems in fusion reactions $^{46}$Ti+$^{46}$Ti and $^{58}$Ni+$^{58}$Ni, these
studies proved that the semiclassical method including the coupled channel between the entrance channel with the bound channels is established clear enhancements in describing the total fusion reaction cross section and the fusion barriers distribution down and up the Coulomb barrier.

The goal of this paper focuses on adopting Discretized Coupled-Channels method (CDCC) for semiclassical approach to study the effect of the coupled-channels and show how it can be used to evaluate total fusion reaction cross section $\sigma_{\text{fus}}$ and the fusion probability $P_f$ for the systems $^{40}\text{Ar}+^{144,148,154}\text{Sm}$. The semiclassical theory calculations have been implemented and coded using Fortran codenamed (SCF) developed by H. D. Marta et al., [13], compared with the full quantum mechanical calculations were performed using the CCFULL developed by K. Hagino et al., [14], and the results will be compared with the empirical data.

2. Theory description of complete fusion

2.1. Penetration probability

Recently, the direct reactions among heavy ions for bombarding energies down the Coulomb barrier have been proved by the validity semiclassical approach description. Since the cross sections increase strongly for bombarding energies up the Coulomb barrier it is of interest to study the expansion of the semiclassical theory to such energies [15,16]. The nucleus-nucleus interaction potential is formed from confluence among the nuclear attraction, the Coulomb repulsion, and the centrifugal force [17,18];

$$V(r) = V_N(r) + V_C(r) + V_{\text{rot}}^I(r)$$

$r$ is the distance between the center of target and projectile, $V_N(r)$ is the nuclear potential, $V_C(R)$ is the Coulomb potential, and $V_{\text{rot}}^I(r) = \frac{\hbar^2 I(I+1)}{2\mu r^2}$ is the effective centrifugal potential.

The fusion reactions are depending on quantum mechanics in single channel descriptions, of one frequently uses a complex potential (the optical potential), whose real part is given by Eq. (1). The sum of the three potentials gives rise to a Coulomb potential barrier, with height $V_B$. The potential has also a negative imaginary part $W_F$, very intense and with a short range, that accounts for the incident flux lost to the fusion channel [18,19]. Owing to the short wavelengths involved in heavy ion collisions the transmission coefficients are frequently evaluated by semiclassical approximations, like the WKB [18,19,20], the WKB approximation and it corresponds to using the classical action as the phase of the wave function. In the development of the tunnelling theory, several authors introduced concepts and recipes in order to get the tunnelling probability as close as possible to the exact result obtained from the solution of the Schrödinger equation (SE) in one dimension [19,21] as given;

$$T_I^{\text{WKB}}(E) = \exp[-2\Phi^{\text{WKB}}(E)]$$

where $\Phi^{\text{WKB}}$ is the integral

$$\Phi^{\text{WKB}}(E) = \int_{x_1}^{x_2} \kappa(x)dx = \int_{x_1}^{x_2} \frac{2\mu}{\hbar} (V_I(x) - E) dx$$

where $x_1$ and $x_2$ are two classical turning points (CTP) which are the solutions of $V_I(x_1) = V_I(x_2) = E$. In spite of several shortcomings, Eq. (2) gives fairly accurate results for smooth barriers and for energies not too close to the top of the barrier [22]. It becomes progressively worse as the energy approaches $V_B$. Furthermore, the WKB penetration coefficient takes the constant value $T_I^{\text{WKB}} = 1$, but its quantum mechanical equivalent is equal to 1/2 at the barrier, and rise up to one as the energy increases at energies up the barrier.

In 1935, Kemble [23] exhibited that the WKB approximation can be enhanced if one uses a better connection, he got the express [19,22];

$$T_I^{K}(E) = \exp[-2\Phi^{\text{WKB}}(E)]/[1 + \exp[-2\Phi^{\text{WKB}}(E)]]$$

(4)
Kemble’s approximation remains correct as the energy approaches the barrier, leading to the valid result at \( E = V_B \), namely \( T_1 = 1/2 \).

2.2. The semiclassical coupling channels theory

The semiclassical coupled channels calculations are employed the Continuum Discretized Coupled-Channel (CDCC) method, based on the semiclassical theory of Alder and Winther (AW) which was consists of classical mechanics that handle the relative motion, whereas the intrinsic motion \( \xi \) is treated as a time-dependent quantum mechanics problem for study the Coulomb excitation [5]. The Hamiltonian system in the coupled channel calculations can be written as [24];

\[
\mathcal{H} = h(r) + h(\xi) + V(\xi, r)
\]  

(5)

Where, the relative motion between the center of mass es of the two nuclei involved in the collision is describe by \( h(r) \), the internal states of each of them \( h(\xi) \) and \( V(\xi, r) \) the interaction between those for all degrees of freedom. The eigen function set are [24,25];

\[
\psi_\xi(\xi) \delta(\xi) \psi_\xi(\xi) = \delta_{\xi\xi}
\]  

(6)

Solving the classical equations of motion with the Hamiltonian for a given variable \( r \) and incident energy \( E_{\text{c.m.}} \), the classical trajectory \( r_l(t) \) is determined. Then, the internal wave function for the excitable nucleus is found by solving the time dependent Schrödinger equation for the Hamiltonian is [24,26]

\[
\mathcal{H}(\xi, t) = h(\xi) + V(\xi, r_l(t)) \equiv h(\xi) + V(\xi, t)
\]  

(7)

i.e.,

\[
\mathcal{H}(\xi, t)\phi(\xi, t) = i\hbar \frac{\partial \phi(\xi, t)}{\partial t}
\]  

(8)

Expanding \( \phi(\xi, t) \) in terms of a properly truncated set of eigen functions of \( \hbar \), Eq. (8) leads to one obtains the Alder-Winther equations

\[
i\hbar \dot{\psi}_\xi(t) = \sum_{v} V_{g,\psi}(t) e^{i(\xi_v - \xi_\psi)t} \psi_\psi(\psi; \q, v = 0, 1, ..., N)
\]  

(9)

The initial conditions \( \psi_\xi(l, t \rightarrow -\infty) = \delta_{\xi,0} \), are used to solve these equations which mean that before the collision the projectile was in its ground state at \( (t \rightarrow -\infty) \). The final population of channel \( \psi \) in a collision with angular momentum \( l \) is \( P_{l}^{(\psi)} = |a_\psi(l, t \rightarrow +\infty)|^2 \) and the cross section is [25,26,27]

\[
\sigma_\psi = \frac{\pi}{k^2} \sum_l (2l + 1) P_{l}^{(\psi)}
\]  

(10)

To expand this method to fusion reactions, we deal with the quantum mechanical problem in a coupled channel of the fusion cross sections. For simplicity, we assume that all channels are bound and have spin zero. The fusion cross sections are sum of contributions from each channel. Carrying out partial-wave expansions we get

\[
\sigma_F = \sum_\psi \left[ \frac{\pi}{k^2} \sum_l (2l + 1) P_{l}^{(\psi)} \right]
\]  

(11)

With
\[ P^F (\varrho) = \frac{4k}{E} \int dr \left| u_{q\ell}(k_\varrho, r) \right|^2 W^F_{\varrho}(r) \]  

(12)

Above, \( u_{q\ell}(k_\varrho, r) \) indicates to the radial wave function for the \( \ell \)th-partial-wave in channel \( \varrho \) and \( W^F_{\varrho} \) is the absolute value of the imaginary part of the optical potential associated to fusion in that channel [27].

3. Barrier distribution

The fusion excitation function was derivatized to extracting the barrier distribution as the second derivative of \( (E_{\sigma_F}) \) with respect to the energy [2,28]. The point difference method was using to found the second derivative as given below. The barrier distribution is defined at energy \( (E_1 + E_2 + E_3)/4 \) as

\[ \frac{d(E_{\sigma_F})}{dE} = 2 \left( \frac{(E_{\sigma_F})_3 - (E_{\sigma_F})_2}{E_3 - E_2} - \frac{(E_{\sigma_F})_2 - (E_{\sigma_F})_1}{E_2 - E_1} \right) \left( \frac{1}{E_3 - E_1} \right) \]  

(13)

where \( (E_{\sigma_F})_i \) are evaluated at energies \( E_i \). Here \( \Delta E \) is the energy step taken for extracting the second derivative. The statistical error \( \delta_c \) associated with the second derivative at energy \( E \) was calculated using the equation

\[ \delta_c = \left( \frac{E}{\Delta E^2} \right) \left( (\delta \sigma_F)_1^2 + 4(\delta \sigma_F)_2^2 + (\delta \sigma_F)_3^2 \right)^{1/2} \]  

(14)

Where in the cross sections are obtained the absolute errors indicate by \( \langle \delta \sigma_F \rangle \). Since \( \delta_c \) is proportional to the value of \( \sigma_F \), for cross sections measured with a fixed percentage error, at higher energies the barrier distribution becomes less and the cross sections are high.

4. Results and Discussions

The data have been analyzed by our employed to the coupled channel formalism. The coupled channel calculations for fusion cross sections \( \sigma_F \), the fusion barrier distributions \( P_F \) and fusion probabilities \( P_F \) with single channel were performed using the SCF codes in semiclassical approach for the systems \( ^{40}\text{Ar}+^{144,148,154}\text{Sm} \). Our calculated results of \( \sigma_F \), \( P_F \) and \( P_F \) compared with the corresponding experimental data and with full quantum mechanical calculations using the CCFULL code. The Akyüz-Winther potential parameters used in the present calculations are tabulated in Table 1.

| System       | \( V_0(\text{MeV}) \) | \( r_0(\text{fm}) \) | \( a_0(\text{fm}) \) | \( V_B(\text{MeV}) \) |
|--------------|-------------------------|----------------------|----------------------|----------------------|
| \( ^{40}\text{Ar}+^{144}\text{Sm} \) | 243.9                   | 1.10                 | 0.70                 | 129.18               |
| \( ^{40}\text{Ar}+^{148}\text{Sm} \) | 295.9                   | 1.00                 | 0.90                 | 129.26               |
| \( ^{40}\text{Ar}+^{154}\text{Sm} \) | 88.0                    | 1.20                 | 0.60                 | 128.92               |

We study the effect of channel coupling and with single channel on heavy ions fusion reactions which represented by solid and dashed (red and blue) curves, for the semiclassical and the full quantum mechanical results respectively. By using chi square method to distinguish between the cases of enhancement and suppression in the results compared experimental data.

In figure 1, panels (a, b and c) shown the results of fusion cross section \( \sigma_F \), the fusion barrier distribution \( D_F \) and fusion probability \( P_F \) for the fusion \( ^{40}\text{Ar}+^{144}\text{Sm} \) in semiclassical and the full quantum mechanical. Experimental cross sections of this fusion were published in 1985 [29]. With respect to expectations of barrier penetration model calculations, they presented a big enhancement, for energies under the Coulomb barrier, which in this case is coupling of fusion cross sections \( \sigma_F \). The best values \( (q^2 = 0.000769, 0.000327) \) for coupling channel and single channel are \( (\chi^2 = 0.033283, 0.829249) \) in semiclassical and the full quantum mechanical. Above Coulomb barrier, the
results were surprising form \(\chi^2 = 0.003358, 0.001383\) in coupling case compare with single case \(\chi^2 = 0.000737, 0.001383\). Form fig.1, and chi square values we found that the calculations of the full quantum mechanical are the best due to vibration motion for two nuclei up to one and two-phonon with deformation parameters \(J_0 = 0.314, 0.08\) [30] for Argon and samarium nuclei respectively. Experimental fusion barrier distribution and fusion probability results respect to the calculations were

\[
\chi^2 = 0.000009, 0.000022
\]

Under barrier the least values are given by \(\chi^2 = 0.000045, 0.000049\) and \(\chi^2 = 0.000683, 0.000144\) for coupling in semiclassical and the full quantum mechanical respectively. We seem, the measured values above barrier the best agreement with both our calculations.

We employed the coupled-channel calculations to analyze the data [29], in reaction \(^{40}\text{Ar} + ^{148}\text{Sm}\) for fusion cross section \(\sigma_F\), the fusion barrier distribution \(D_F\) and fusion probability \(P_F\). The potential used in the calculations was a Woods-Saxon parametrization of the Akyüz-Winther potential as shown Table 1. The results are shown in Fig. 2 panels (a, b and c), where the vibrational states of the project and target with one-phonon states. It can be seen that the coupling to the excitation channels for this reaction brings in an additional enhancement in semiclassical calculations under Coulomb barrier more than full quantum mechanical calculations from Fig. 2., panels (a, b and c) and the chi square values. The chi square values were given by \(\chi^2 = 0.000050, 0.001383\) for fusion cross section \(\sigma_F\), \(\chi^2 = 0.000004, 0.000110\) the fusion barrier distribution \(D_F\) and \(\chi^2 = 0.000005, 0.000066\) for fusion probability \(P_F\) in the semiclassical and full quantum mechanical calculations respectively. Under Coulomb barrier the semiclassical calculations in a good agreement by taken into consideration of all excitation states. The semiclassical and the full quantum mechanical calculations including coupling and no coupling effects above barrier are converged with experimental data as shown in Fig.2.

Fig.1: The calculations of semiclassical theory (red curves) are compared with full quantum mechanical calculations (blue curves) and with the empirical data (black filled circles) [29] for \(^{40}\text{Ar} + ^{144}\text{Sm}\) system. Panel (a) for the total fusion reaction cross sections \(\sigma_F\) (mb), Panel (b) for the fusion reaction barriers distribution and \(D_F\) (mb/MeV) and Panel (c) for fusion probability \(P_F\).

Fig.2: The calculations of semiclassical theory (red curves) are compared with full quantum mechanical calculations (blue curves) and with the empirical data (black filled circles) [29] for \(^{40}\text{Ar} + ^{148}\text{Sm}\) system. Panel (a) for the total fusion reaction cross sections \(\sigma_F\) (mb), Panel (b) for the fusion reaction barriers distribution and \(D_F\) (mb/MeV) and Panel (c) for fusion probability \(P_F\).
Exact coupled channel calculations were performed in the semiclassical mechanical with the full quantum mechanical. The results of $\sigma_F$, $D_F$, and $P_F$, are shown in Fig. 3, panels (a, b and c). The target 154Sm is taken rotation motion in the case of quantum mechanical calculations including coupling to the state (2+) which has experimental value of 0.081973 [31] with the deformation parameter ($\beta_2 = 0.27, \beta_3 = 0.105$) taken from Ref. [32], while the projectile 40Ar is taken to be inert.

The best calculated values of chi-square values obtained are ($\chi^2 = 0.000009, 0.000031, 0.000025$), which corresponds to the semiclassical calculations including channel coupling are in best agreement with the experimental data [33] for $\sigma_F, D_F$ and $P_F$ under the Coulomb barrier. Compare with the minimum values obtained are ($\chi^2 = 0.000017, 0.023036, 0.009747$), which correspond to the full quantum calculations including coupling.

The best calculated value obtained is $\chi^2 = 0.000001$ for $\sigma_F$ which corresponds to the semiclassical calculations including no coupled and coupled channel, which means that they are able to reproduce the experimental data better than other calculations above barrier. The chi-square values are found to be ($\chi^2 = 0.000007, 0.000001$) for $D_F$ and $P_F$ of semiclassical calculations including coupling in comparison with the experimental data which means that they are perfect match with the corresponding experimental data. While the quantum mechanical calculations including coupling the chi-square values are found to be ($\chi^2 = 0.000004$) for $\sigma_F$ which to be more near to semiclassical calculations including coupling with the experimental data. From that means that semiclassical calculations are perfect match with the corresponding experimental data.

Fig.3: The calculations of semiclassical theory (red curves) are compared with full quantum mechanical calculations (blue curves) and with the empirical data (black filled circles) [33] for $^{40}\text{Ar}+^{154}\text{Sm}$ system. Panel (a) for the total fusion reaction cross sections $\sigma_F$ (mb), Panel (b) for the fusion reaction barriers distribution and $D_F$ (mb/MeV) and Panel (c) for fusion probability $P_F$.

5. Conclusion
We studied an expansion of the semiclassical theory of Alder and Winther to calculate the cross sections $\sigma_F$, the fusion barriers distribution $D_F$ and fusion probability $P_F$. The semiclassical mechanical results were exhibited to be in very good agreement with the experimental data. As calculations are much converged than full quantum calculations, thus providing a powerfully tool for the analysis of heavy ion fusion reactions.

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