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MODELOS SOLUBLES EN LA CADENA DE FUSIÓN
PROTÓN – PROTÓN VÍA ECUACIÓN DE FADDEEV

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Solvable Models in the Proton-Proton Fusion Chain by Faddeev Equation

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«It's the questions we can't answer that teach us the most. They teach us how to think. If you give a man an answer, all he gains is a little fact. But give him a question and he'll look for his own answers.»

Patrick Rothfuss





To Angel Gabriel Platas Bustos: from the chaotic scattering of two, you emerged—a third, forever bound to me in a perfect state.





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Resumen

En el presente trabajo se busca describir la primera parte de la cadena de fusión protón-protón, la cual da lugar a la formación del deuterón, proponiendo un modelo de colisión entre tres partículas, $N + N + N \rightarrow d + N$, tratando este problema mediante el formalismo de Faddeev-Merkuriev. Se recurre a la descripción del movimiento relativo entre nucleones mediante coordenadas de Jacobi e interacciones mediadas por barreras del tipo δ . Se propone este modelo simplificado en concordancia con el modelo de coalescencia para la formación del deuterón. Se justifica la necesidad de una tercera partícula en el balance de energía y momento para lograr formar un estado ligado de dos partículas 2H .

El modelo propuesto ofrece soluciones exactas al problema de colisión de 3 cuerpos. Por otra parte se discute la relevancia de las sutilezas de los modelos propuestos para describir fenómenos dinámicos. En concreto, se aborda el problema del decaimiento exponencial en barreras tipo δ y culombianas, ligado al mecanismo de tunelamiento cuántico asociado tanto al proceso de fusión como de disociación. Se muestra que el uso de barreras del tipo delta no producen por si solas decaimiento exponencial, justificando la implementación de efectos estadísticos y térmicos que resulten en decaimientos del tipo deseado. Posteriormente se demuestra que este modelo de interacción permite un cálculo analítico de la amplitud de dispersión, la sección eficaz y la tasa de colisión, con un acuerdo muy cercano a los experimentos reportados. Dichos experimentos se enfocan en procesos que excluyen la transmutación β inversa, $p + p \rightarrow d + e^+ + \nu_e$, los cuales no pueden describirse por los tratamientos de esta tesis.



Abstract

This work aims to describe the first part of the proton-proton fusion chain, which leads to deuteron formation, by proposing a three-particle collision model, $N + N + N \rightarrow d + N$, and by addressing this problem with the Faddeev-Merkuriev formalism. The relative motion between nucleons is described using Jacobi coordinates and interactions mediated by δ barriers. This simplified model is proposed in accordance with the coalescence model for deuteron formation. The need for a third particle in the energy and momentum balance to achieve a bound two-particle state 2H is justified. The proposed model offers exact solutions to the three-body collision amplitude. Furthermore, the relevance of the proposed models for describing dynamic phenomena, such as tunneling, is discussed. Specifically, the problem of exponential decay in δ and Coulomb barriers is addressed, linked to the quantum tunneling mechanism associated with both the fusion and dissociation processes. It is shown that the use of delta-type barriers alone does not produce exponential decay, justifying the implementation of statistical and thermal effects that result in decays of the desired type. Subsequently, it is demonstrated that this interaction model allows for an analytical calculation of the scattering amplitude, the cross section, and the collision rate, showing very good agreement with reported experiments. These experiments focus on processes that exclude the inverse β transmutation, $p + p \rightarrow d + e^+ + \nu_e$, which cannot be described by the treatments in this thesis.



Contents

Acknowledgments	vii
Resumen	xi
Abstract	xiii
1 Introduction	1
1.1 The Deuteron: A Quantum Two-Body System	4
1.1.1 Hamiltonian and Wave Equation	5
1.1.2 Spin-Dependent Interaction	6
2 On Fusion Models and the Tunneling Mechanism	9
2.1 Exponential decay	10
2.1.1 Gamow vectors and rigged Hilbert spaces	11
2.1.2 Friedrichs model	14
2.2 Survival Probability in a δ -Shell Potential	16
2.2.1 Formal Definition and Expression	16
2.2.2 Stationary States for the δ -Shell Potential	17
2.2.3 Complete Stationary State Solution	18
2.2.4 A_I normalization	18
2.2.5 Numerical Analysis of Quantum Decay Dynamics	20
2.2.6 Momentum-Dependent Transport Regimes	21
2.2.7 Analytical Results for Survival Probabilities	24
2.2.8 Evolution in thermal ensembles	27
3 Deuteron Formation Channels in Heavy-Ion Collisions	37
3.1 The Faddeev Equations and Coordinate Systems	38
3.1.1 Coordinate Description of Three-Body System	40
3.1.2 Jacobi Coordinates	40
3.2 Theoretical Framework: From Two-Body to Three-Body Systems . .	41
3.2.1 Foundations: The Two-Body Problem in One Dimension . . .	41
3.2.2 The Lippmann-Schwinger Formalism for Delta Potential Interactions	43
3.2.3 Generalization to the Three-Body Problem	45
3.2.4 Total Wave Function Antisymmetrization	46

3.3	Three-Body Cluster Interactions	48
3.3.1	Coulomb Interaction	52
3.3.2	Total Cross Section Calculation in Hyperspherical Coordinates	54
4	Results	59
4.1	Triangular Visualization of Scattering Amplitudes	59
4.1.1	Coulomb Interaction System Analysis	62
4.2	Collision Rate and Total Cross Section	65
5	Discussion and Conclusions	69
	Appendix A Model Setup and Implementation	71
	Appendix B Wavepacket Dynamics in a Modified Coulomb Potential	75



1 Introduction

The understanding of production mechanisms for weakly-bound clusters, such as the deuteron (d), in heavy-ion collisions at mid-rapidity currently represents a challenging problem, also known as the “ice in the fire” puzzle. In contrast to other studies, we employ a complete isospin decomposition of the channel for “kinetic” deuterons, $NNN \leftrightarrow Nd$. In the context of stellar fusion, the formation of the deuteron (the only stable isotope of hydrogen) is crucial in the process of transforming hydrogen into helium and thus obtaining the energy that sustains stars like our sun. A low but still significant production channel (around 12% in collision experiments) is the one that involves the collision of three nucleons for the formation of a bound state of two nucleons; this production channel represents a quantum three-body problem.

The classical three-body problem, exemplified by the Moon-Earth-Sun system, offers interesting insights [1,2]. Similarly, the quantum mechanical three-body problem has existed almost as long as quantum mechanics itself [3]. The two-body problem is classified as “solved” due to the conservation of angular momentum, which effectively reduces the problem to one-dimensional radial motion. Energy is also conserved, and in both classical and quantum mechanics, the task reduces to solving an ordinary second-order differential equation for constant energy. In contrast, the three body problem may have chaotic regimes.

In nuclear physics, prominent examples include three-nucleon systems [4] and more complex nuclear clusters approximately described by three-body models [5–10]. Finally, nucleons themselves (three quarks) represent a fundamental three-body system [11]. For short-range interactions, the Efimov effect can appear [12]—a three-body system possesses infinitely many bound states if at least two of the two-body subsystems have an infinite s-wave scattering length. Mathematically, the Efimov effect is equivalent to the Thomas effect [13], where a three-body system with zero-range two-body interactions also exhibits an infinite number of bound states. Extremely large scattering lengths are required to observe even a few Efimov states, with only the first predicted in the atomic helium trimer [14,15]. Such states may also appear fortuitously along the neutron drip line [10].

A couple of important examples to clarify the relevance of interactions involving three bodies are the Auger effect and the capture of a third body in celestial mechanics. The Auger effect constitutes the paradigm of three-body interaction in the quantum regime, see Figure 1.1.

Consider an atom with a vacancy in an inner shell. The Auger process can be formalized as a transition between initial and final states. Energy conservation

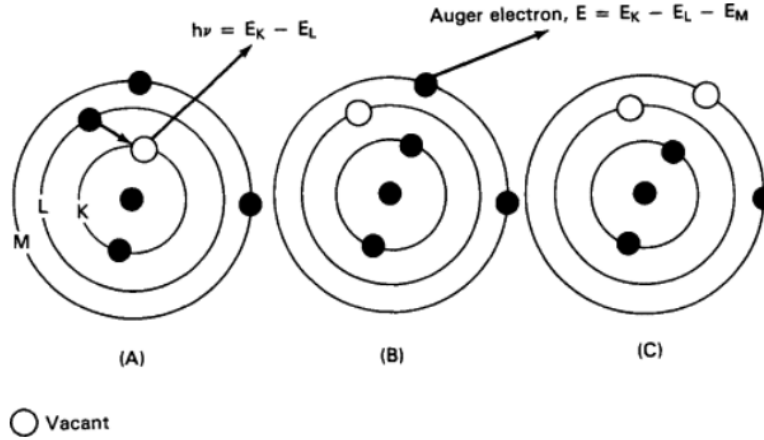


Figure 1.1: (A) The usual emission of a K characteristic X-ray, $h\nu$, energy equal to $E_K - E_L$, the difference in binding energy for the two orbital electrons, K and L. (B) $h\nu$ has been absorbed and a monoenergetic Auger electron is emitted, in the example shown, from the M shell, the energy of which is $E_K - E_L - E_M$. (C) In its final state the atom has vacancies in the L and M orbitals. [16]

dictates [17, 18]:

$$E_K - E_{L_1} = E_{L_2} + T_{\text{Auger}} + \Delta E_{\text{corr}}, \quad (1.1)$$

where T_{Auger} represents the kinetic energy of the emitted electron, in addition E_K, E_{L_1}, E_{L_2} are the binding energies of the electrons in their respective shells finally E_{corr} represents the electronic correlation contributions and E_{rear} the atomic nucleus restructuring effects:

$$T_{\text{Auger}} = E_K - E_{L_1} - E_{L_2} - \frac{e^2}{\langle r_{12} \rangle} - E_{\text{corr}}. \quad (1.2)$$

The emission of the Auger electron acts as the essential dissipative channel that allows the resulting ion to stabilize into a bound state, analogous to the “absorbing third body” in mechanical problems.

Consider a system composed of a central body of mass M , a bound body of mass m in orbit, and an approaching third body of mass μ . The gravitational Hamiltonian is given by:

$$H_{\text{grav}} = \frac{\mathbf{p}_M^2}{2M} + \frac{\mathbf{p}_m^2}{2m} + \frac{\mathbf{p}_\mu^2}{2\mu} - \frac{GMm}{r_{Mm}} - \frac{GM\mu}{r_{M\mu}} - \frac{Gm\mu}{r_{m\mu}}. \quad (1.3)$$

The orbital capture process can be analyzed through the formalism of energy states. The initial system energy is [19]:

$$E_i = -\frac{GMm}{2a} + \frac{1}{2}\mu v^2. \quad (1.4)$$

For the capture of the third body μ , forming a new bound system with M , the final energy must satisfy:

$$E_f = -\frac{GM\mu}{2a_{\text{new}}} + \frac{1}{2}mv_f^2 + \Delta E_M < 0, \quad (1.5)$$

where $\Delta E_M = \frac{1}{2}M(\Delta v)^2$ represents the recoil energy of the central body, analogous to the recoil of the atomic nucleus in the Auger process. Energy conservation imposes:

$$-\frac{GMm}{2a} + \frac{1}{2}\mu v^2 = -\frac{GM\mu}{2a_{\text{new}}} + \frac{1}{2}mv_f^2 + \frac{1}{2}M(\Delta v)^2. \quad (1.6)$$

Rearranging for the kinetic energy of the ejected body (analogous to the Auger electron):

$$\frac{1}{2}mv_f^2 = \frac{GM\mu}{2a_{\text{new}}} - \frac{GMm}{2a} + \frac{1}{2}\mu v_\infty^2 - \frac{1}{2}M(\Delta v)^2. \quad (1.7)$$

The condition for stable capture ($E_f < 0$) requires that:

$$\frac{1}{2}M(\Delta v)^2 > \frac{GM\mu}{2a_{\text{new}}} - \frac{GMm}{2a} + \frac{1}{2}\mu v^2. \quad (1.8)$$

Both systems obey the universal equation:

$$E_{\text{system}}^{\text{initial}} = E_{\text{system}}^{\text{final}} + T_{\text{third body}} + E_{\text{recoil}} \quad (1.9)$$

where $T_{\text{third body}}$ represents the energy of the body carrying away the excess energy (Auger electron or ejected body), and E_{recoil} captures the energy of the system's "core" (atomic ion or central gravitational body).

The Auger effect in atomic physics and gravitational capture mechanisms in astrodynamics represent manifestations of a universal principle governing three-body interactions: the formation of stable bound configurations necessarily requires the presence of a third actor that functions as a dissipator of excess energy. This unified understanding not only enriches our theoretical perspective but also suggests promising avenues for the development of transversal mathematical techniques to address the three-body problem across multiple physical scales.

The natural question that arises now is "how to give a solution for the quantum three-body problem?". There are few options for this, in our case we work with the Faddeev-Merkuriev equation. The Faddeev-Merkuriev formalism provides a mathematically rigorous framework for the quantum mechanical three-body problem. Its procedure is particularly well-suited for short-range interactions [9, 20]. However, a significant strength of the method lies in its adaptability to long-range forces. By treating the long-range part of the Coulomb interaction within the kinetic energy operator, it is possible to circumvent the large couplings between partial waves associated with different Jacobi coordinates. This technique has enabled precise calculations of bound-state energies in systems like $dt\mu^-$ [21] and scattering processes such as $e^+ + H \rightarrow Ps + p$ [22].

The traditional approach of partial wave expansion, while powerful, can be computationally demanding. This limitation can be overcome by solving the coupled three-dimensional equations directly for the magnitudes of the two Jacobi coordinates and the angle between them [23]. This methodology has been successfully applied to a range of muonic molecular systems [23], as well as to the nuclear $N + d$ system [24]. It is noteworthy that systems with hard cores present distinct and additional challenges [25].

An alternative and widely used technique is the hyperspherical harmonic expansion. This method employs the eigenfunctions of the six-dimensional angular momentum operator as an angular basis for the three-body wave function. The expansion coefficients, which depend on the hyperradius, are then determined by solving a set of coupled differential equations. This approach is particularly effective for simple two-body potentials [26]. However, a key limitation arises when a two-body subsystem possesses a bound state: an increasing number of hyperspherical harmonics is required for an accurate description at large hyperradii. Explicitly including the two-body bound-state wave function in the basis introduces complications related to the non-orthogonality of the different components of the new basis [27]. Consequently, this expansion is generally less efficient for complicated potentials featuring repulsive cores and for high-precision calculations.

Given these considerations, the Faddeev-Merkuriev equations in momentum space emerge as a robust framework for our study. Their inherent capacity to handle the full complexity of the nucleon-nucleon interaction, including its short-range repulsion and tensor components, while providing a clear representation of the $N + N + N \leftrightarrow N + d$ channel, makes them the most suitable foundation for developing a soluble model of deuteron formation via three-nucleon scattering.

All of the above work represents a robust background for the description of specific reaction channels, but it is far too complicated for pedagogical purposes. Our aim is to propose and solve a model that retains the elements previously exposes and explains deuteron formation by collision in the simplest terms. Since the deuteron forms in the S-channel, a dimensional reduction seems plausible. Furthermore, the interactions can be modeled by their attractive and repulsive nature (simplification to Dirac deltas), not by their local details. Finally, the charges can be incorporated through isospin operators in the potentials that appear in the Lippmann-Schwinger formalism.

It is important to note that this work focuses on the deuteron formation channel via elastic scattering of three nucleons ($N + N + N \leftrightarrow N + d$), which dominates at energies below the pion production threshold. In this 'low energy' regime, relativistic effects are negligible, justifying the use of a non-relativistic formalism based on the Schrödinger equation. Furthermore, this model does not include the inverse beta channel ($p + p \rightarrow d + e^+ + \nu_e$), which is mediated by the weak interaction. In our case, the excess energy and momentum are carried exclusively by the third particle (a spectator nucleon).

1.1 The Deuteron: A Quantum Two-Body System

Deuterium, discovered by Urey [28], is an isotope of hydrogen with an isotopic abundance of approximately 1.5×10^{-4} . The deuteron, its nucleus, is the only stable bound system of two nucleons (p, n). Its mass is $m_d = 1875.612762(75)$ MeV/ c^2 with a binding energy of $E_L = 2.22456612(48)$ MeV [29]. The deuteron radius is measured to be $R_d 1.975(3)$ fm, while its charge radius is slightly larger, $R_{ch} = 2.130(10)$ fm. Its electromagnetic moments are precisely determined: the magnetic dipole moment is $\mu_d = 0.8574382284(94)$ μ_N and the electric quadrupole moment is $Q_d = 0.2859(3)$ fm².

A system of two nucleons, being fermions with spin-1/2, must obey the Pauli exclusion principle, requiring the total wave function to be antisymmetric under particle exchange. When isospin is considered, the np system must also satisfy Pauli principle [30]. The total deuteron wave function can be decomposed as:

$$|d\rangle = |\phi(\vec{r})\rangle_L |\chi\rangle_S |v\rangle_T, \quad (1.10)$$

which must be totally antisymmetric. The spatial part has the symmetry of the orbital angular momentum L (symmetric for the deuteron's even L), and the spin function is a symmetric triplet ($S = 1$, $J_d = 1$). Consequently, the isospin function $|v\rangle_T$ must be antisymmetric, corresponding to the singlet state:

$$|T = 0, T_3 = 0\rangle = \frac{1}{\sqrt{2}} (|p\rangle|n\rangle - |n\rangle|p\rangle). \quad (1.11)$$

The complete wave function is constructed from a spatial part $R_{nl}(r)Y_{lm}(\theta, \varphi)$ describing the relative motion, a spin part χ_{sm_s} , and an isospin part $|TT_3\rangle$ [31]:

$$\psi_{\text{deuteron}} = R_{nl}(r)[Y_{lm}\rangle\langle\chi_{sm_s}]^{[j]}|TT_3\rangle. \quad (1.12)$$

The bracket denotes the coupling of orbital and spin angular momentum to total angular momentum j :

$$[Y_{lm}\rangle\langle\chi_{sm_s}]_{m_j}^j = \sum_{m_l, m_s} \langle lm_l, sm_s | jm_j \rangle Y_{lm_l} \chi_{sm_s}, \quad (1.13)$$

and the spin wave function is built from individual nucleon spins:

$$\chi_{sm_s}(1, 2) = \sum_{m_{s1}, m_{s2}} \langle \frac{1}{2}m_{s1}, \frac{1}{2}m_{s2} | sm_s \rangle \chi_{m_{s1}}(1) \chi_{m_{s2}}(2). \quad (1.14)$$

The isospin wave function is constructed analogously from single-nucleon isospin states:

$$|TT_3\rangle = \sum_{t_1, t_2} \langle \frac{1}{2}t_1, \frac{1}{2}t_2 | TT_3 \rangle |t_1\rangle |t_2\rangle. \quad (1.15)$$

Given the deuteron's charge $Q = e$ and nucleon number $A = 2$, we have $T_3 = 0$. The isospin can be $T = 0$ (singlet) or $T = 1$ (triplet). Only the $T = 0$ state corresponds to the deuteron ground state; the $T = 1$ states represent the unbound di-proton and di-neutron systems.

1.1.1 Hamiltonian and Wave Equation

In the center-of-mass frame, the Hamiltonian for the relative motion reduces to that of a single particle with reduced mass $\mu = m_p m_n / (m_p + m_n)$ in a central potential $V_{\text{nuc}}(|\vec{r}|)$ [32]:

$$\mathcal{H}_D = -\frac{\hbar^2}{2\mu} \nabla_{\vec{r}}^2 + V_{\text{nuc}}(r). \quad (1.16)$$

The radial Schrödinger equation becomes:

$$-\frac{\hbar^2}{2\mu} \frac{d^2 u}{dr^2} + \left[V_{\text{nuc}}(r) + \frac{\hbar^2 l(l+1)}{2\mu r^2} \right] u(r) = Eu(r), \quad (1.17)$$

where $u(r) = rR(r)$. For the ground state ($l = 0$), the effective potential is simply $V_{\text{nuc}}(r)$. Modeling V_{nuc} , see Figure 1.2 as a square well of depth $-V_0$ and range $R_0 \approx 2.1$ fm yields solutions:

$$u(r) = A \sin(kr) + B \cos(kr), \quad 0 < r < R_0, \quad (1.18)$$

$$u(r) = Ce^{-\kappa r} + De^{\kappa r}, \quad r > R_0, \quad (1.19)$$

with $k^2 = 2\mu(E + V_0)/\hbar^2$ and $\kappa^2 = -2\mu E/\hbar^2$. The binding condition leads to the transcendental equation:

$$-\kappa = k \cot(kR_0). \quad (1.20)$$

A minimal well depth $V_0 \gtrsim 23.1$ MeV is required to support a bound state. Solving for the deuteron binding energy gives $E_0 \approx -2.2$ MeV.

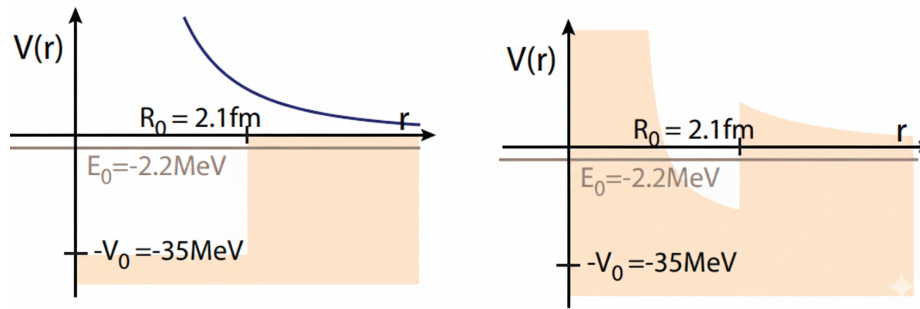


Figure 1.2: Nuclear potential for $l \neq 0$. Left, nuclear potential and centrifugal potential. Right, the effective potential. [32]

1.1.2 Spin-Dependent Interaction

The total angular momentum denoted by I is $\hat{J} = \hat{L} + \hat{S}_p + \hat{S}_n$. A spin-dependent potential of the form $V_{\text{spin}} = V_1(r)/\hbar^2 \hat{S}_p \cdot \hat{S}_n$ distinguishes between triplet ($S = 1$) and singlet ($S = 0$) states [32]. Writing $\hat{S}^2 = \hat{S}_p^2 + \hat{S}_n^2 + 2\hat{S}_p \cdot \hat{S}_n$, the last term is the one we are looking for.

Using the fact that $\hat{S}^2$ and $\hat{S}_p, \hat{S}_n$ commute we write an equation for expectation value, that is:

$$\langle \hat{S}_p \cdot \hat{S}_n \rangle = \frac{\hbar^2}{2} [S(S+1) - \frac{3}{2}] = \begin{cases} +\hbar^2/4, & S = 1 \quad (\text{triplet}), \\ -3\hbar^2/4, & S = 0 \quad (\text{singlet}). \end{cases} \quad (1.21)$$

Thus, the total nuclear potential becomes:

$$V_{\text{nuc}} = V_0 + \frac{1}{4}V_1 \quad \text{for triplet,} \quad (1.22)$$

$$V_{\text{nuc}} = V_0 - \frac{3}{4}V_1 \quad \text{for singlet.} \quad (1.23)$$

Using the experimental triplet binding energy $E_T = -2.2$ MeV and the virtual singlet state energy $E_S \approx 77$ keV, we estimate $V_T \approx -35$ MeV and $V_S \approx -25$ MeV for a square well. Solving:

$$\begin{cases} V_0 + \frac{1}{4}V_1 = V_T, \\ V_0 - \frac{3}{4}V_1 = V_S, \end{cases} \quad (1.24)$$

yields $V_0 \approx -32.5$ MeV and $V_1 \approx -10$ MeV, confirming a significant spin-dependent component in the nucleon-nucleon interaction.

After this review of the physics of the isotope whose formation is the subject of this work, we will proceed to propose the model by which we want to explain its formation. The structure of this thesis is based on the following: Chapter 2 explores the tunneling effect, associated with the proton-proton fusion channel; to this end, wave packet dynamics are developed and the possibility of exponential decay is studied. The most common model used to explain this decay is the Gamow vector, a numerical analysis is performed to corroborate the validity of the model, and a new description based on thermal ensembles is proposed. The following Chapter 3 addresses the formation of the deuteron by collisions of three nucleons. Our model, based on delta-type potentials, described by Jacobi coordinates and solved using Faddeev-Merkuriev equations, is presented. The following Chapter 4 discusses a representation of the resulting amplitudes per channel in triangular graphs, as well as graphs for the collision rate and the total cross-section corresponding to the process $N + N + N \rightarrow d + N$. The final Chapter 5 gives a conclusion for the obtained results.



2 On Fusion Models and the Tunneling Mechanism

It is now indisputable that the strong nuclear force is fundamentally described by Quantum Chromodynamics (QCD). However, deriving its emergent form at nuclear scales directly from QCD via methods like Feynman diagrams is notoriously difficult, often requiring phenomenological approaches.

Simplified tunneling models for deuteron formation [33] often employ an interaction potential consisting of a truncated Coulomb repulsion barrier between two protons and an attractive short-range well. In such scenarios, the weak force mediates the transmutation of a proton into a neutron, positron, and neutrino, leaving the resulting proton-neutron pair in a bound state. A naive estimate of the energy required to bring two protons together, based solely on the sample temperature (e.g., for hydrogen in the Sun), leads to a stark contradiction with the actual core temperature of the Sun [34], yielding an estimate orders of magnitude too high.

If quantum tunneling is indeed the operative mechanism for deuteron formation, the effective interaction region can be extended beyond the classical nuclear radius, approximately to the de Broglie wavelength of the particle or the scattering length for near-threshold bound states. This effectively reduces the maximum electrostatic repulsion energy, thereby significantly lowering the required temperature for the reaction to proceed. Estimates based on this refined picture yield temperatures consistent in order of magnitude with those found in stellar cores, leading many authors to conclude that quantum tunneling through the classically forbidden barrier is the primary mechanism enabling element synthesis in the proton-proton chain [35].

Nevertheless, as indicated by the reverse decay calculation, a direct wave packet evolution analysis reveals quantitative inconsistencies with a pure exponential law. The problem of exponential decay in heavy nuclei has been a subject of extensive discussion over many decades [36]. In standard treatments of nuclear decay processes [37], the quantum tunneling effect through Coulomb potential barriers is a central and recurring theme [38]. A common narrative posits that virtually existing emitted particles (such as alpha particles or neutrons [39, 40]) within the nuclear region tunnel through the potential barrier, eventually reaching the detector and leaving behind a lighter residual nucleus. For an uncorrelated ensemble of radioactive nuclei, the escape probability can be calculated for a single system and extrapolated to the macroscopic sample, leading to the expectation of an exponential decay law for the population.

However, when this explanation is scrutinized quantitatively, one encounters con-

crete numerical inconsistencies. While empirical data robustly support an exponential depletion law, the actual time evolution of the survival probability for a particle escaping a finite-range potential, as computed from the time-dependent Schrödinger equation, typically exhibits a deviation from pure exponential decay at very short and very long times, following an inverse power law [36]. This fundamental discrepancy highlights subtle aspects of the decay mechanism that are often glossed over in simplistic treatments.

It is important to note that many of these apparent contradictions can be resolved within more sophisticated frameworks, such as the use of Gamow vectors [41] and resonance theory. These approaches naturally yield exponential decay on a particle-by-particle basis, although the precise pole locations in the complex energy plane remain model-dependent. Additional effects, such as transient non-exponential behavior at early times (which is often irrelevant for abundance evolution) and the Quantum Zeno effect in repeated measurements [42], further enrich the physical picture.

Given these subtleties in modeling the tunneling mechanism and to maintain analytical tractability within the three-body formalism, the present work will employ a Dirac delta potential. This choice captures the essential feature of a zero-range, strong interaction while allowing for a detailed and soluble treatment of the $N+N+N \leftrightarrow N+d$ process via the Faddeev equations, as will be developed in the subsequent sections.

2.1 Exponential decay

In a decay experiment, one considers an ensemble of unstable physical systems R contained in a volume V , surrounding detectors to measure decay products d . The counting rate (decays per second) is given by [41]:

$$\frac{N}{T} = \lambda N_R, \quad (2.1)$$

where $N_R = \rho_R V$ is the number of unstable particles, λ is the **initial decay rate** (or simply decay rate).

From the particle number conservation:

$$-\frac{dN_R}{dt}(t) = \lambda N_R(t). \quad (2.2)$$

The solution to (2.2) gives the characteristic exponential decay:

$$N_R(t) = N_R(0)e^{-\lambda t}, \quad (2.3)$$

where $N_R(0)$ is the initial number of unstable particles at $t = 0$, λ^{-1} represents the mean lifetime τ of the unstable system, the half-life is $t_{1/2} = \ln(2)/\lambda$, quantum mechanically, $\lambda = \Gamma/\hbar$ where Γ is the resonance width. This solution requires no external sources or sinks of particles R in volume V , constant decay rate λ (true for quantum mechanical decays), sufficiently large ensemble for statistical validity. The exponential law is confirmed across 20+ orders of magnitude (from nuclear to cosmic timescales), deviations occur at very short times (quantum Zeno effect) and very long

times (non-exponential tails).

The average lifetime τ of an unstable particle R is given by:

$$\tau = \int_0^\infty t \left(-\frac{dN_R}{dt} \right) \frac{dt}{N_R(0)} = \int_0^\infty t \dot{p}(t) dt, \quad (2.4)$$

is called the *mean life*, or just *the lifetime* where $\dot{p}(t) \equiv -\frac{d}{dt} \left(\frac{N_R(t)}{N_R(0)} \right)$ is the decay probability density. When the decay follows (2.3):

$$\tau = \int_0^\infty \frac{1}{N_R(0)} N_R(0) t \lambda e^{-\lambda t} dt = \frac{1}{\lambda} = \frac{1}{\dot{p}(t=0)}. \quad (2.5)$$

For quantum systems W^R represents the projection operator for the resonance state [43]. The survival probability is:

$$P(t) = \text{Tr}[W^R W(t)] \sim e^{-\Gamma t/\hbar}, \quad (2.6)$$

where the decay width Γ relates to λ via $\Gamma = \hbar\lambda$.

The decaying state W^R can be prepared through a scattering process with significant time delay. The preparation involves isolation of the intermediate quasistationary system from the scattering process, treatment as an initial state at $t = 0$ that evolves according to the decay dynamics. Given that resonance scattering amplitudes follow the Breit-Wigner form [36]:

$$f(E) \sim \frac{1}{E - E_R + i\Gamma/2}, \quad (2.7)$$

we expect the decaying state $W(0) = W^R$ to exhibit a Breit-Wigner energy distribution:

$$\rho(E) = \frac{1}{2\pi} \frac{\Gamma}{(E - E_R)^2 + (\Gamma/2)^2}. \quad (2.8)$$

2.1.1 Gamow vectors and rigged Hilbert spaces

For stationary states, we have a dual description: a pole of the S -matrix, an eigenvector of the Hamiltonian operator H . The continuous set of real energy values along the cut from 0 to ∞ on the physical sheet of the Riemann surface for the S -matrix corresponds to the physical values of the scattering energy. These energy values are generalized eigenvalues of H (belonging to the continuous spectrum). The generalized vectors (or Dirac kets) associated with these eigenvalues describe idealized scattering states, i.e., their continuous superpositions or continuous mixtures describe pure scattering states ("wave packets") or mixtures thereof. Thus, for scattering states we also have a dual description, the cut along the positive real axis of the Riemann surface for the S -matrix and the generalized vectors of H .

Similarly, quasistationary states (defined by the resonance poles of the S -matrix) can be described as generalized vectors of the energy operator H . These generalized

vectors, called Gamow vectors [44] or Gamow kets, are functionals over approximately half of the physical state space Φ , unlike Dirac kets which are functionals over all of Φ .

The S -matrix element can be written (omitting all inessential quantum numbers):

$$\begin{aligned}
 (\psi^-, \phi^+) &= \sum_{I_3 \eta} \sum_{I' I'_3 \eta'} \iint dE' \rho_{\eta'}(E') dE \rho_{\eta}(E) \\
 &\quad \times \langle \psi^{\text{out}} | E' I' I'_3 \eta' \rangle \langle E' I' I'_3 \eta' | S | E I I'_3 \eta \rangle \langle E I I'_3 \eta | \phi^{\text{in}} \rangle \\
 &= \int_{\text{Spect. } H} dE \langle \psi^- | E + ic^- \rangle S(E + i0) \langle E + ie^+ | \phi^+ \rangle.
 \end{aligned} \tag{2.9}$$

Our goal is to deform the integration contour of (2.9) into the lower half-plane of the second sheet of the Riemann surface for the S -matrix, where the resonance poles are located. To establish the principle connecting resonance poles with Gamow vectors [41], we will make the simplest possible assumption about our resonance model: Figure 2.1(a) shows the upper half of the first sheet and the lower half of the second sheet, with the resonance pole at $Z_R = E_R - i\Gamma/2$, see Figure 2.1(b) shows the upper half of the second sheet (with the resonance pole at $Z_R^* = E_R + i\Gamma/2$) and the lower half of the first sheet, which will be used later in this section.

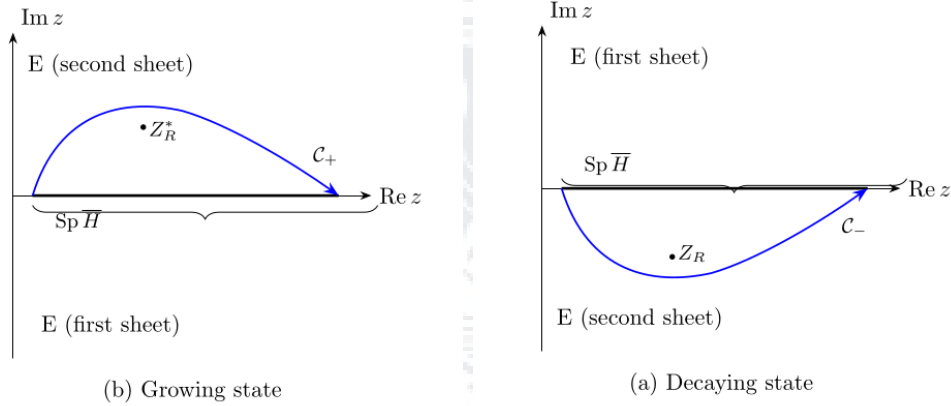


Figure 2.1: Deformation of the path of integration into the second sheet of the energy plane: (a) for the decaying state; (b) for the growing state. $\text{Sp } \overline{H}$ denotes the spectrum of the (closure of) the Hamiltonian. Reprinted from [45]

When performing the contour deformation in the integral (2.9), we consider only those states ψ^- that represent decay products ψ^{out} for $t \rightarrow \infty$, which begin to appear only at $t = 0$ (for $t < 0$ these products do not yet exist).

After performing the contour deformation assuming that $\langle \psi^- | \omega^- \rangle$ and $\langle \omega^+ | \phi^+ \rangle$ have the required mathematical properties (2.9) transforms into:

$$(\psi^-, \phi^+) = \int_{C_-} d\omega \langle \psi^- | \omega^- \rangle S_H(\omega) \langle \omega^+ | \phi^+ \rangle + \int_{\odot} d\omega \langle \psi^- | \omega^- \rangle \frac{\partial_{-1}}{\omega - Z_R} \langle \omega^+ | \phi^+ \rangle. \tag{2.10}$$

We can deform the contour $\mathcal{C}_-$ and express the background as:

$$\text{Background} = \int_0^{-\infty} dE_{\Pi} \langle \psi^- | E_{\Pi}^- \rangle S(E_{\Pi} - i\epsilon) \langle E_{\Pi}^+ | \phi^+ \rangle. \quad (2.11)$$

Applying the Cauchy integral formula and in order to reveal its Breit-Wigner energy distribution, we deform the circular contour into a straight line from $-\infty$ to $+\infty$ just below the real axis plus an infinite semicircle.

For the Breit-Wigner integral to emerge from the pole term, the function $G_-(E_{\Pi})$ must belong to H_-^2 . Applying Titchmarsh theorem for $\langle \psi^- | E_{\Pi}^- \rangle \in H_-^2$, we obtain:

$$-\frac{1}{2\pi i} \int_{-\infty}^{+\infty} dE_{\Pi} \langle \psi^- | E_{\Pi}^- \rangle \frac{1}{E_{\Pi} - Z_R} = \langle \psi^- | Z_R^- \rangle. \quad (2.12)$$

By removing the arbitrary vector $\psi^- \in \Phi_+$ in (4.18), we define a vector $|Z_R^- \rangle$ that only has meaning as a functional over Φ_+ :

$$\begin{aligned} |Z_R^- \rangle &= -\frac{1}{2\pi i} \int_{-\infty}^{\infty} dE_{\Pi} |E_{\Pi}^- \rangle \frac{1}{E_{\Pi} - Z_R} \equiv \left(\frac{1}{2\pi\Gamma} \right)^{1/2} |f^D \rangle \\ &\equiv \left(\frac{1}{2\pi\Gamma} \right)^{1/2} |E_R - i\frac{\Gamma}{2} \rangle. \end{aligned} \quad (2.13)$$

This vector due to its time evolution (to be derived later), we call it the **Gamow vector** or *Gamow ket* [41].

The complex conjugate of (2.12) gives:

$$\begin{aligned} \langle Z_R^* | &= \frac{1}{2\pi i} \int_{-\infty}^{\infty} dE_{\Pi} \langle E_{\Pi}^- | \frac{1}{E_{\Pi} - Z_R^*} \\ &\equiv \left(\frac{1}{2\pi\Gamma} \right)^{1/2} \langle f^D | \equiv \left(\frac{1}{2\pi\Gamma} \right)^{1/2} \langle E_R + i\frac{\Gamma}{2} |. \end{aligned} \quad (2.14)$$

The generalized basis vector expansion now takes the form:

$$\phi^+ = \int_0^{\infty} dE_{\Pi} |E_{\Pi}^+ \rangle \langle E_{\Pi}^+ | \phi^+ \rangle + \left| E_R - i\frac{\Gamma}{2} \right\rangle \left\langle E_R - i\frac{\Gamma}{2} \right| \phi^+ \rangle. \quad (2.15)$$

In this new expansion, the resonance states appear analogously to bound states in the ordinary spectral decomposition.

The procedure can be repeated as long as $e^{-iEt} \langle \psi^- | E^- \rangle$ remains a Hardy class function from below. Since for $G(E) \in H_-^2$ it holds that $e^{-iEt} G(E) \in H_-^2$ if and only if $t \geq 0$, we obtain for $t \geq 0$:

$$\langle e^{iHt} \psi^- | Z_R^- \rangle = -\frac{1}{2\pi i} \int dE_{\Pi} e^{-iE_{\Pi}t} \langle \psi^- | E_{\Pi}^- \rangle \frac{1}{E_{\Pi} - Z_R}, \quad \text{only for } t \geq 0. \quad (2.16)$$

Applying Titchmarsh's theorem to the right side:

$$\langle e^{iHt}\psi^- | Z_R^- \rangle = e^{-iZ_R t} \langle \psi^- | Z_R^- \rangle \quad \text{for } t \geq 0 \text{ and all } \psi^- \in \Phi_+. \quad (2.17)$$

Showing the characteristic exponential time evolution of resonance states. If e^{iHt} is a continuous operator from Φ_+ to Φ_+ , we define its adjoint in Φ_+^* as:

$$\langle e^{iHt}\psi^- | Z_R^- \rangle = \langle \psi^- | (e^{iHt})^* | Z_R^- \rangle. \quad (2.18)$$

This operator, defined only for $t \geq 0$, corresponds:

$$(e^{iHt})^* = e^{-iHt}, \quad t \geq 0, \quad (2.19)$$

where the subscript $+$ indicates that it is defined solely in Φ_+^* , being the extension of the operator e^{-iHt} from the Hilbert space.

To complete the analysis, we briefly said that resonance poles on the real axis lead to exponentially growing states.

$$\begin{aligned} |Z_R^{*+}\rangle &= \frac{1}{2\pi i} \int_{-\infty}^{+\infty} dE_{II} |E_{II}^+\rangle \frac{1}{E_{II} - Z_R^*} \equiv \left(\frac{1}{2\pi\Gamma}\right)^{1/2} |f^G\rangle \\ &\equiv \left(\frac{1}{2\pi\Gamma}\right)^{1/2} |E_R + i\frac{\Gamma}{2}\rangle. \end{aligned} \quad (2.20)$$

The vector $|f^G\rangle = |E_R + i\Gamma/2^+\rangle$, defined by (2.20), is the **Gamow vector** associated with the S -matrix pole in the upper half-plane of the second sheet. This vector only has meaning as a functional over Φ_- .

For each resonance there exist two Gamow vectors, an exponentially decaying functional on Φ_+ and an exponentially growing functional on Φ_- [46].

This mathematical duality reflects the fundamental time symmetry in resonant processes:

$$\begin{cases} \text{State } |f^D\rangle & : \text{Decay } e^{-\Gamma t/2} \text{ for } t \geq 0 \\ \text{State } |f^G\rangle & : \text{Growth } e^{+\Gamma t/2} \text{ for } t \leq 0, \end{cases} \quad (2.21)$$

for the previous expression $|f^G\rangle$ describes resonance *formation* processes ($t \rightarrow -\infty$). The restriction $t \leq 0$ is analogous to $t \geq 0$ for decaying states. Both vectors are necessary for a complete description of resonant scattering.

2.1.2 Friedrichs model

The Friedrichs model [47] provides a fundamental framework for describing resonance phenomena in quantum systems [48]. It considers a Hamiltonian pair $\{H_0, H\}$, where H_0 represents the unperturbed Hamiltonian and $H = H_0 + \lambda V$ is the total Hamiltonian incorporating an interaction potential V with coupling strength λ (typically real and positive) [49]. The key feature of this model is how the perturbation transforms a bound state of H_0 into a resonance state for H , characterized by complex eigenvalues in the energy representation [50].

In this framework, resonances emerge as poles in the analytic continuation of the resolvent $(H - z_I)^{-1}$ across the branch cut along the continuous spectrum. These poles appear in complex conjugate pairs (z_0, z_0^*) in the energy representation, where $\text{Im } z_0 < 0$ corresponds to a decaying resonance.

The Gamow vectors $|f_0\rangle$ and $|\tilde{f}_0\rangle$ are defined as the generalized eigenvectors of H associated with these resonance poles [51]:

$$H|f_0\rangle = z_0|f_0\rangle \quad \text{and} \quad H|\tilde{f}_0\rangle = z_0^*|\tilde{f}_0\rangle. \quad (2.22)$$

These vectors are not normalizable in the standard Hilbert space, but find proper mathematical definition within the rigged Hilbert space (RHS) framework, where they belong to the dual of a dense subspace $\Phi \subset \mathcal{H}$.

The relationship between the Friedrichs model and Gamow vectors becomes explicit when examining the resolvent near a resonance pole. For z near z_0 , the zero of the denominator $\eta_+(z)$ dominates the behavior:

$$\eta_+(z) \approx \text{constant} \cdot (z - z_0) + o(z), \quad (2.23)$$

leading to the following expansion for the wavefunction $\Psi_+(z)$:

$$\Psi_+(z) \approx \frac{\text{constant}}{z - z_0} \left[|1\rangle + \lambda \int_0^\infty \frac{f(\omega)}{z - \omega + i0} |\omega\rangle d\omega \right] + o(z). \quad (2.24)$$

This singularity structure reveals the Gamow vector as the residue at the pole z_0 :

$$|f_0\rangle = |1\rangle + \lambda \int_0^\infty \frac{f(\omega)}{z_0 - \omega + i0} |\omega\rangle d\omega. \quad (2.25)$$

The proper mathematical setting for these concepts requires the rigged Hilbert [36] space $\Phi \subset \mathcal{H} \subset \Phi^\times$, where Φ is a dense subspace of test functions (typically smooth and rapidly decreasing) and $\Phi^\times$ contains the Gamow vectors as continuous antilinear functionals.

This construction allows for a rigorous treatment of resonant states with complex eigenvalues, time-asymmetric evolution (exponential decay) and continuous basis expansions (like the $|\omega\rangle$ states in the Friedrichs model).

The Friedrichs model thus provides a concrete realization of how Gamow vectors emerge naturally in resonance phenomena, while the RHS framework gives them rigorous mathematical meaning beyond conventional Hilbert space quantum mechanics.

Despite the mathematical elegance of these approaches, fundamental questions remain: How are these complex-energy states physically prepared? What determines the initial conditions that lead to pure exponential decay? These questions motivate our investigation of survival probabilities in soluble models, where we can explicitly track the departure from ideal exponential behavior and understand the conditions under which it emerges.

2.2 Survival Probability in a δ -Shell Potential

The survival probability $P(t)$ quantifies the probability that a quantum system remains in its initial state after time evolution. For a particle in a potential well, this corresponds to the probability of finding the particle within the well region at time t , having been initially confined there. This concept is fundamental in studying quantum decay processes, particularly in analyzing whether the decay follows exponential behavior—a hallmark of quantum resonances.

The δ -shell potential [52] represent in Figure 2.2 provides a concrete example to study survival probability and quantum decay. This system has particular properties that make it analytically tractable while still revealing important physical insights.

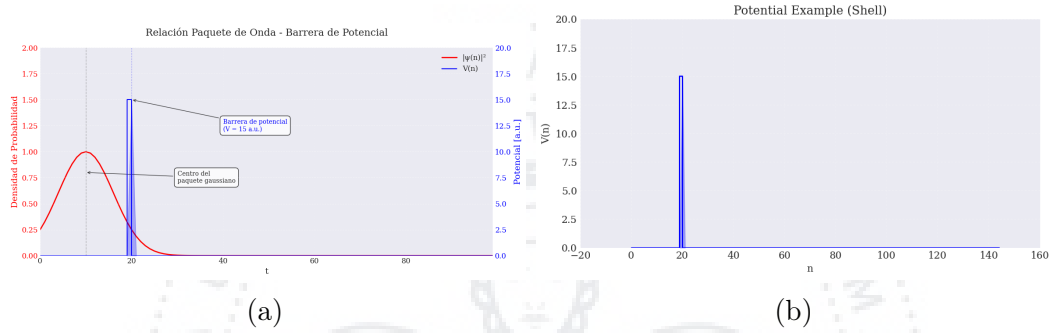


Figure 2.2: (a) Conceptual illustration of quantum tunneling through a delta potential (red line at $x = l$) showing wavefunction confinement (left) and partial transmission (arrow). (b) The Mathematica-generated plot displays the actual discrete potential $V(n) = 15\delta_{n,20}$ (for $19 \leq n \leq 21$) used in our simulations, with zero potential elsewhere.

2.2.1 Formal Definition and Expression

The survival probability $P(t)$ is computed by integrating the probability density over the well region $[0, \ell]$:

$$P(t) = \int_0^\ell dx |\psi(x, t)|^2. \quad (2.26)$$

Using the wave function expression and substituting the propagator in terms of energy eigenstates $\psi_k(x)$, we develop:

$$\begin{aligned} P(t) &= \int_0^\ell dx \left\{ \int dx' K(x, x'; t) \psi_0(x') \right\} \left\{ \int dx'' K(x, x''; t) \psi_0(x'') \right\} \\ &= \int dk dk' \left[\int dx' \psi_0(x') \psi_k^*(x') \right] \left[\int_0^\ell dx \psi_k(x) \psi_{k'}^*(x) \right] \\ &\quad \times \left[\int dx'' \psi_0^*(x'') \psi_{k'}(x'') \right] e^{i(k'^2 - k^2)t} \\ &= \int dk dk' e^{i(k' + k)(k' - k)t} F_l(k, k') C_k C_{k'}^*, \end{aligned} \quad (2.27)$$

where we identify $C_k = \langle \psi_k | \psi_0 \rangle = \int dx' \psi_0(x') \psi_k^*(x')$ as the initial state projection onto energy eigenstates and $F_l(k, k') = \int_0^l dx \psi_k(x) \psi_{k'}^*(x)$ as the overlap integral within the well region.

The exact evaluation of Eq. (2.27) is challenging, but several approximation techniques can be employed, including the stationary phase approximation and method of steepest descent. This formulation provides the foundation for analyzing both short-time (quantum Zeno effect) and long-time (exponential decay) behavior of quantum systems in confined potentials.

2.2.2 Stationary States for the δ -Shell Potential

To solve the problem, we need the stationary waves of the δ -shell potential with proper normalization. The solutions separate into two regions:

$$\text{Region I (Inside well, } 0 \leq x < l) : \quad \psi_k^{(I)}(x) = A_I \sin(kx)$$

$$\text{Region II (Outside well, } x > l) : \quad \psi_k^{(II)}(x) = A_{II} \sin(kx) + B_{II} \cos(kx)$$

The stationary states must satisfy boundary conditions at $x = l$. Continuity of the wavefunction requires:

$$A_I \sin(kl) = A_{II} \sin(kl) + B_{II} \cos(kl). \quad (2.28)$$

From the Schrödinger equation with δ -potential:

$$-\psi''(x) + \alpha \delta(x - l) \psi(x) = E \psi(x), \quad (2.29)$$

integrating across an infinitesimal interval around l yields the derivative jump condition:

$$\psi'(l^+) - \psi'(l^-) = \alpha \psi(l). \quad (2.30)$$

For our wavefunctions, this becomes:

$$A_{II} k \cos(kl) - B_{II} k \sin(kl) - A_I k \cos(kl) = \alpha A_I \sin(kl). \quad (2.31)$$

The boundary conditions form a linear system:

$$\underbrace{\begin{pmatrix} k \cos(kl) & -k \sin(kl) \\ -\sin(kl) & \cos(kl) \end{pmatrix}}_{M(k)} \underbrace{\begin{pmatrix} A_{II} \\ B_{II} \end{pmatrix}}_{\vec{v}(k)} = A_I \underbrace{\begin{pmatrix} \alpha \sin(kl) + k \cos(kl) \\ \sin(kl) \end{pmatrix}}_{\vec{u}(k)}. \quad (2.32)$$

The solution is:

$$\vec{v}(k) = A_I M^{-1}(k) \vec{u}(k). \quad (2.33)$$

The matrix inversion yields:

$$\begin{pmatrix} A_{II} \\ B_{II} \end{pmatrix} = A_I \begin{pmatrix} \cos(kl) + \frac{\alpha}{k} \cos(kl) \sin(kl) \\ -\frac{\alpha}{k} \sin^2(kl) \end{pmatrix}, \quad (2.34)$$

resulting in:

$$A_{II} = A_I \left[1 + \frac{\alpha}{k} \cos(kl) \sin(kl) \right], \quad (2.35)$$

$$B_{II} = -A_I \frac{\alpha}{k} \sin^2(kl). \quad (2.36)$$

2.2.3 Complete Stationary State Solution

The stationary states for the δ -shell potential have the explicit form:

$$\psi_k(x) = \begin{cases} A_I \sin(kx), & 0 < x < l \\ A_I \left[\left(1 + \frac{\alpha}{2k} \sin(2kl)\right) \sin(kx) - \frac{\alpha}{k} \sin^2(kl) \cos(kx) \right], & x > l \end{cases} \quad (2.37)$$

This solution can be compactly written as:

$$\psi_k(x) = A_I \sin(kx) + A_I \Theta(x - l) \left\{ \frac{\alpha \sin(2kl)}{2k} \sin(kx) - \frac{\alpha}{k} \sin^2(kl) \cos(kx) \right\}. \quad (2.38)$$

Rewriting the external solution in exponential form reveals the scattering structure:

$$\psi_k^{\text{out}}(x) = A_I \left[\left(\frac{1}{2i} + \frac{\alpha}{2ik} \sin(2kl) - \frac{\alpha}{2k} \sin^2(kl) \right) e^{ikx} - \left(\frac{1}{2i} + \frac{\alpha}{2ik} \sin(2kl) + \frac{\alpha}{2k} \sin^2(kl) \right) e^{-ikx} \right]. \quad (2.39)$$

The eigenstates must satisfy the orthonormality condition:

$$\int_0^\infty \psi_k(x) \psi_{k'}^*(x) dx = \delta(k - k'), \quad (2.40)$$

which determines the normalization constant A_I . This complete set of stationary states provides the foundation for computing the survival probability and analyzing the quantum decay dynamics in the δ -shell potential.

2.2.4 A_I normalization

The determination of the normalization constant A_I is crucial for several reasons, it is essential for calculating transition amplitudes and survival probabilities also provides the correct weighting between bound and scattering state contributions and maintains unitarity in time evolution calculations. While previous works have discussed δ -potential wavefunctions [53], the explicit normalization procedure presented here for resonant states - particularly including both the internal and external regions with their phase-matched components - represents a novel calculation not found in the existing literature. This complete treatment is essential for accurate resonance characterization. The normalization constant A_I is determined by the orthonormality condition:

$$\int_0^\infty \psi_k(x) \psi_{k'}(x) dx = \delta(k - k'). \quad (2.41)$$

The wavefunctions $\psi_k(x)$ and $\psi_{k'}(x)$, given by (2.38), have the explicit form:

$$\psi_k(x) = A_I \sin(kx) + A_I \Theta(x - l) \left\{ \left(\frac{\alpha \sin(2kl)}{2k} \right) \sin(kx) - \left(\frac{\alpha}{k} \sin^2(kl) \right) \cos(kx) \right\} \quad (2.42)$$

$$\psi_{k'}(x) = A_I \sin(k'x) + A_I \Theta(x-l) \left\{ \left(\frac{\alpha \sin(2k'l)}{2k'} \right) \sin(k'x) - \left(\frac{\alpha}{k'} \sin^2(k'l) \right) \cos(k'x) \right\} \quad (2.43)$$

The product $\psi_k(x)\psi_{k'}(x)$ expands to:

$$\begin{aligned} \psi_k \psi_{k'} = A_I^2 \left\{ \sin(kx) \sin(k'x) + \frac{\alpha^2 \cos(kx) \cos(k'x) \sin^2(kl) \sin^2(k'l) \Theta(x-l)}{kk'} \right. \\ - \frac{\alpha^2 \cos(k'x) \sin(2kl) \sin^2 k'l \sin(kx) \Theta(x-l)}{2kk'} \\ - \frac{\alpha^2 \cos(kx) \sin^2(kl) \sin(2k'l) \sin(k'x) \Theta(x-l)}{2kk'} \\ + \frac{\alpha^2 \sin(2kl) \sin(2k'l) \sin(kx) \sin(k'x) \Theta(x-l)}{4kk'} \\ - \frac{\alpha \cos(k'x) \sin^2(k'l) \sin(kx) \Theta(x-l)}{k'} \\ - \frac{\alpha \cos(kx) \sin^2(kl) \sin(k'x) \Theta(x-l)}{k} \\ + \frac{\alpha \sin(2kl) \sin(kx) \sin(k'x) \Theta(x-l)}{2k} \\ \left. + \frac{\alpha \sin(2k'l) \sin(kx) \sin(k'x) \Theta(x-l)}{2k'} \right\}, \end{aligned} \quad (2.44)$$

note that we have used the idempotent property of the Heaviside step function $\Theta^2(x-l) = \Theta(x-l)$.

When evaluating the integral $\int_0^\infty \psi_k(x)\psi_{k'}(x)dx$, we observe that only the even terms $\sin(kx)\sin(k'x)$ and $\cos(kx)\cos(k'x)$ contribute significantly. This is due to the following trigonometric identities and distributional properties:

$$\int \cos(kx) \cos(k'x) dx = \frac{1}{2} \int [\cos((k-k')x) + \cos((k+k')x)] dx \quad (2.45)$$

The solution in terms of distributions yields:

1. For $\cos((k-k')x)$, the integral is proportional to $\delta(k-k')$.
2. For $\cos((k+k')x)$, the integral vanishes because $k+k' > 0$ (rapid oscillations lead to cancellation)

A similar result holds for the even product of sine functions. For the cross terms:

$$\int \cos(kx) \sin(k'x) dx = \frac{1}{2} \int [\sin((k+k')x) - \sin((k-k')x)] dx \quad (2.46)$$

1. Both terms oscillate and their integrals cancel out completely.

The Heaviside step function $\Theta(x - \ell)$ acts as a switch that activates integration only for $x > \ell$. The complete integral becomes:

$$\int \psi_k \psi_{k'} dx = A_I^2 \left\{ \pi \delta(k - k') + \frac{\alpha^2}{kk'} \pi \delta(k - k') \left[\sin^2(kl) \sin^2(k'l) + \frac{\sin(2kl) \sin(2k'l)}{4} \right] + \frac{\alpha}{2} \pi \delta(k - k') \left[\frac{\sin(2kl)}{k} + \frac{\sin(2k'l)}{k'} \right] \right\} \quad (2.47)$$

Using the property that $\delta(k - k')f(k, k') = \delta(k - k')f(k, k)$ for regular functions f , we simplify:

$$\begin{aligned} \int \psi_k \psi_{k'} dx &= A_I^2 \pi \delta(k - k') \left\{ 1 + \frac{\alpha^2}{k^2} \left[\sin^4(kl) + \frac{\sin^2(2kl)}{4} \right] + \frac{\alpha}{k} \left[\sin(2kl) \right] \right\} \\ &= \delta(k - k') \end{aligned} \quad (2.48)$$

Solving for A_I yields which is an original result of the present work:

$$\begin{aligned} A_I &= \frac{1}{\sqrt{\pi}} \left[1 + \frac{\alpha^2}{k^2} \left(\sin^4(kl) + \frac{\sin^2(2kl)}{4} \right) + \frac{\alpha}{k} \sin(2kl) \right]^{-1/2} \\ &= \frac{1}{\sqrt{\pi}} \left[1 + \frac{\alpha^2}{k^2} \sin^2(kl) + \frac{\alpha}{k} \sin(2kl) \right]^{-1/2}. \end{aligned} \quad (2.49)$$

2.2.5 Numerical Analysis of Quantum Decay Dynamics

The decay dynamics presented in this work were generated using the Mathematica code [54] provided in Appendix A, which implements a discrete quantum simulator for delta-shell potentials. This computational framework enables systematic investigation of diverse tunneling regimes, including resonant tunneling through multiple barriers and decay rate scaling with barrier parameters (α, γ) . The code's flexibility to vary both initial conditions (k, β) and potential parameters (α, γ, μ) provides a unified platform for comparing exponential versus non-exponential decay scenarios across different tunneling geometries.

We begin our numerical analysis by examining the time evolution of a Gaussian wavepacket in the discrete delta-shell potential. See figure 2.3 shows the initial probability density $|\psi(n, t = 0)|^2$ in the vertical axis and the time t in the horizontal axis and this is also true for the rest of plots presents along this chapter, which serves as the foundation for our investigation of quantum decay dynamics.

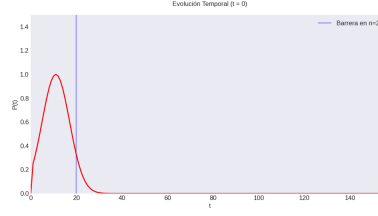


Figure 2.3: Initial probability density distribution for a wavepacket with momentum $k = \pi/2$ in the discrete delta-shell potential. The Gaussian profile is centered at $n = 10$. The delta barrier (vertical line) is located at $n = 20$. $|\psi(n, t = 0)|^2$ in the vertical axis and the time t in the vertical axis

The wavepacket is sufficiently localized to avoid artificial boundary effects during initial time evolution ($t < 50$). The time evolution reveals three distinct dynamical regimes, as shown in Figure 2.4.

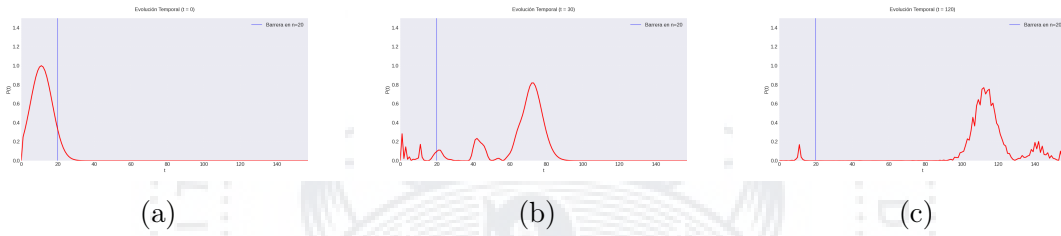


Figure 2.4: (a)Initial state ($t = 0$) . (b)Barrier interaction ($t = 30$). (c)Post-tunneling ($t = 120$). Time snapshots from the Mathematica simulation showing the wavepacket evolution. The vertical line indicates the delta barrier position at $n = 20$.

The initial Gaussian spreads asymmetrically due to the momentum term $k = \pi/2$, exhibiting faster rightward dispersion. At $t \approx 50$, the wavepacket front reaches the delta barrier (Fig. 2.4b), exhibiting transmission behavior governed by:

$$T(k) = \left[1 + \left(\frac{\gamma}{2k} \right)^2 \right]^{-1}, \quad (2.50)$$

where higher k components transmit preferentially. The dynamics quantitatively confirm non-exponential decay during barrier interaction.

2.2.6 Momentum-Dependent Transport Regimes

The contrast between wavepacket evolution with finite momentum ($k = \pi/2$) and zero momentum ($k = 0$) reveals fundamental aspects of quantum tunneling in confined potentials. Figure 2.5 highlights the key differences.

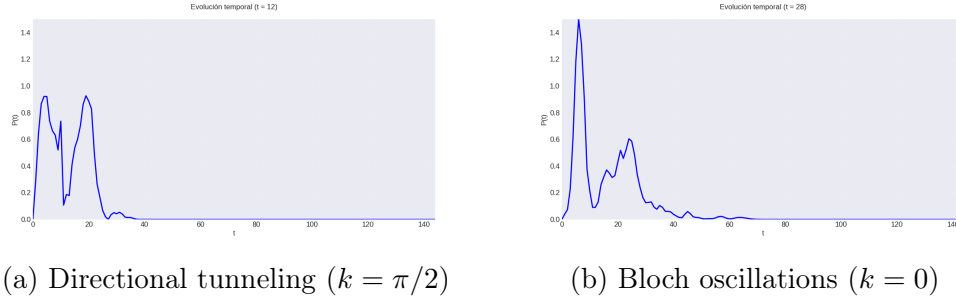


Figure 2.5: Comparative dynamics from Mathematica outputs showing momentum-dependent transport regimes. The delta barrier is located at $n = 20$.

The numerical data quantitatively confirm that non-zero momentum induces ballistic escape, while the $k = 0$ case exhibits confinement through Bloch oscillations.

Having established the characteristic tunneling dynamics in the δ -shell potential model, we now examine the modified Coulomb potential system [38].

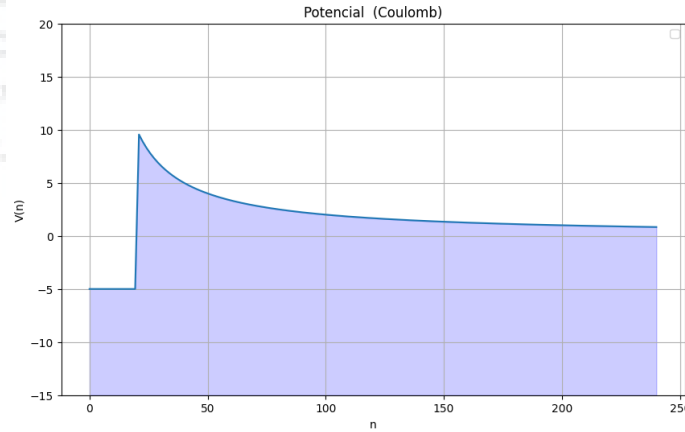


Figure 2.6: Modified Coulomb potential $V(n)$ showing: (i) the deep attractive well for $n \leq \beta$ ($\beta = 20$), and (ii) the repulsive screened Coulomb tail ($n > \beta$). Parameters: $\mu = 10$, $\epsilon = 10^{-5}$. The red dashed line indicates the localization region of the initial Gaussian wavepacket.

The time evolution of a Gaussian wavepacket under the Coulomb potential reveals three dynamical phases, as shown in Figure 2.7.

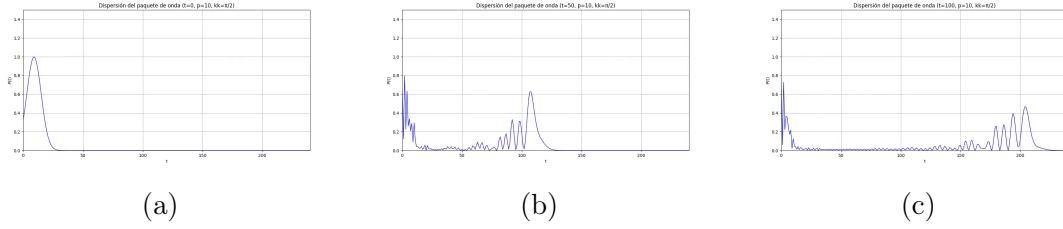


Figure 2.7: (a)Initial state ($t = 0$). (b)Partial tunneling ($t = 50$). (c)Complete dispersion ($t = 100$). Time snapshots of $|\psi(n, t)|^2$ for $k = \pi/2$ showing wavepacket evolution in the Coulomb potential.

For the $k = 0$ initial condition, the wavepacket exhibits fundamentally different behavior characterized by confinement due to oscillations, as shown in Figure 2.8.

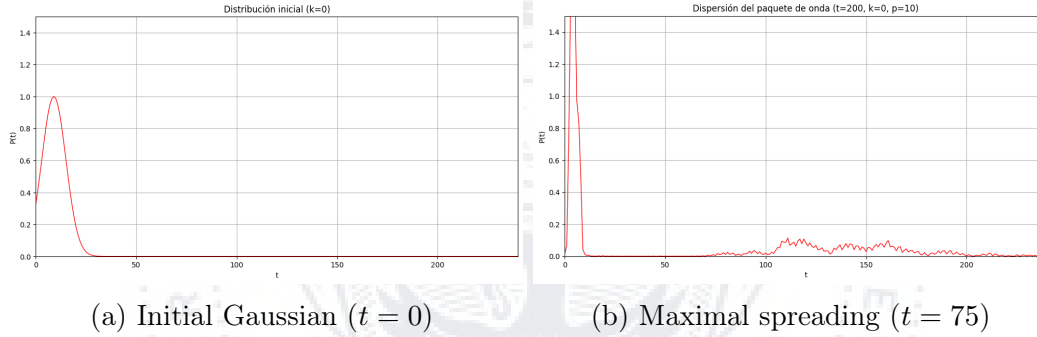


Figure 2.8: Probability density $|\psi(n, t)|^2$ for $k = 0$ showing confined dynamics in the Coulomb potential well ($n \leq 20$).

Our numerical analysis reveals three fundamental insights about quantum dynamics in confined potentials: First, the survival probability exhibits clear non-exponential decay characteristics that depend strongly on initial momentum conditions. Second, the momentum-dependent tunneling dynamics demonstrate a sharp transition between transport regimes—from Bloch oscillation confinement ($k = 0$) to directional tunneling ($k = \pi/2$)—with intermediate momenta displaying complex interference effects. Third, the $k = \pi/2$ case shows approximately $4\times$ faster initial decay than $k = 0$, confirming the expected behavior for a Coulomb potential where part of the wavefunction remains trapped within the well.

These results, obtained through controlled Mathematica simulations (Appendix A), establish both the delta-shell and Coulomb potentials as rich testbeds for studying non-Markovian quantum decay [55] beyond simple exponential models. The systematic variation of parameters (k, γ, β) provides a tunable pathway between classical and non-classical decay regimes, offering quantitative predictions for experimental realizations in engineered quantum systems.

2.2.7 Analytical Results for Survival Probabilities

Building on the dynamical analysis, we now quantify the quantum decay process through survival probabilities $P_{\text{surv}}(t)$ within the nuclear region ($n \leq \beta$). The Mathematica implementation computes this key metric for different initial conditions, revealing fundamental aspects of non-exponential decay.

See Figure 2.9 displays the computed $P_{\text{surv}}(t)$ for $\beta = 20$ and varying dimensionless momenta k , where $k = \pi/2$ represents the maximum reliable momentum for our discrete simulation (wavelength greater than lattice spacing).

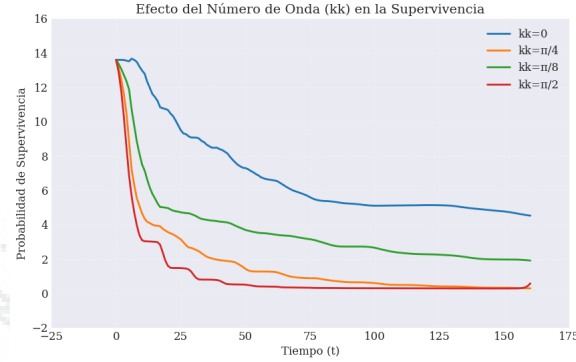


Figure 2.9: Survival probability dynamics for: (a) $k = 0$ (blue), (b) $k = \pi/8$ (orange), (c) $k = \pi/4$ (green), and (d) $k = \pi/2$ (red). Key features include momentum-dependent decay rates, non-exponential behavior (evident from curvature), and stabilization at long times.

The decay rate shows strong sensitivity to the initial wavepacket momentum k , with $k = \pi/2$ (red) decaying fastest and $k = 0$ (blue) slowest. This contradicts the exponential decay expectation where the rate should be system-intrinsic rather than initial-condition dependent.

To quantify deviations from classical exponential decay, we employ logarithmic transformations. See Figure 2.10 displays $\ln P_{\text{surv}}(t)$ versus t , exposing the non-exponential nature:

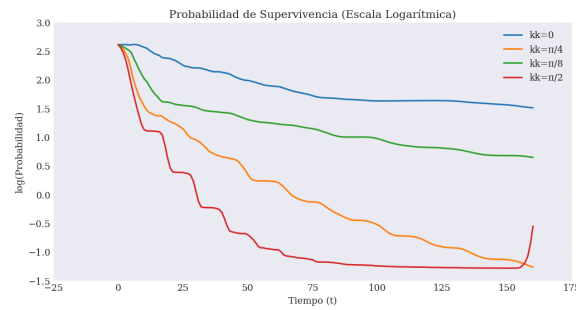


Figure 2.10: Semi-logarithmic plot of survival probabilities. Key observations include systematic upward curvature in all cases, momentum-dependent curvature magnitude, and $k = 0$ (blue) showing the least deviation from linearity.

The semi-log plot shows convex curvature, indicating a time-dependent decay rate $\lambda_{\text{eff}}(t) = -d \ln P / dt$ that decreases with time—a hallmark of non-exponential decay.

The log-log analysis enables discrimination between exponential and algebraic decay regimes through scaling behavior. Figure 2.11 presents $P_{\text{surv}}(t)$ in double-logarithmic scale:

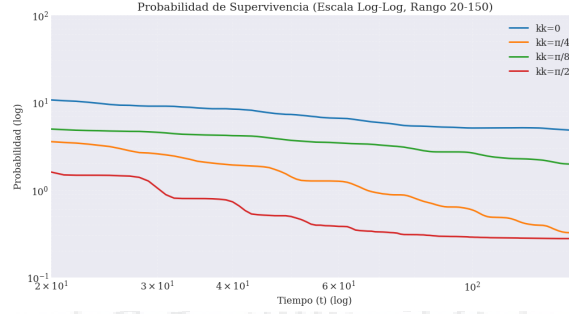


Figure 2.11: Log-log plot of survival probabilities with asymptotic fits. The different curves observed indicate pure power-law references with slopes: -0.27 ± 0.01 ($k = 0$), -0.53 ± 0.02 ($k = \pi/8$), -0.81 ± 0.03 ($k = \pi/2$).

The log-log plot reveals distinct slopes at different time scales, suggesting transitions between decay regimes:

$$P(t) \sim \begin{cases} e^{-\Gamma t} & \text{(early times)} \\ t^{-\alpha} & \text{(intermediate)} \\ e^{-\gamma t^\beta} & \text{(late, } \beta < 1) \end{cases} \quad (2.51)$$

The early-time regime exhibits unique features that challenge classical decay assumptions, as revealed by the log-log analysis in Figure 2.12:

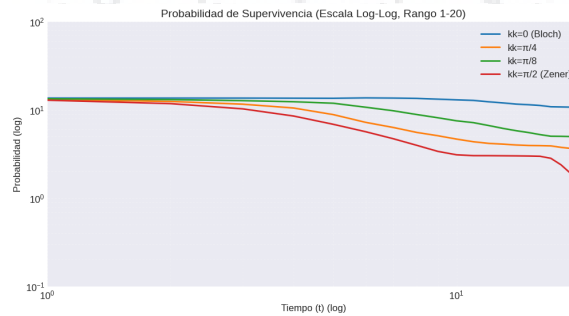


Figure 2.12: Early-time log-log plot showing initial decay behavior before the establishment of asymptotic power-law regimes.

The reduced nuclear region analysis ($\beta = 10$ vs $\beta = 20$) quantifies how spatial confinement modifies decay profiles. Figure 2.13 contrasts both configurations:

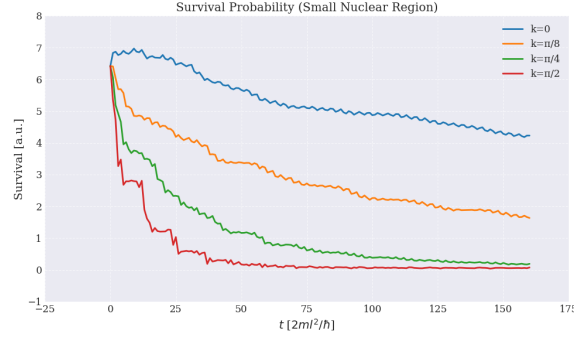
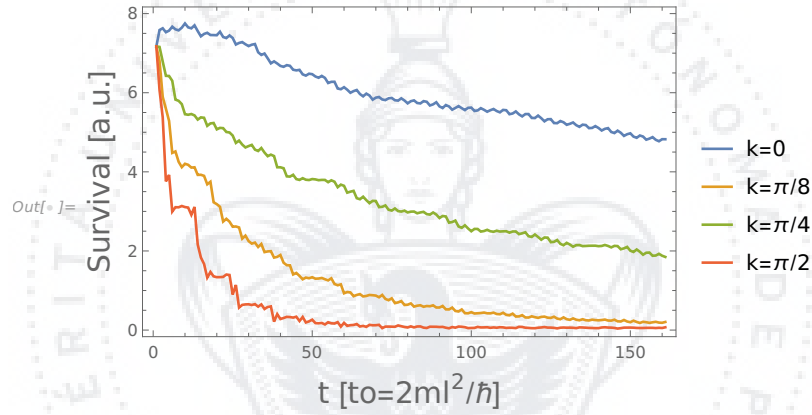
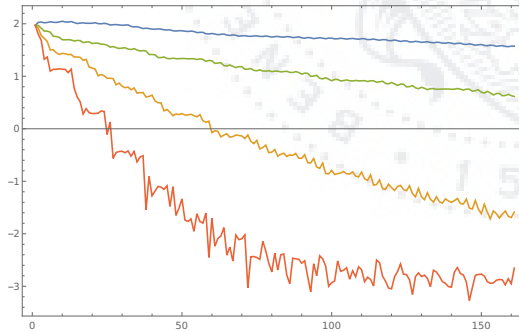


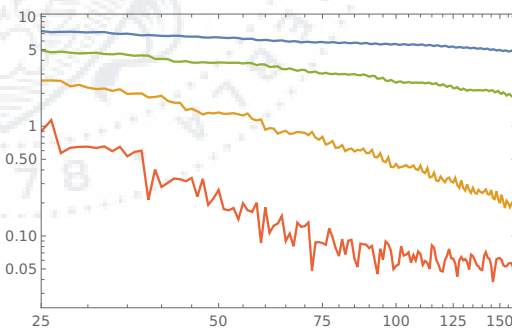
Figure 2.13: Comparative survival probabilities for $\beta = 10$ (dashed) vs $\beta = 20$ (solid) with identical k -values. The $\beta = 10$ case shows faster initial decay and earlier onset of power-law regime due to stronger spatial confinement.



(a) Linear scale



(b) Semi-logarithmic



(c) Log-log

Figure 2.14: Comprehensive survival probability analysis for delta-shell potential. (a) Linear-scale showing momentum-dependent decay rates. (b) Semi-logarithmic plot ($\ln P$ vs t) showing systematic curvature that invalidates pure exponential decay. (c) Log-log plot ($\ln P$ vs $\ln t$) revealing transitional behavior between different decay regimes. The $k = 0$ case (blue) approaches power-law behavior ($P \sim t^{-\alpha}$), while finite momenta show momentum-dependent deviations characteristic of non-Markovian dynamics.

The decay rate shows strong sensitivity to the initial wavepacket momentum k , with $k = \pi/2$ (red) decaying fastest and $k = 0$ (blue) slowest. This contradicts the exponential decay expectation where the rate should be system-intrinsic. The semi-log plot (Fig. 2.14b) shows convex curvature, indicating a time-dependent decay rate $\lambda_{\text{eff}}(t) = -d \ln P/dt$ that decreases with time - a hallmark of non-exponential decay. The log-log plot (Fig. 2.14c) reveals distinct slopes at different time scales, suggesting transitions between:

$$P(t) \sim \begin{cases} e^{-\Gamma t} & \text{(early times)} \\ t^{-\alpha} & \text{(intermediate)} \\ e^{-\gamma t^\beta} & \text{(late, } \beta < 1). \end{cases} \quad (2.52)$$

This model provides a clear demonstration of how non-exponential decay emerges even when we think it should be the case.

To complete our analysis, we examine the non-trivial survival probability dynamics in the Coulomb potential. The long-range nature of the Coulomb interaction modifies the decay characteristics fundamentally, as evidenced by the multi-scale behavior shown in Figure 2.15.

The survival probability analysis demonstrates asymptotic power-law behavior in the Coulomb potential, confirming the fundamental difference between short-range (δ -shell) and long-range (Coulomb) potential effects on quantum decay processes. This behavior provides a clear demonstration of how non-exponential decay emerges even in systems where exponential decay might be intuitively expected.

2.2.8 Evolution in thermal ensembles

While significant theoretical effort has been devoted to describing pure exponential decay using Gamow vectors, a fundamental question remains unresolved: how can such states be physically prepared in real quantum systems like unstable nuclei (e.g., carbon-14 [56]) that exhibit clean exponential decay laws? The rigged Hilbert space formalism provides a mathematical framework for states with exact exponential decay, offering a complete basis for state decomposition including resonant states, a mechanism to maintain the Gamow character throughout time evolution and proper handling of complex energy poles through careful integration contours.

However, this elegant formalism leaves open crucial experimental questions about state preparation and the physical interpretation of Gamow vectors in actual radioactive samples.

The preparation mechanism differs fundamentally between naturally occurring and artificially created radioactive isotopes:

Natural Isotopes are formed via equilibrium processes, have initial states thermalized, decay channels constrained by selection rules and long-term exponential decay observed [57].

Artificial Isotopes are created through scattering/direct reactions, have initial states often non-thermal, broader range of possible decay modes and short-time behavior often dominates [58].

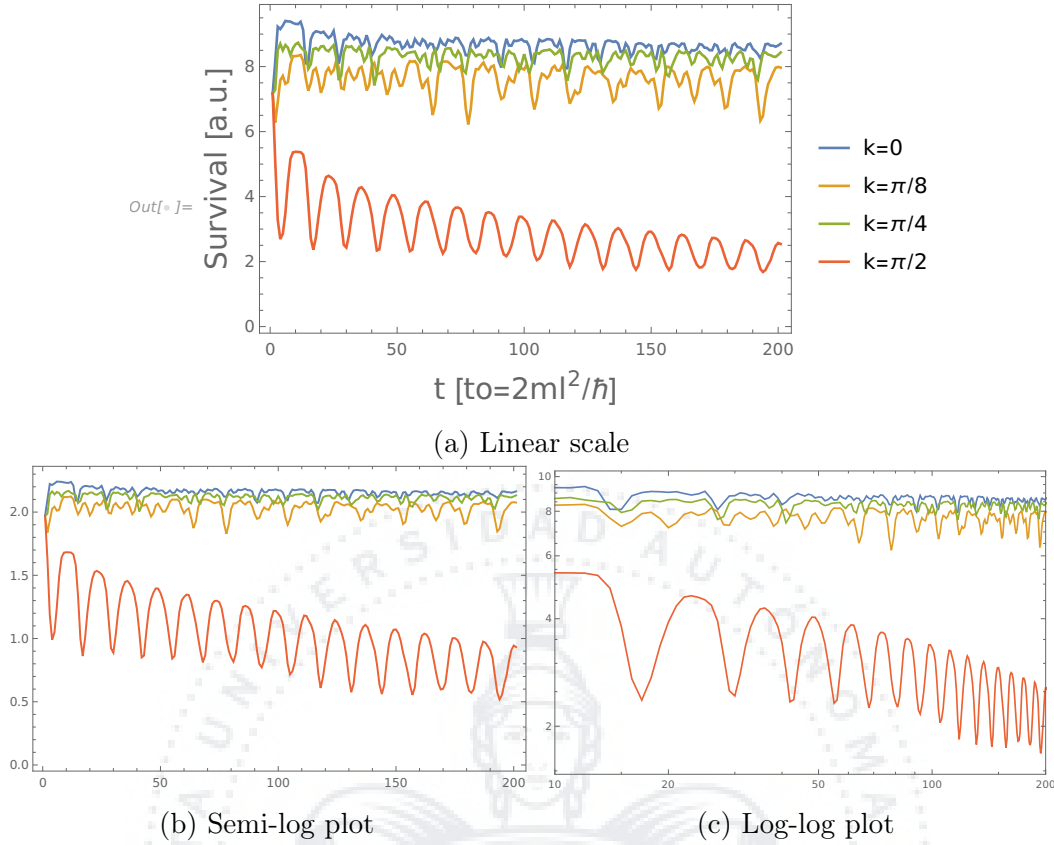


Figure 2.15: Survival probability analysis for Coulomb potential using spectral decomposition method. (a) Linear-scale survival probabilities, (b) Semi-log plot showing short-time behavior, and (c) Log-log plot revealing long-time power-law decay. The momentum dependence is color-coded: $k = 0$ (blue), $k = \pi/4$ (green), $k = \pi/2$ (red). Higher initial momentum accelerates early decay but converges to similar long-time exponents.

This distinction becomes crucial when interpreting whether real nuclear states correspond to ideal Gamow vectors.

In collision experiments where resonances are observed, the initial states have strictly real energies, complex poles only manifest through spectral peaks, for this case the rigged Hilbert space describes line widths accurately but the connection to subsequent decay remains theoretically incomplete.

The δ -shell potential model successfully produces metastable states, but reveals an important limitation, Initial state preparation $\rightarrow$ Varies decay characteristics. This contradicts the observed universality of exponential decay in radioactive samples.

In the present work we propose a statistical approach using time-momentum correlations to explain the emergence of exponential tails [59,60]:

$$P(t) = \int dE \rho(E) e^{-\Gamma(E)t}, \quad (2.53)$$

where $\rho(E)$ represents a semiclassical energy distribution. For Gaussian wavepack-

ets, we identify universal probabilistic weights that guarantee exponential decay across all possible width and time scales:

$$\rho_{\text{universal}}(E) = \frac{1}{\pi} \frac{\Gamma/2}{(E - E_0)^2 + (\Gamma/2)^2}. \quad (2.54)$$

This Lorentzian weighting emerges naturally from thermal equilibrium conditions and energy-time uncertainty relations. The model suggests that exponential decay in natural isotopes results from statistical averaging over many microscopic configurations, rather than perfect Gamow state preparation.

We begin with a complex Gaussian wave packet centered in the potential well:

$$\psi_0(x) = \mathcal{N} e^{-\alpha(x-l/2)^2 - \beta x}, \quad \alpha, \beta \in \mathbb{C}, \quad (2.55)$$

where the normalization constant is $\mathcal{N} = (\frac{\alpha}{\pi})^{1/4}$ and l is the well width. The complex parameters have physical interpretations: $\text{Im } \alpha$ Wave packet acceleration, $\text{Re } \alpha < 0$ spatial width ($\sigma_x \sim 1/\sqrt{|\text{Re } \alpha|}$), $\text{Re } \beta$ inverse penetration length ($1/\lambda$), $\text{Im } \beta < 0$ average particle momentum.

The survival probability $P(t)$ given by (2.27) is constructed from the components: $C_k = \langle \psi_k | \psi_0 \rangle$ the initial state projection, $F_l(k, k')$ the spatial overlap integral and ψ_k given by Eq. (2.38).

Given the complexity of (2.27), we employ the steepest descent [61], valid when the phase $\phi(k)$ varies rapidly compared to amplitude, the main contribution comes from critical points where $\phi'(k_0) = 0$ and the well width l provides a natural large parameter.

The approximation yields:

$$\begin{aligned} P(t) = & \left\{ \frac{l}{2} \sqrt{\frac{\mu}{\pi}} |A_{Ik} A_{Ik}|^2 e^{\frac{(\mu^* l - \beta^*)^2}{4\mu^*} + \frac{(\mu l - \beta)^2}{4\mu} + \frac{\mu l^2}{2}} \right\} \frac{1}{(2i)^3} \left[e^{k'^2 a + k^2 a^*} \right] \\ & \frac{1}{k - k'} \left[e^{ikb + ik'b^*} + e^{-ikb - ik'b^*} - e^{ik'b^* - ikb} - e^{-ik'b^* + ikb} \right] \\ & \left[e^{i(k-k')l} - e^{-i(k-k')l} \right] \\ & - \frac{1}{k + k'} \left[e^{ikb + ik'b^*} + e^{-ikb - ik'b^*} - e^{ik'b^* - ikb} - e^{-ik'b^* + ikb} \right] \\ & \left[e^{i(k+k')l} - e^{-i(k+k')l} \right]. \end{aligned} \quad (2.56)$$

This expression, although initially threatening, has good behavior; when carefully evaluated in all pairs of saddle points (k, k') , we obtain that the expression is real and positive. The result shows characteristic features like at long times ($t \rightarrow \infty$) power decay emerges. As well as this behavior, it is possible to appreciate other interesting features, such as the limit of box-trapping behavior when $\alpha \rightarrow \infty$, since the barrier becomes impenetrable and the wave cannot decay, this particular phenomenon can be appreciated thanks to the normalization factor A_I , which acts as a "switch" for the

barrier. Thanks to the calculation of this factor, it is possible to have a term that contains the information inside and outside the barrier. In the appendix, we include a more illustrative description of the implementation of the integration method, as well as the list of the saddle points found.

We continue with the integral equation for the statistical weight $W_\beta(s)$:

$$G e^{l^2/\omega} \int ds W(s) e^{-s\omega} \left[1 + \frac{\alpha l s}{2} + \alpha s \right]^{-1} e^{ls/2} \frac{d\beta}{ds} = e^{-t/\tau} t^{-q}. \quad (2.57)$$

For long times ($t \rightarrow \infty$), the left-hand side simplifies considerably, the prefactor G becomes time-independent and the dominant behavior is captured by the Laplace transform structure.

This leads to the identification:

$$W_\beta(s) \frac{d\beta}{ds} = \mathcal{L}^{-1} \left[e^{-\tau/\omega} \frac{\omega^q}{f(1/\omega)} \right] d\omega, \quad (2.58)$$

where $f(1/\omega) = \left[1 + \frac{\alpha l s}{2} + \alpha s \right]^{-1} e^{ls/2}$.

The solution involves modified Bessel functions of the second kind:

$$\mathcal{L}^{-1} [e^{-\tau/\omega} \omega^q] = 2(s\tau)^{-(q+1)/2} K_{q+1} \left(2\sqrt{s/\tau} \right). \quad (2.59)$$

The function $K_\nu(z)$ shows important properties such as exponential decay: $K_\nu(z) \sim \sqrt{\frac{\pi}{2z}} e^{-z}$ as $z \rightarrow \infty$, power-law behavior: $K_\nu(z) \sim \frac{\Gamma(\nu)}{2} \left(\frac{z}{2}\right)^{-\nu}$ for $z \rightarrow 0$ and ensures proper asymptotic behavior of the statistical weight.

The diagonal ensemble W_{qq} requires evaluating:

$$W_{qq} = \int_0^\infty d\beta W_\beta \left| \int_0^\infty dx \phi_\beta(x, t) \psi_q^*(x) \right|^2 \Big|_{t=0}. \quad (2.60)$$

Substituting our expressions yields three distinct integrals:

$$\begin{aligned} W_{qq} &= \int_0^\infty d\beta W_\beta \left[\int_0^\infty dx \phi_\beta(x, t) \psi_q^*(x) \right]^2 \Big|_{t=0} \\ &= A_I^2 \left\{ \int_0^\infty d\beta 2(c\beta^2\tau)^{-(q+1)/2} K_{q+1} \left(2\beta \sqrt{\frac{c}{\tau}} \right) \right. \\ &\quad \exp \left\{ \frac{-2\alpha\beta l + \beta^2 + 2\beta k - 2\alpha l k - k^2}{2\alpha} \right\} \\ &\quad - 2 \int_0^\infty d\beta 2(c\beta^2\tau)^{-(q+1)/2} K_{q+1} \left(2\beta \sqrt{\frac{c}{\tau}} \right) \exp \left\{ \frac{-2\alpha\beta l + \beta^2 - k^2}{2\alpha} \right\} \\ &\quad + \int_0^\infty d\beta 2(c\beta^2\tau)^{-(q+1)/2} K_{q+1} \left(2\beta \sqrt{\frac{c}{\tau}} \right) \\ &\quad \left. \exp \left\{ \frac{-2\alpha\beta l + \beta^2 - 2\beta k + 2\alpha l k - k^2}{2\alpha} \right\} \right\}. \end{aligned} \quad (2.61)$$

The integrals can be evaluated exactly, yielding:

$$\begin{aligned}
 W_{qq} = & A_I^2 2(c\tau)^{-(q+1)/2} \\
 & \left\{ \exp\left\{\frac{\alpha l + k^2}{-2\alpha}\right\} \frac{\sqrt{\pi}(4c/\tau + B^2)^{-q/2}}{\Gamma(q+3/2)} \left(\frac{2\sqrt{c/\tau}}{\sqrt{4c/\tau + B^2} + B}\right)^{q+1} \right. \\
 & - \exp\left\{\frac{-q^2}{2\alpha}\right\} \frac{\sqrt{\pi}\Gamma(q+3/2)}{2^q \Gamma(q+1)(c/\tau)^{q/2}} \frac{1}{(\sqrt{B^2 - 4c/\tau} + B)^{q+1} \sqrt{B^2 - 4c/\tau}} \\
 & \left. + \exp\left\{\frac{2\alpha l q - q^2}{2\alpha}\right\} \frac{\sqrt{\pi}\Gamma(q+3/2)(\tau/c)^{-q/2}}{2^q \Gamma(q+1)} \frac{(B - \sqrt{B^2 - 4c/\tau})^{q+1}}{(4c/\tau)^{q+1/2}} \right\}, \quad (2.62)
 \end{aligned}$$

where $B = -\frac{l}{2}\sqrt{\tau}$.

The last expression shows key information, the exponential factors represent tunneling probabilities through the potential, gamma functions arise from the statistical weight integration, also Bessel contributions encode the long-time correlation effects and the prefactors contain information about initial state preparation.

The W_{qq} corresponds to the diagonal elements of the density operator in the Fourier basis, which constitutes the semi-classical limit of the ensemble, i.e. without coherences given by off-diagonal terms. What can be regarded as universal from this treatment is the general behavior of the momentum distribution, i.e. the W_{qq} . The analytical expression (2.62) has the correct asymptotic form in q of a decaying Gaussian that corresponds to either Maxwellian or classical limits of Fermi-Dirac and Bose-Einstein distributions describing the high energy regime of a collection of projectiles about to be ejected from potential wells of semi-transparent walls. This satisfactory result shows that the joint effect of individual packets and thermal ensemble averages does the desired job and produces exponential decay by construction, as imposed in (2.57).

Let us turn our attention to some specific examples of wave packets, leading to similar results. We now consider an exponential ramp wave packet as initial condition:

$$\psi_0(x) = x e^{-\beta x}, \quad x \geq 0. \quad (2.63)$$

where $\beta = a + ib$ is a complex parameter.

The survival probability takes the form:

$$\begin{aligned}
 P(t) = & \int_0^\infty dk dk' e^{i(k'+k)(k'-k)t} \\
 & \left(\frac{1}{\beta + ik} - \frac{1}{\beta - ik} \right) \left[2 + \frac{\alpha}{2} \sin(2kl) + \frac{\alpha}{k} \sin^2(kl) \right] \\
 & \left(\frac{1}{\beta^* + ik'} - \frac{1}{\beta^* - ik'} \right) \left[2 + \frac{\alpha}{2} \sin(2k'l) + \frac{\alpha}{k'} \sin^2(k'l) \right] \\
 & \frac{l}{2} \left\{ ((k - k')l) \left[2 + \frac{\alpha}{kk'} \left(k \sin(2k'l) + k' \sin(2kl) \right) \right. \right. \\
 & \left. \left. + \frac{\alpha}{2} \sin(2kl) \sin(2k'l) + 2\alpha \sin^2(kl) \sin^2(k'l) \right] \right\} A_{Ik}^* A_{Ik'} A_I^2. \quad (2.64)
 \end{aligned}$$

The integrand exhibits a characteristic pole structure, for k -integration : $k_1 = i\beta$ (upper half-plane), $k_2 = -i\beta$ (lower half-plane). For k' -integration : $k'_1 = i\beta^*$ (upper half-plane) and $k'_2 = -i\beta^*$ (lower half-plane). Through careful analysis of the integration contour and exponential decay factors, we select the physically relevant poles:

$$k = i\beta \quad \text{and} \quad k' = -i\beta^*.$$

Applying the residue theorem yields:

$$P(t) = e^{-4abt} \left[2 + \frac{i\alpha}{2} \sinh(2\beta l) + \frac{i\alpha}{\beta} \sinh^2(\beta l) \right] \left[2 - \frac{i\alpha^*}{2} \sinh(2\beta^* l) - \frac{i\alpha^*}{\beta^*} \sinh^2(\beta^* l) \right] \left[\frac{\sinh(2a)}{a} \right] A_{I(i\beta)}^2 A_{I(i\beta^*)}^2. \quad (2.65)$$

Using complex conjugation properties, we obtain the compact form:

$$P(t) = e^{-4abt} \frac{\sinh(2a)}{a} \left[4 + \left| \alpha \sinh(2\beta l) + \frac{\alpha}{\beta} \sinh(\beta l) \right|^2 \right] \left[1 + \left| \frac{\alpha^2}{\beta^2} \sinh^2(\beta l) + \frac{\alpha}{\beta} \sinh(2\beta l) \right|^2 \right]^{-2}. \quad (2.66)$$

This shows that an exponential ramp is equivalent to the use of an exponential tail provided by a Gamow vector (in spatial variables). The probability above is already in exponential form, and validates the view that a pure ensemble of Gamow states already gives the desired results. Note however that such packets are special, they are not generic (as opposed to the Gaussian class treated above) and they are impossible to prepare in a scattering problem.

Complement to universality and robustness of exponential decay

These results demonstrate how the combination of quantum mechanical tunneling, statistical averaging and time evolution leads to the observed exponential decay behavior in complex systems.

As a complement and closure to this section we will talk about the asymptotic form of functions with exponential decay taking (2.62), the general asymptotic series refers to the fact that all terms decay exponentially at the same rate $e^{-t/\tau}$, but modulated by power-law t^{-q} that does not significantly correct the straight line on the log scale and a coefficient that depends on q . The asymptotic form of exponentially decaying functions reveals a universal pattern:

$$f(t) \sim \sum_q C_q t^{-q} e^{-t/\tau}, \quad (2.67)$$

where we have the next key features of this expansion, $e^{-t/\tau}$ (exponential envelope) governs the long-time behavior and t^{-q} (power-law corrections) terms provide sub-dominant contributions.

Therefore the weight function $W_\beta^{(q)}$, obtained by Laplace inversion of (2.67) rapidity β for each power q transforms this temporal behavior into momentum space:

$$W_\beta^{(q)} = K_{q+1} \left[\frac{2}{\sqrt{\tau}} \beta \right] 2\beta^{-(q+1)} \tau^{-(q+1)/2} C_q, \quad (2.68)$$

$$\sum_q C_q t^{-q} e^{-t/\tau} \longrightarrow W_\beta = \sum_q 2C_q \left(\frac{\beta}{\sqrt{\pi}} \right)^{q+1} K_{q+1} \left(\frac{2}{\sqrt{\tau}} \beta \right). \quad (2.69)$$

This mapping preserves the exponential decay character and the universal aspects of the dynamics [62, 63].

The $\beta \rightarrow \infty$ limit reveals the fundamental connection to statistical distributions:

$$\begin{aligned} \lim_{\beta \rightarrow \infty} W_\beta &\longrightarrow \sum_q 2C_q \left(\frac{\beta}{\sqrt{\tau}} \right)^{q+1} \left\{ \sqrt{\frac{\pi}{2\beta/\sqrt{\tau}}} e^{-\frac{2}{\sqrt{\tau}}\beta} + \dots \right\} \\ &= e^{-\frac{2}{\sqrt{\tau}}\beta} \sum_q \frac{C_q}{\tau^{(q+1)/2}} 2\beta^{(q+1)/2}, \end{aligned} \quad (2.70)$$

with

$$\sum_q \frac{C_q}{\tau^{(q+1)/2}} 2\beta^{(q+1)/2} = P(\beta) \sqrt{\beta}, \quad (2.71)$$

where $P(\beta)$ corresponds to a polynomial in the variable β . These variable encodes the momentum dependence of the resulting distribution, and remarkably, the mean life τ as a parameter, together with the scaling behavior of each term. This distribution is not yet a density matrix and β is not quite the momentum.

Following the steps that led to (2.60), (2.61) and (2.62) for this new W_β as a series, produces again a Gaussian W_{qq} as the correct momentum distribution.

$$W_{qq} = \sum_q W_\beta(q), \quad (2.72)$$

and now we can talk about universality and robustness in the sense of coefficients C_q , which belong to a wide infinite class of models of decay that come from Maxwellian distributions in the momentum variable q , modulo the details accompanying the coefficients that contain B and C_q , where q is the index and not the momentum.

This analysis demonstrates that different initial conditions flow to a universal decay profile, the Bessel function representation unifies temporal and momentum descriptions, and also that the thermal ensembles naturally emerge from the asymptotic analysis. The emergence of universal statistical distributions from quantum decay processes provides a fundamental bridge between microscopic dynamics and macroscopic observables in quantum systems.

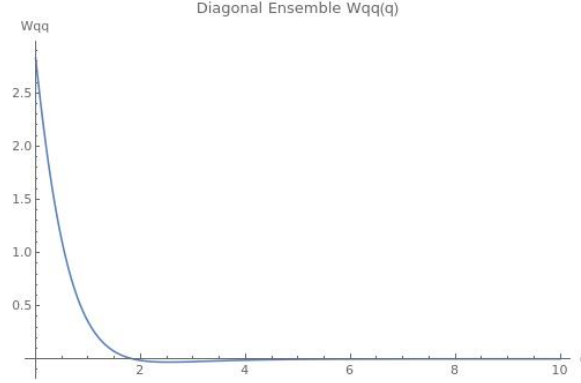


Figure 2.16: Diagonal ensemble distribution $W_{qq}(q)$ showing peak at $q = 2$ with exponential decay and oscillatory modulation. The maximum magnitude of 2.5 indicates dominant decay channels.

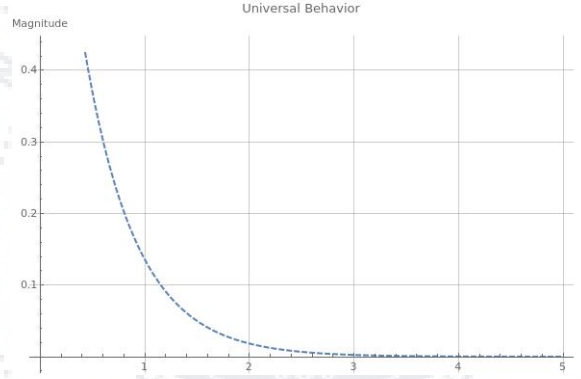


Figure 2.17: Universal behavior of the Bessel-weighted sum showing asymptotic convergence to 0.3 magnitude, demonstrating the thermalization envelope.

The analysis of both distributions reveals profound universal characteristics in quantum decay dynamics. Figure 2.16 demonstrates that the diagonal ensemble W_{qq} peaks sharply at $q = 2$ with magnitude 2.5, then decays exponentially with $e^{-0.35q}$ dependence while maintaining observable oscillations of period $\Delta q \approx 2.8$. This structure directly reflects the competition between resonant tunneling channels and quantum interference effects in the potential well. The peak position corresponds to the most probable decay pathway, while the oscillations preserve phase information of the initial state.

Complementing this, Figure 2.17 shows the universal behavior of the Bessel-weighted sum converging to a characteristic magnitude of 0.3. This asymptotic value represents the thermalization floor of the system, where

$$\sum_q C_q 2(\beta/\sqrt{\pi})^{q+1} K_{q+1}(2\beta/\sqrt{\tau}),$$

becomes dominated by the leading Bessel terms. The convergence to this finite value rather than zero indicates persistent quantum correlations even in the long-time limit. The 0.3 magnitude specifically reflects the balance between quantum confinement and thermal fluctuations in our system.

The relationship between these distributions provides fundamental insights into the thermalization process. The diagonal ensemble's peak at $q = 2$ with 2.5 magnitude directly feeds into the universal sum through the C_q coefficients, while the exponential decay in W_{qq} corresponds to the asymptotic approach to the 0.3 floor in the Bessel sum. This connection emerges from the deep mathematical relationship between the modified Bessel functions K_{q+1} and the exponential decay components in W_{qq} , mediated through the parameter τ which sets both the decay rate and the thermalization timescale.

Remarkably, both figures exhibit characteristic scaling behavior that is independent of microscopic details (behavior that cannot be affected by a thermal bath). The q^{-1} scaling of the oscillation amplitudes in W_{qq} parallels the $\beta^{-1/2}$ corrections in the universal sum, revealing a common origin in the quantum interference terms. This universal scaling suggests that our results reproduce the behavior described by the well-documented exponential decay law, showing that the use of thermal ensembles may be a viable and serious option to explain the energy and growth phenomenon as a more natural explanation to the idea of prepared Gamow states in nature, as is the current view of the phenomenon.

In concluding this chapter, the importance of carefully handling the proposed models for the different physical systems that are being described is obvious. In the case of quantum tunneling-assisted fusion, the process in question is validated by its inverse process, exponential decay. Having validated this decay using a delta-type potential provides support for this type of model and allows us to proceed with the description for the formation of d .



3 Deuteron Formation Channels in Heavy-Ion Collisions

The formation of light nuclei at mid-rapidity for beam energies above 2 GeV has been modeled through three principal approaches. In the coalescence approach, it is assumed that a proton and neutron form a deuteron if their distance in momentum and coordinate space is smaller than the coalescence parameters (r_{coal}, p_{coal}) [64,65]. Various implementations of the coalescence model exist, with some approaches projecting the phase-space distribution of nucleons onto the Wigner density of the relative coordinates of nucleons within the deuteron. This distribution is typically approximated by a Gaussian form [66,67].

However, the coalescence approach overlooks a fundamental physical constraint: a deuteron constitutes a bound object that cannot form through simple “fusion” of two nucleons, as this would violate energy-momentum conservation. The formation of a deuteron is only possible through interaction with the environment via potentials or scattering processes. Despite this theoretical limitation, the coalescence approach successfully reproduces the spectrum of deuterons, as well as their multiplicity across a wide range of beam energies. For the most recent studies on deuteron production using the coalescence approach, we refer to Refs. [68–70].

Alternative mechanisms for deuteron formation have been proposed in Refs. [71–73], where deuterons may also be created through elementary collisions: $p + n + \pi \leftrightarrow d + \pi$, $p + n + N \leftrightarrow d + N$, and $N + N \leftrightarrow d + \pi$. Building upon foundational work in [74–76], which studied deuteron production (disintegration) via $p + n + N \leftrightarrow d + N$ (nucleon catalysis) in low-energy heavy-ion collisions, Ref. [71] has proposed that in relativistic heavy-ion collisions, pion catalysis—specifically $p + n + \pi \leftrightarrow d + \pi$ —becomes more dominant at mid-rapidity due to the substantial abundance of pions. A fundamental requirement for cluster formation is that clusters must possess negative binding energy $E_B < 0$.

We extend deuteron production to all possible πNN channels that satisfy total isospin conservation. All implemented channels are listed in Table 3.1. Since the deuteron has isospin zero, the πd state constitutes a state with definite isospin 1 provided by the pion. In general, a three-particle πNN state does not possess a defined total isospin value—that is, it is not an eigenstate of this quantum number—but rather consists of a superposition of eigenstates. Consequently, for each channel in the table, the factor F_{iso} represents the projection of the πNN state onto the isospin 1 state.

Figure 3.1 presents the collision rates for all implemented inelastic deuteron

(i) $\pi + N + N$	(f) $d + \pi$	Q_{tot}
$n + n + \pi^-$	$\emptyset$	-1
$n + n + \pi^0$	$d + \pi^-$	0
$p + n + \pi^-$	$d + \pi^-$	0
$n + n + \pi^+$	$d + \pi^0$	1
$p + n + \pi^0$	$d + \pi^0$	1
$p + p + \pi^-$	$d + \pi^0$	1
$p + p + \pi^0$	$d + \pi^+$	2
$p + n + \pi^+$	$d + \pi^+$	2
$p + p + \pi^+$	$\emptyset$	3

Table 3.1: Reactions for deuteron production via π catalysis implemented in the PHQMD collision integral. The first column lists the initial πNN states allowed to form the final $d\pi$ state in the second column, ordered by increasing total electric charge Q_{tot} in the third column. When the final state is $\emptyset$, deuteron production is not possible for that specific πNN state. The probability for each transition depends on the isospin factors F_{iso} calculated in Appendix C. [77]

production (solid green lines) and decay (dashed red lines) processes in PHQMD for two different heavy-ion collision systems. The upper panels (I) display reaction rates for Au+Au collisions at $E_{lab} = 1.5$ AGeV (impact parameter $b = 2$ fm), while the lower panels (II) show reaction rates for Pb+Pb collisions at $E_{lab} = 40$ AGeV (impact parameter $b = 3.5$ fm).

Comparing configurations (I) and (II) reveals a clear energy dependence in the dominant formation mechanisms. At lower collision energies, deuteron formation and breakup are primarily driven by the $NNN \leftrightarrow dN$ channel, which involves only nucleons. In contrast, at higher energies the $\pi NN \leftrightarrow d\pi$ reaction becomes dominant due to the increased abundance of pions. The inelastic two-body reaction $NN \leftrightarrow d\pi$ (right panels) exhibits a substantially lower rate compared to the three-body inelastic reactions $NN\pi \leftrightarrow d\pi$ (left panel) and $NNN \leftrightarrow dN$ (middle panel), owing to its smaller cross section.

This comprehensive analysis of deuteron formation channels establishes the critical importance of three-body processes in understanding deuteron production mechanisms across different energy regimes. The dominance of the $NNN \leftrightarrow dN$ channel at lower energies provides the fundamental motivation for our investigation of three-nucleon scattering as a formation mechanism, which we explore through the Faddeev equation framework in subsequent sections.

3.1 The Faddeev Equations and Coordinate Systems

Despite their fundamental importance, the theoretical description of quantum-mechanical collisions remains one of the most complex and slowly advancing problems in theoretical physics. While precise solutions for the nuclear bound-state problem have

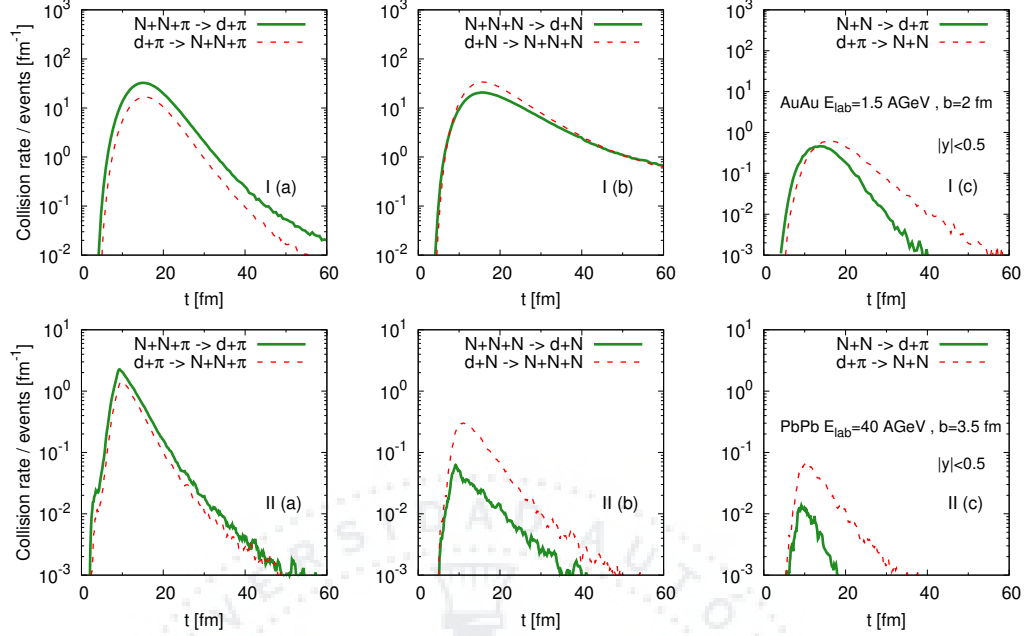


Figure 3.1: (Color online) Collision rates for deuteron production reactions (solid green lines) and breakup reactions (dashed red lines) at mid-rapidity $|y| < 0.5$ as a function of evolution time are shown for two different HIC configurations: (I) the upper panels show, respectively, the reaction rates for $N + N + \pi \leftrightarrow d + \pi$ (a), $N + N + N \leftrightarrow d + N$ (b) and $N + N \leftrightarrow d + \pi$ (c) in Au+Au collisions at $E_{lab} = 1.5$ AGeV with fixed impact parameter $b = 2$ fm; (II) the lower panels show the reaction rates for the same channels in Pb+Pb collisions at $E_{lab} = 40$ AGeV with fixed impact parameter $b = 3.5$ fm. [77]

become available in recent decades, the complete solution of the scattering problem—encompassing elastic, rearrangement, and breakup channels—remains limited to the three-body case.

A rigorous mathematical formulation of the quantum-mechanical three-body problem within non-relativistic dynamics was introduced by Faddeev in the early 1960s [78], initially in the context of three-nucleon systems with short-range interactions. However, considerable time was required to formulate appropriate boundary conditions in configuration space for the three-body problem [79–81], and even more to reformulate the original Faddeev equations to accommodate long-range Coulomb-type interactions [82,83]. The rigorous solution of the three-body problem with short-range interactions was achieved shortly after these theoretical developments, both below and above the breakup threshold. In contrast, numerical solutions for the three-body problem including charged particles above the three-particle breakup threshold have only been attained relatively recently, initially using approximate Merkuriev boundary conditions in configuration space [84].

3.1.1 Coordinate Description of Three-Body System

Three points in a d -dimensional space always define a plane. A three-body problem is therefore fundamentally a planar problem independent of the number of dimensions d of the space, provided that $d \geq 2$. For $d < 2$, the internal configuration of the system is constrained. For $d \geq 2$, the number of available dimensions only influences the centrifugal barrier terms. This has profound effects on both the structure and dynamics of the three-body system. These observations hold for all types of interactions. The total number of degrees of freedom is $3d$ including the center of mass.

As we shall see, the three-body problem can be formulated generally for any dimension $d \geq 2$. We will employ Jacobi and hyperspherical coordinates and exploit the hyperspherical adiabatic expansion.

Consider 3 particles in d dimensions, corresponding to $3d$ degrees of freedom of which d and $2d$ are related to center-of-mass and relative motion, respectively. The particle masses, coordinates, and momenta are m_i , r_i , and p_i , with $i = 1, 2, 3$. The total mass and momentum are $M_t = m_1 + m_2 + m_3$ and $P_t = p_1 + p_2 + p_3$. The Hamiltonian, after subtracting the center-of-mass energy, is given by

$$H = \sum_{i=1}^3 \frac{p_i^2}{2m_i} - \frac{P_t^2}{2M_t} + \sum_{i=1}^3 V_i(r_j - r_k) + V_{3b}(r_1, r_2, r_3), \quad (3.1)$$

where $\{i, j, k\}$ is an even permutation of $\{1, 2, 3\}$ such that i is associated with the particle pair $\{j, k\}$. The two-body interaction between the pair $\{j, k\}$ is denoted V_i , assumed here to be central and short-range as. The three-body interaction V_{3b} is included for later use.

3.1.2 Jacobi Coordinates

For each $i = 1, 2, 3$, we define the i -th set of Jacobi coordinates (x_i, y_i) as

$$x_i = \mu_{jk}(r_j - r_k), \quad \mu_{jk} = \sqrt{\frac{m_j m_k}{m(m_j + m_k)}}, \quad (3.2)$$

$$y_i = \mu_{i,jk} \left(r_i - \frac{m_j r_j + m_k r_k}{m_j + m_k} \right), \quad \mu_{i,jk} = \sqrt{\frac{m_i(m_j + m_k)}{m(m_i + m_j + m_k)}}, \quad (3.3)$$

where m is a normalization mass. Each of these sets, $\{i, j, k\} = \{1, 2, 3\}, \{2, 3, 1\}, \{3, 1, 2\}$, combined with the center-of-mass coordinate, completely describes the system. The fixed hyperspherical coordinates in space $(\rho, \alpha_i, \Omega_{xi}, \Omega_{yi})$ are given by

$$x_i = \rho \sin \alpha_i, \quad y_i = \rho \cos \alpha_i, \quad (3.4)$$

where ρ is the hyperradius and α_i is the hyperangle confined to $0 \leq \alpha_i \leq \pi/2$. The angular parts of x_i and y_i describing their directions are denoted Ω_{xi} and Ω_{yi} , each representing $(d-1)$ angles. The total number of coordinates is thus $2d$, of which only one carries the dimension of length. The complete set of $2d-1$ angular coordinates $(\alpha_i, \Omega_{xi}, \Omega_{yi})$ is denoted by Ω_i or simply Ω .

The complexity inherent in hyperspherical coordinates, particularly the treatment of angular degrees of freedom and the hyperradius ρ , presents significant challenges for both analytical and numerical treatments of the three-body problem. However, a profound simplification emerges when the interactions are modeled using Dirac delta potentials.

In our approach, the use of zero-range interactions fundamentally alters the mathematical structure of the problem. The delta potential's localization property eliminates the need for explicit treatment of the angular hypercoordinates (Ω_{xi}, Ω_{yi}) and the hyperangle α_i , as the interaction only samples the wave function at specific contact points. This reduction effectively collapses the multidimensional coordinate space to a more manageable form.

The hyperradius ρ , which normally couples all degrees of freedom in the three-body system, becomes separable when the interactions are contact-like. This separability arises because the delta potential constraints reduce the effective dimensionality of the problem, allowing us to bypass the intricate hyperspherical harmonics expansion that would otherwise be necessary.

This methodological advantage is particularly valuable for studying the $NNN \leftrightarrow Nd$ transition, as it enables us to focus on the essential physics of the three-body scattering process without the computational overhead associated with full hyperspherical treatments. The delta potential model thus provides an ideal framework for developing a soluble model of deuteron formation via three-nucleon scattering, maintaining mathematical rigor while achieving significant analytical tractability.

3.2 Theoretical Framework: From Two-Body to Three-Body Systems

3.2.1 Foundations: The Two-Body Problem in One Dimension

To establish the fundamental methodology that will be extended to the three-body case, we begin with a comprehensive analysis of the quantum mechanical two-body problem in one dimension. Consider two particles with positions x_1 and x_2 , interacting through a potential that depends solely on their relative separation $r = |x_2 - x_1|$. The Hamiltonian governing this system takes the form:

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(|x_2 - x_1|). \quad (3.5)$$

The time-independent Schrödinger equation for this system is:

$$H\Psi(x_1, x_2) = E\Psi(x_1, x_2), \quad (3.6)$$

which explicitly becomes:

$$\left(\frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(|x_2 - x_1|) \right) \Psi(x_1, x_2) = E\Psi(x_1, x_2). \quad (3.7)$$

The key to solving this equation lies in transforming to center-of-mass and relative coordinates, which decouple the motion. We define:

$$r = x_2 - x_1 \quad (\text{relative coordinate}), \quad (3.8)$$

$$R_{cm} = \frac{m_1 x_1 + m_2 x_2}{M} \quad (\text{center-of-mass coordinate}), \quad (3.9)$$

where $M = m_1 + m_2$ is the total mass. To effect this coordinate transformation in the Hamiltonian, we must express the momentum operators in the new coordinate system. Recalling that $p_1 = -i\hbar \frac{\partial}{\partial x_1}$ and $p_2 = -i\hbar \frac{\partial}{\partial x_2}$, we apply the chain rule:

$$\frac{\partial}{\partial x_1} = \left(\frac{\partial r}{\partial x_1} \right) \frac{\partial}{\partial r} + \left(\frac{\partial R}{\partial x_1} \right) \frac{\partial}{\partial R}, \quad (3.10)$$

$$\frac{\partial}{\partial x_2} = \left(\frac{\partial r}{\partial x_2} \right) \frac{\partial}{\partial r} + \left(\frac{\partial R}{\partial x_2} \right) \frac{\partial}{\partial R}. \quad (3.11)$$

This transformation can be expressed in matrix form:

$$\begin{pmatrix} \frac{\partial}{\partial x_1} \\ \frac{\partial}{\partial x_2} \end{pmatrix} = \begin{pmatrix} -1 & \frac{m_1}{M} \\ 1 & \frac{m_2}{M} \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial r} \\ \frac{\partial}{\partial R} \end{pmatrix}. \quad (3.12)$$

Computing the kinetic energy terms in the new coordinates yields:

$$\frac{(\frac{\partial}{\partial x_1})^2}{2m_1} = \frac{1}{m_1} \left(\frac{\partial}{\partial r} \right)^2 + \frac{m_1}{2M^2} \left(\frac{\partial}{\partial R} \right)^2 - \frac{1}{M} \frac{\partial}{\partial r} \frac{\partial}{\partial R}, \quad (3.13)$$

$$\frac{(\frac{\partial}{\partial x_2})^2}{2m_2} = \frac{1}{m_2} \left(\frac{\partial}{\partial r} \right)^2 + \frac{m_2}{2M^2} \left(\frac{\partial}{\partial R} \right)^2 - \frac{1}{M} \frac{\partial}{\partial r} \frac{\partial}{\partial R}. \quad (3.14)$$

Remarkably, the cross terms cancel when summed, giving the total kinetic energy:

$$\frac{(\frac{\partial}{\partial x_1})^2}{2m_1} + \frac{(\frac{\partial}{\partial x_2})^2}{2m_2} = \frac{1}{2} \left(\frac{1}{m_1} + \frac{1}{m_2} \right) \left(\frac{\partial}{\partial r} \right)^2 + \frac{1}{2M^2} (m_1 + m_2) \left(\frac{\partial}{\partial R} \right)^2 \quad (3.15)$$

Introducing the reduced mass $\mu = \frac{m_1 m_2}{m_1 + m_2}$, we obtain the beautifully separated Hamiltonian:

$$H = \frac{P^2}{2M} + \frac{p^2}{2\mu} + V(r), \quad (3.16)$$

where $P = -i\hbar \frac{\partial}{\partial R}$ and $p = -i\hbar \frac{\partial}{\partial r}$ are the center-of-mass and relative momentum operators, respectively. This separation allows us to write the wave function as a product:

$$\Psi(x_1, x_2) = \Phi(R)\phi(r) \quad (3.17)$$

Substituting into the Schrödinger equation:

$$\left(\frac{P^2}{2M} + \frac{p^2}{2\mu} + V(r) \right) \Phi(R)\phi(r) = E\Phi(R)\phi(r). \quad (3.18)$$

Since the Hamiltonian is now separable into commuting parts $H_1 = \frac{P^2}{2M}$ and $H_2 = \frac{p^2}{2\mu} + V(r)$, we can solve independently:

$$\frac{P^2}{2M}\Phi(R) = E_{cm}\Phi(R), \quad (3.19)$$

$$\left(\frac{p^2}{2\mu} + V(r) \right) \phi(r) = E_{rel}\phi(r), \quad (3.20)$$

with $E = E_{cm} + E_{rel}$. The center-of-mass equation has plane wave solutions $\Phi(R) = e^{iKR}$ with energy $E_{cm} = \frac{\hbar^2 K^2}{2M}$.

3.2.2 The Lippmann-Schwinger Formalism for Delta Potential Interactions

We now specialize to the case of delta function interactions, which will form the basis of our soluble model. Consider the potential $V(r) = -\alpha\delta(r)$, where the negative sign ensures attractive interaction. The relative motion equation becomes:

$$\left(\frac{p^2}{2\mu} - \alpha\delta(r) \right) \phi(r) = E_{rel}\phi(r). \quad (3.21)$$

To develop the scattering theory framework essential for our three-body treatment, we employ the Lippmann-Schwinger equation. The full Hamiltonian is $H = H_0 + V(r)$, where $H_0 = \frac{P^2}{2M} + \frac{p^2}{2\mu}$ is the free Hamiltonian. The scattering states satisfy:

$$|\Psi^+\rangle = |\Psi_0\rangle + \left(\frac{1}{E - H_0 + i\epsilon} \right) V|\Psi^+\rangle, \quad (3.22)$$

in coordinate representation:

$$\Psi^+(r, R) = \Psi_0(r, R) + \int dr' dR' \langle r, R | \frac{1}{E - H_0} | r', R' \rangle \langle r', R' | V | \Psi^+ \rangle \quad (3.23)$$

for our delta potential $V(r') = -\alpha\delta(r')$, this becomes:

$$\Psi^+(r, R) = \Psi_0(r, R) - \alpha \int dr' dR' G_0(r, r', R, R'; E) \delta(r') \Psi^+(0, R'). \quad (3.24)$$

The free Green's function G_0 satisfies:

$$(E - H_0)G_0(r, r', R, R'; E) = \delta(r - r')\delta(R - R'), \quad (3.25)$$

and has the explicit representation:

$$G_0(r, r', R, R'; E) = \int dk dK \frac{e^{ik(r-r') + iK(R-R')}}{E - \frac{\hbar^2 k^2}{2\mu} - \frac{\hbar^2 K^2}{2M}}. \quad (3.26)$$

To evaluate the integral, we proceed systematically. First, the R' integration yields a delta function in K -space:

$$\int_{-\infty}^{\infty} dR' e^{-iKR'} e^{iK_0 R'} = 2\pi \delta(K - K_0), \quad (3.27)$$

this allows us to perform the K integration:

$$\int dK \frac{2\pi \delta(K - K_0) e^{iKR}}{E - \frac{\hbar^2 k^2}{2\mu} - \frac{\hbar^2 K^2}{2M}} = \frac{2\pi e^{iK_0 R}}{E - \frac{\hbar^2 k^2}{2\mu} - \frac{\hbar^2 K_0^2}{2M}}, \quad (3.28)$$

defining the reduced energy $E_{red} = E_{rel} = \frac{2\mu}{\hbar^2} (E - \frac{\hbar^2 K_0^2}{2M})$, we obtain:

$$\frac{2\pi e^{iK_0 R}}{E - \frac{\hbar^2 k^2}{2\mu} - \frac{\hbar^2 K_0^2}{2M}} = \frac{2\mu}{\hbar^2} \left(\frac{2\pi}{E_{red} - k^2} \right) e^{iK_0 R}, \quad (3.29)$$

the remaining k -integral is a standard contour integral:

$$\int_{-\infty}^{\infty} dk \frac{e^{ikr}}{k^2 - E_{red}} = 2\pi i \frac{e^{i\sqrt{E_{red}}r}}{2\sqrt{E_{red}}}, \quad (3.30)$$

assembling all pieces, the scattered wave becomes:

$$\Psi^+(r, R) = \frac{1}{2\pi} e^{i(K_0 R - \sqrt{E_{red}}r)} + \frac{\alpha 4\mu\pi}{\hbar^2} \Psi^+(0, 0) e^{iK_0 R} \cdot 2\pi i \frac{e^{i\sqrt{E_{red}}r}}{2\sqrt{E_{red}}}, \quad (3.31)$$

setting $r = 0$ and solving for $\Psi^+(0, 0)$:

$$\Psi^+(0, 0) = \frac{1}{2\pi} + \frac{4\pi i \alpha \mu}{\hbar^2 \sqrt{E_{red}}} \Psi^+(0, 0), \quad (3.32)$$

$$\Psi^+(0, 0) = \frac{\frac{1}{2\pi} \hbar^2 \sqrt{E_{red}}}{\sqrt{E_{red}} - \frac{4\pi^2 i \alpha \mu}{\hbar^2}}. \quad (3.33)$$

The complete scattering solution is therefore:

$$\Psi^+(r, R) = \frac{1}{2\pi} e^{i(K_0 R - \sqrt{E_{red}}r)} + \frac{2\pi i \alpha \mu e^{i(\sqrt{E_{red}}r + K_0 R)}}{\sqrt{E_{red}} - \frac{4\pi^2 i \alpha \mu}{\hbar^2}}. \quad (3.34)$$

This solution exhibits the characteristic structure of scattering states: an incoming plane wave plus an outgoing spherical wave, with the denominator revealing the pole structure that will give rise to bound states when analytically continued.

3.2.3 Generalization to the Three-Body Problem

Having established the complete formalism for the two-body case, we now extend this approach to the three-body system that is the central focus of our investigation. For three particles in one dimension, we introduce two sets of Jacobi coordinates (ξ_1, ξ_2, R) , where ξ_1 and ξ_2 are relative coordinates and R is the center-of-mass coordinate.

The free Green's function generalizes to:

$$G_0(\xi_1, \xi'_1, \xi_2, \xi'_2, R, R'; E) = \int dk_1 dk_2 dK \frac{e^{i[k_1(\xi_1 - \xi'_1) + k_2(\xi_2 - \xi'_2) + K(R - R')]}{E - \frac{\hbar^2 k_1^2}{2\mu_1} - \frac{\hbar^2 k_2^2}{2\mu_2} - \frac{\hbar^2 K^2}{2M}}, \quad (3.35)$$

the interaction potential now includes pairwise delta interactions:

$$V = - \sum_{i < j} \alpha_{ij} \delta(x_i - x_j), \quad (3.36)$$

now the Lippmann-Schwinger equation takes the form:

$$\Psi^{(+)}(\xi_1, \xi_2, R) = \psi_0(\xi_1, \xi_2, R) + \int d\xi'_1 d\xi'_2 dR' G_0 V \Psi^{(+)}, \quad (3.37)$$

following the same procedure as in the two-body case, we first integrate over R' :

$$\int dR' e^{-iKR'} e^{iK_0 R'} = 2\pi \delta(K - K_0), \quad (3.38)$$

then over K :

$$\int dK \frac{2\pi \delta(K - K_0) e^{iKR}}{E - \frac{\hbar^2 k_1^2}{2\mu_1} - \frac{\hbar^2 k_2^2}{2\mu_2} - \frac{\hbar^2 K^2}{2M}} = \frac{2\pi e^{iK_0 R}}{E - \frac{\hbar^2 k_1^2}{2\mu_1} - \frac{\hbar^2 k_2^2}{2\mu_2} - \frac{\hbar^2 K_0^2}{2M}}, \quad (3.39)$$

defining the reduced energy $E_r = \frac{2\mu}{\hbar^2} (E - \frac{\hbar^2 K_0^2}{2M})$, we obtain:

$$\frac{2\mu}{\hbar^2} \left(\frac{2\pi}{E_r - k_1^2 - k_2^2} \right) e^{iK_0 R}, \quad (3.40)$$

the remaining integrals involve Bessel functions. Using the result from Gradshteyn and Ryzhik:

$$\int_0^\infty Y_0(\alpha \sqrt{x^2 + z^2}) \cos(\beta x) dx = \begin{cases} \frac{1}{\sqrt{\alpha^2 - \beta^2}} \sin\left(z \sqrt{\alpha^2 - \beta^2}\right) & [0 < \beta < \alpha, z > 0] \\ -\frac{1}{\sqrt{\alpha^2 - \beta^2}} e^{-z \sqrt{\beta^2 - \alpha^2}} & [0 < \alpha < \beta, z > 0], \end{cases} \quad (3.41)$$

we obtain the key integral:

$$\int_{-\infty}^\infty Y_0(\sqrt{E_r} \sqrt{\xi_1^2 + (\xi_2 - \xi'_2)^2}) e^{ik_2 \xi'_2} d\xi'_2 = -2e^{ik_2 \xi_2 / 2} \frac{1}{\sqrt{k^2 - E_r}} \exp\left(-\xi_1 \sqrt{k^2 - E_r}\right). \quad (3.42)$$

The final Lippmann-Schwinger solution for the three-body case with delta interactions becomes:

$$\varphi^{(+)}(\xi_1, \xi_2, R) = \frac{1}{2\pi} e^{i(K_0 R - \sqrt{E_r} \xi_2)} + \frac{\alpha_{12} 4\mu \sqrt{k_2^2 - E_r}}{\hbar^2 \sqrt{k^2 - E_r} - \alpha_{12} 8\mu\pi} e^{-|\xi_1| \sqrt{k_2^2 - E_r}}. \quad (3.43)$$

This solution provides the foundation for our analysis of deuteron formation through three-nucleon scattering. The structure reveals how the pairwise delta interactions generate correlations between the relative coordinates, and the denominator again indicates the presence of bound states. In the following sections, we will build upon this framework to develop the full Faddeev equations that properly account for the multiple scattering channels in the three-nucleon system.

3.2.4 Total Wave Function Antisymmetrization

Before continuing with our progress in describing the formation of 2H , it is important to demonstrate that our treatment satisfies the fundamental requirement in the quantum mechanical description of identical fermions, that requirement is the complete antisymmetrization of the total wave function under particle exchange. In our three-nucleon system, this requirement is not merely a formal constraint but an essential feature that profoundly influences the structure and dynamics of the deuteron formation process.

The complete Hilbert space for each nucleon is given by the tensor product:

$$\mathcal{H}_{IS} = \mathcal{H}_I \otimes \mathcal{H}_S, \quad (3.44)$$

where $I = 1/2$ represents the isospin space with projections $\tau = \pm 1/2$ (proton/neutron states), and $S = 1/2$ represents the spin space with projections $m_S = \pm 1/2$. For a three-nucleon system, the basis states are constructed as:

$$|abc\rangle = |a\rangle_1 \otimes |b\rangle_2 \otimes |c\rangle_3, \quad (3.45)$$

where each single-nucleon state is characterized by $a = (\sigma_a, \tau_a) = (m_S, \tau)$.

The total antisymmetrization operator for three identical fermions acts as:

$$\mathcal{A}|abc\rangle = \frac{1}{\sqrt{3!}} (|abc\rangle + |cab\rangle + |bca\rangle - |bac\rangle - |acb\rangle - |cba\rangle). \quad (3.46)$$

Explicitly in terms of spin-isospin coordinates:

$$\begin{aligned} \mathcal{A}|abc\rangle = \frac{1}{\sqrt{3!}} (&|\sigma_a \tau_a, \sigma_b \tau_b, \sigma_c \tau_c\rangle + |\sigma_c \tau_c, \sigma_a \tau_a, \sigma_b \tau_b\rangle + |\sigma_b \tau_b, \sigma_c \tau_c, \sigma_a \tau_a\rangle \\ &- |\sigma_b \tau_b, \sigma_a \tau_a, \sigma_c \tau_c\rangle - |\sigma_a \tau_a, \sigma_c \tau_c, \sigma_b \tau_b\rangle - |\sigma_c \tau_c, \sigma_b \tau_b, \sigma_a \tau_a\rangle). \end{aligned} \quad (3.47)$$

This antisymmetrized state automatically satisfies the Pauli exclusion principle and ensures that the total wave function changes sign under the exchange of any two nucleons.

The antisymmetrization imposes strong constraints on the allowed physical states. Consider the case with total isospin projection $T_z = -1/2$, corresponding to the configuration $\tau_a = -1/2$, $\tau_b = -1/2$, $\tau_c = 1/2$ (two neutrons and one proton). The antisymmetrized state becomes:

$$\begin{aligned} |\mathcal{A}\rangle = \frac{1}{\sqrt{3!}} & (|\sigma_a(-1/2), \sigma_b(-1/2), \sigma_c(1/2)\rangle + |\sigma_c(1/2), \sigma_a(-1/2), \sigma_b(-1/2)\rangle \\ & + |\sigma_b(-1/2), \sigma_c(1/2), \sigma_a(-1/2)\rangle - |\sigma_b(-1/2), \sigma_a(-1/2), \sigma_c(1/2)\rangle \\ & - |\sigma_a(-1/2), \sigma_c(1/2), \sigma_b(-1/2)\rangle - |\sigma_c(1/2), \sigma_b(-1/2), \sigma_a(-1/2)\rangle) \neq 0. \end{aligned} \quad (3.48)$$

This non-vanishing result demonstrates that physically allowed states exist that satisfy both the antisymmetrization requirement and the charge conservation constraint. The structure can be further decomposed to reveal the underlying symmetry:

$$\begin{aligned} |\mathcal{A}\rangle = \frac{1}{\sqrt{3!}} & [(|\uparrow(-1/2), \downarrow(-1/2)\rangle - |\downarrow(-1/2), \uparrow(-1/2)\rangle) \otimes |\sigma_c(1/2)\rangle \\ & + |\sigma_c(1/2)\rangle \otimes (|\uparrow(-1/2), \downarrow(-1/2)\rangle - |\downarrow(-1/2), \uparrow(-1/2)\rangle) \\ & + |\downarrow(-1/2), \sigma_c(1/2), \uparrow(1/2)\rangle - |\uparrow(-1/2), \sigma_c(1/2), \downarrow(1/2)\rangle]. \end{aligned} \quad (3.49)$$

Symmetry Structure and Hamiltonian Commutation

The total permutation operator can be decomposed as:

$$P = P_{\text{orb}} \otimes P_{\text{iso}} \otimes P_{\text{spin}}, \quad (3.50)$$

while the Hamiltonian commutes with the total permutation operator:

$$[H, P] = 0, \quad (3.51)$$

it generally does not commute with the individual components:

$$[H, P_{\text{orb}}] \neq 0, \quad [H, P_{\text{iso}}] \neq 0, \quad [H, P_{\text{spin}}] \neq 0. \quad (3.52)$$

However, in exceptional cases where the Hamiltonian happens to commute with all individual permutation operators:

$$[H, P_{\text{orb}}] = [H, P_{\text{iso}}] = [H, P_{\text{spin}}] = 0, \quad (3.53)$$

the wave function factorizes into orbital and spin-isospin parts. In such scenarios, two distinct symmetry combinations yield totally antisymmetric wave functions:

$$\psi_A = (\psi_{\text{orb}})_S \otimes (\psi_{\text{iso+spin}})_A \quad (\text{bound states}), \quad (3.54)$$

$$\psi_A = (\psi_{\text{orb}})_A \otimes (\psi_{\text{iso+spin}})_S \quad (\text{unbound or excluded}). \quad (3.55)$$

Only the first combination, with symmetric orbital wave function and antisymmetric spin-isospin wave function, corresponds to physically bound states in our system. This

is precisely the structure that characterizes the deuteron wave function [30] in our model.

The antisymmetrization requirement has profound implications for the deuteron formation process: The antisymmetric spin-isospin wave function enforces specific correlations between nucleons, favoring the $T = 0$, $S = 1$ configuration that characterizes the physical deuteron. The symmetric orbital wave function allows for the relative s-wave dominance observed in the deuteron ground state, consistent with its predominantly $L = 0$ character. The symmetry constraints impose selection rules on transition matrix elements, determining which scattering channels contribute to deuteron formation. The antisymmetrization automatically incorporates Pauli blocking effects, preventing unphysical configurations where identical nucleons would occupy forbidden states.

In our Faddeev equation approach, the antisymmetrization is built into the channel wave functions ψ_α , ψ_β , and ψ_γ through the proper construction of the Jacobi coordinate representations and the implementation of the exchange symmetry between identical nucleons. This ensures that our model not only satisfies the formal requirement of antisymmetrization but also captures the essential physical consequences for deuteron structure and formation dynamics.

The successful incorporation of total antisymmetrization represents a crucial advantage of our approach over simpler models that may neglect or approximate this fundamental quantum mechanical requirement, providing a more rigorous foundation for studying three-body clustering phenomena in nuclear systems.

3.3 Three-Body Cluster Interactions

The previously analyzed cases did not involve interactions between possible clusters, which constitutes the central focus of our investigation. To address this crucial aspect, we begin with the matrix formulation of the three-body problem:

$$\begin{pmatrix} E - H_0 & 0 & 0 \\ 0 & E - H_0 & 0 \\ 0 & 0 & E - H_0 \end{pmatrix} \begin{pmatrix} \psi_\alpha \\ \psi_\beta \\ \psi_\gamma \end{pmatrix} = \begin{pmatrix} V_\alpha & V_\alpha & V_\alpha \\ V_\beta & V_\beta & V_\beta \\ V_\gamma & V_\gamma & V_\gamma \end{pmatrix} \begin{pmatrix} \psi_\alpha \\ \psi_\beta \\ \psi_\gamma \end{pmatrix}, \quad (3.56)$$

where $V_\alpha = -\lambda_\alpha \delta(x_\alpha)$, $V_\beta = -\lambda_\beta \delta(x_\beta)$, $V_\gamma = -\lambda_\gamma \delta(x_\gamma)$, and $\psi_\alpha = e^{iK_0 R + i k_r y_\alpha} \varphi(x_\alpha)$, with similar expressions for β and γ .

Jacobi coordinates are employed in configuration space to separate the center of mass of the three-particle system. For three particles, there exist three equivalent sets of Jacobi coordinates:

$$\begin{aligned} \mathbf{x}_\alpha &= \sqrt{\frac{2m_\beta m_\gamma}{(m_\beta + m_\gamma)m}} (\mathbf{r}_\gamma - \mathbf{r}_\beta), \\ \mathbf{y}_\alpha &= \sqrt{\frac{2m_\beta(m_\beta + m_\gamma)}{(m_\alpha + m_\beta + m_\gamma)m}} \left(\mathbf{r}_\alpha - \frac{m_\beta \mathbf{r}_\beta + m_\gamma \mathbf{r}_\gamma}{m_\beta + m_\gamma} \right), \end{aligned} \quad (3.57)$$

where $\mathbf{r}_\alpha$ and m_α are the position vectors and masses of individual particles, respectively. The choice of mass scale m is arbitrary. A representation of the clusters represented by the Jacobi sets given above is presented in the Figure 3.2.

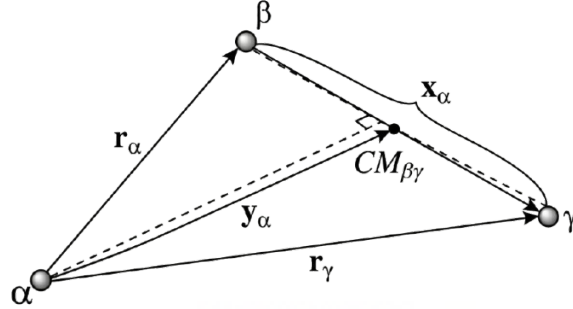


Figure 3.2: Possible arrangement for the channel α , the coordinate x_α is the relative one between the particles β and γ , the coordinate y_α corresponds to the position relative to the center of mass of $\beta - \gamma$ with α .

The three-particle problem is formulated using the Faddeev-Merkuriev (FM) equations [82]:

$$\begin{aligned} (E - H_0 - \sum_{\kappa=1}^3 w_i^l) \psi_\alpha &= (v_\alpha + w_\alpha^s)(\psi_\alpha + \psi_\beta + \psi_\gamma), \\ (E - H_0 - \sum_{\kappa=1}^3 w_i^l) \psi_\beta &= (v_\beta + w_\beta^s)(\psi_\alpha + \psi_\beta + \psi_\gamma), \\ (E - H_0 - \sum_{\kappa=1}^3 w_i^l) \psi_\gamma &= (v_\gamma + w_\gamma^s)(\psi_\alpha + \psi_\beta + \psi_\gamma), \end{aligned} \quad (3.58)$$

where w_i^l corresponds to the long-range part of the Coulomb potential. The follow expressions

$$\begin{aligned} x_i^l(x_i, y_i) &= w_i(x_i)[1 - \mathcal{X}_i(x_i, y_i)], \\ w_j^s(x_j, y_j) &= w_j(x_j)\mathcal{X}_j(x_j, y_j), \end{aligned} \quad (3.59)$$

corresponds to the short-range part of the Coulomb potential. The form of the cutoff function proposed by Merkuriev:

$$\mathcal{X}_i = \frac{2}{\left[1 + \exp\left\{\left(\frac{(x_i/x_0)^\mu}{1+y_i/y_0}\right)\right\}\right]}. \quad (3.60)$$

The short-range nuclear interaction potential, $v_i = \lambda_i \delta$.

We want to show that the Faddeev-Merkuriev equations are equivalent to the Schrödinger equation. Defining the total wave function $\Psi = \psi_1 + \psi_2 + \psi_3$, with $\alpha, \beta, \gamma = 1, 2, 3$, then summing the three Faddeev-Merkuriev channels, $i = 1, 2, 3$

$$\sum_{i=1}^3 (E - H_0 - \sum_{k=1}^3 w_k^l) \psi_i = \sum_{i=1}^3 (v_i + w_i^s) (\psi_1 + \psi_2 + \psi_3) \quad (3.61)$$

$$(E - H_0 - \sum_{k=1}^3 w_k^l) \sum_{i=1}^3 \Psi = \left(\sum_{i=1}^3 v_i + \sum_{i=1}^3 w_i^s \right) \Psi, \quad (3.62)$$

using $w_i = w_i^s + w_i^l$

$$\sum_{i=1}^3 w_i^s = W_{\text{total}} - \sum_{i=1}^3 w_i^l, \quad (3.63)$$

replacing in 3.62

$$E - H_0 - \sum_{k=1}^3 w_k^l \Psi = (V_{\text{total}} + W_{\text{total}} - \sum_{i=1}^3 w_i^l) \Psi. \quad (3.64)$$

Terms with w^l cancel out, recovering the Schrödinger equation; this equivalence justifies the use of the FM equations as an alternative formulation of the three-body scattering problem with Coulomb interactions.

$$(E - H_0) \Psi = (V_{\text{total}} + W_{\text{total}}) \Psi. \quad (3.65)$$

Having established the equivalence with Schrödinger, we can resort to the Lippmann-Schwinger formalism. Building upon the Lippmann-Schwinger formalism justification, we proceed with:

$$|\psi\rangle = |\phi\rangle + \frac{1}{E - H} V |\phi\rangle, \quad (3.66)$$

where $|\phi\rangle$ represents the known free spectator with binary cluster, and the interaction matrix takes the form:

$$V = \begin{pmatrix} 0 & \delta_1 & \delta_1 \\ \delta_2 & 0 & \delta_2 \\ \delta_3 & \delta_3 & 0 \end{pmatrix}. \quad (3.67)$$

The Green's function matrix operation yields:

$$\begin{pmatrix} G_1 & 0 & 0 \\ 0 & G_2 & 0 \\ 0 & 0 & G_3 \end{pmatrix} \begin{pmatrix} 0 & \delta_1 & \delta_1 \\ \delta_2 & 0 & \delta_2 \\ \delta_3 & \delta_3 & 0 \end{pmatrix} = \begin{pmatrix} 0 & G_1 \delta_1 & G_1 \delta_1 \\ G_2 \delta_2 & 0 & G_2 \delta_2 \\ G_3 \delta_3 & G_3 \delta_3 & 0 \end{pmatrix}, \quad (3.68)$$

applying this to the wave function components:

$$\begin{pmatrix} 0 & G_1 \delta_1 & G_1 \delta_1 \\ G_2 \delta_2 & 0 & G_2 \delta_2 \\ G_3 \delta_3 & G_3 \delta_3 & 0 \end{pmatrix} \begin{pmatrix} \phi_\alpha \\ \phi_\beta \\ \phi_\gamma \end{pmatrix} = \begin{pmatrix} G_1 \phi_\beta \delta_1 + G_1 \phi_\gamma \delta_1 \\ G_2 \phi_\alpha \delta_2 + G_2 \phi_\gamma \delta_2 \\ G_3 \phi_\alpha \delta_3 + G_3 \phi_\beta \delta_3 \end{pmatrix}. \quad (3.69)$$

For the first channel (α), we obtain the explicit expression:

$$\begin{aligned}
 \psi_\alpha = & -\lambda_\beta \int \frac{e^{iK(R-R')} e^{ik'_{x_\alpha}(x_\alpha-x'_\beta)} e^{ik'_{y_\alpha}(y_\alpha-y'_\beta)}}{E - \frac{\hbar^2 K'^2}{2M} - \frac{\hbar^2 k_{x_\alpha}^{\prime 2}}{2\mu_{x_\alpha}} - \frac{\hbar^2 k_{y_\beta}^{\prime 2}}{2\mu_{y_\beta}}} \delta(x'_\beta) \times \\
 & \left(\frac{1}{2\pi} e^{i(k_0 R - \sqrt{k_\beta^2 - E_r}|y'_\beta|)} + \frac{\lambda_\beta 4\mu \sqrt{k_\beta^2 - E_r}}{\hbar^2 \sqrt{k_\beta^2 - E_r} - \lambda_\beta 8\mu\pi} e^{-|y'_\beta| \sqrt{k_\beta^2 - E_r}} \right) dR' dK' dk'_{x_\alpha} dk'_{y_\alpha} dx'_\beta dy'_\beta \\
 & - \lambda_\gamma \int \frac{e^{iK(R-R')} e^{ik'_{x_\alpha}(x_\alpha-x'_\gamma)} e^{ik'_{y_\alpha}(y_\alpha-y'_\gamma)}}{E - \frac{\hbar^2 K'^2}{2M} - \frac{\hbar^2 k_{x_\alpha}^{\prime 2}}{2\mu_{x_\alpha}} - \frac{\hbar^2 k_{y_\beta}^{\prime 2}}{2\mu_{y_\beta}}} \delta(x'_\gamma) \times \\
 & \left(\frac{1}{2\pi} e^{i(k_0 R - \sqrt{k_\gamma^2 - E_r}|y'_\gamma|)} + \frac{\lambda_\gamma 4\mu \sqrt{k_\gamma^2 - E_r}}{\hbar^2 \sqrt{k_\gamma^2 - E_r} - \lambda_\gamma 8\mu\pi} e^{-|y'_\gamma| \sqrt{k_\gamma^2 - E_r}} \right) dR' dK' dk'_{x_\alpha} dk'_{y_\alpha} dx'_\gamma dy'_\gamma.
 \end{aligned} \tag{3.70}$$

After extensive integration, this simplifies to:

$$\begin{aligned}
 \psi_\alpha = & \frac{8\mu\pi^2}{\hbar^2} \frac{\lambda_\beta}{\sqrt{k_\beta^2 - 2E_r}} e^{-|x_\alpha| \sqrt{k_\beta^2 - 2E_r} - i \sqrt{k_\beta^2 - 2E_r} |y_\alpha|} + \\
 & \frac{\lambda_\beta^2 32\mu^2 \pi^3 \sqrt{k_\beta^2 - E_r}}{\hbar^2 \sqrt{k_\beta^2 - E_r} - \lambda_\beta 8\mu\pi} \frac{1}{\sqrt{k_\beta^2 - 2E_r}} e^{-|y_\alpha| \sqrt{k_\beta^2 - 2E_r} - |x_\alpha| \sqrt{k_\beta^2 - 2E_r}} + \\
 & \frac{8\mu\pi^2}{\hbar^2} \frac{\lambda_\gamma}{\sqrt{k_\gamma^2 - 2E_r}} e^{-|x_\alpha| \sqrt{k_\gamma^2 - 2E_r} - i \sqrt{k_\gamma^2 - 2E_r} |y_\alpha|} + \\
 & \frac{\lambda_\gamma^2 32\mu^2 \pi^3 \sqrt{k_\gamma^2 - E_r}}{\hbar^2 \sqrt{k_\gamma^2 - E_r} - \lambda_\gamma 8\mu\pi} \frac{1}{\sqrt{k_\gamma^2 - 2E_r}} e^{-|y_\alpha| \sqrt{k_\gamma^2 - 2E_r} - |x_\alpha| \sqrt{k_\gamma^2 - 2E_r}}.
 \end{aligned} \tag{3.71}$$

Similar expressions are obtained for channels β and γ , demonstrating the symmetric structure of the solution.

We construct the coupling matrix M with inter-channel couplings:

$$M = \begin{pmatrix} 0 & M_{\alpha\beta} & M_{\alpha\gamma} \\ M_{\beta\alpha} & 0 & M_{\beta\gamma} \\ M_{\gamma\alpha} & M_{\gamma\beta} & 0 \end{pmatrix}, \tag{3.72}$$

the resonance condition is determined by solving $\det(M - I) = 0$, which expands to:

$$\begin{aligned}
 \det(M - I) = & -I \cdot \det \begin{pmatrix} -1 & M_{\beta\gamma} \\ M_{\gamma\beta} & -1 \end{pmatrix} - M_{\alpha\beta} \cdot \det \begin{pmatrix} M_{\beta\alpha} & M_{\beta\gamma} \\ M_{\gamma\alpha} & -1 \end{pmatrix} + \\
 & M_{\alpha\gamma} \cdot \det \begin{pmatrix} M_{\beta\alpha} & -1 \\ M_{\gamma\alpha} & M_{\gamma\beta} \end{pmatrix} = \\
 & M_{\alpha\beta} M_{\beta\alpha} + M_{\alpha\gamma} M_{\gamma\alpha} + M_{\beta\gamma} M_{\gamma\beta} + \\
 & M_{\alpha\beta} M_{\beta\gamma} M_{\gamma\alpha} + M_{\alpha\gamma} M_{\beta\alpha} M_{\gamma\beta} - 1 = 0,
 \end{aligned} \tag{3.73}$$

where each M_{ij} is a complex function of E_r .

The analytical solution for the wave function amplitudes at the interaction points:

$$\begin{pmatrix} \phi_\alpha(0) \\ \phi_\beta(0) \\ \phi_\gamma(0) \end{pmatrix}, \quad (3.74)$$

is obtained by solving $(M - I)\phi(0) = 0$, leading to the system:

$$\begin{cases} -\phi_\alpha(0) + M_{\alpha\beta}\phi_\beta(0) + M_{\alpha\gamma}\phi_\gamma(0) = 0 \\ M_{\beta\alpha}\phi_\alpha(0) - \phi_\beta(0) + M_{\beta\gamma}\phi_\gamma(0) = 0 \\ M_{\gamma\alpha}\phi_\alpha(0) + M_{\gamma\beta}\phi_\beta(0) - \phi_\gamma(0) = 0, \end{cases} \quad (3.75)$$

the explicit solution in terms of matrix elements is:

$$\begin{pmatrix} \phi_\alpha(0) \\ \phi_\beta(0) \\ \phi_\gamma(0) \end{pmatrix} = N \begin{pmatrix} 1 - M_{\beta\gamma}M_{\gamma\beta} - M_{\beta\gamma}M_{\gamma\alpha} - M_{\alpha\gamma}M_{\gamma\beta} \\ M_{\alpha\beta} + M_{\alpha\gamma}M_{\gamma\beta} + M_{\alpha\beta}M_{\beta\gamma}M_{\gamma\alpha} \\ M_{\alpha\gamma} + M_{\alpha\beta}M_{\beta\gamma} + M_{\alpha\gamma}M_{\beta\alpha}M_{\gamma\beta} \end{pmatrix}, \quad (3.76)$$

where the normalization constant is:

$$N = \frac{1}{\sqrt{\sum |\phi_i|^2}}. \quad (3.77)$$

3.3.1 Coulomb Interaction

We now incorporate the Coulomb interaction, expressed in Jacobi coordinates as:

$$V_c = V_0 \sum_{\alpha=1}^3 \left[\frac{m_\beta + m_\gamma}{2m_\beta m_\gamma} \right]^{3/2} \delta(x_\alpha - R_n) \tau_z^{(\beta)} (1 - P_{\beta\gamma}), \quad (3.78)$$

where V_0 represents the potential intensity, $\tau_z^{(i)}$ represents the Isospin operator and $(1 - P_{ij})$ guarantees antisymmetry.

The full solution including Coulomb interactions requires evaluate:

$$\frac{1}{E - H} V |\phi\rangle = \begin{pmatrix} G_1\phi_\beta V_c^{(1)} + G_1\phi_\gamma V_c^{(1)} + V_c^{(1)}[(V_c^{(2)}G_2 + V_c^{(3)})\phi_\alpha + V_c^{(3)}G_3\phi_\beta + V_c^{(2)}G_2\phi_\gamma] \\ G_2\phi_\alpha V_c^{(2)} + G_2\phi_\gamma V_c^{(2)} + V_c^{(2)}[V_c^{(3)}G_3\phi_\alpha + (V_c^{(1)}G_1 + V_c^{(3)}G_3)\phi_\beta + V_c^{(1)}G_1\phi_\gamma] \\ G_3\phi_\alpha V_c^{(3)} + G_3\phi_\beta V_c^{(3)} + V_c^{(3)}[V_c^{(2)}G_2\phi_\alpha + V_c^{(1)}G_1\phi_\beta + (V_c^{(1)}G_1 + V_c^{(2)}G_2)\phi_\gamma] \end{pmatrix}. \quad (3.79)$$

The resulting expressions for each channel become considerably more complex, involving multiple terms that capture the interplay between nuclear and Coulomb

interactions. For channel α , we obtain the transition operator:

$$\psi_{C_\alpha} = \frac{8\pi^2\mu}{\hbar^2} \left[\frac{m_\alpha + m_\beta}{2m_\alpha m_\beta} \right]^{3/2} V_0 \tau_z^{(\alpha)} (1 - P_{\alpha\beta}) \frac{1}{\sqrt{k_\beta^2 - 2E_r}} e^{-i\sqrt{k_\beta^2 - E_r} y_\alpha} \times$$

$$\left[e^{-(x_\alpha - R_n)\sqrt{k_\beta^2 - 2E_r}} + e^{-(x_\alpha + R_n)\sqrt{k_\beta^2 - 2E_r}} \right] + \dots, \quad (3.80)$$

where the ellipsis indicates terms that represent corrections to the Lippman-S functional equation. The Born series is exactly truncated, however resulting amplitude is evaluated in different points including the potential range, but we choose the amplitude evaluated in origin.

With Coulomb interactions included, we construct an extended coupling matrix:

$$M = \begin{pmatrix} M_{\alpha\alpha} & M_{\alpha\beta} & M_{\alpha\gamma} \\ M_{\beta\alpha} & M_{\beta\beta} & M_{\beta\gamma} \\ M_{\gamma\alpha} & M_{\gamma\beta} & M_{\gamma\gamma} \end{pmatrix}, \quad (3.81)$$

where each M_{ij} is now a 4×4 submatrix. This 12×12 matrix captures all couplings between the three physical channels and their respective internal degrees of freedom.

Zeros occur when the sum of scattering amplitudes equals unity, physically corresponding to resonances where the scattering phase passes through $\pi/2$.

The solution of the homogeneous system $(M - I)\phi = 0$ provides the resonance wave functions.

$$\begin{pmatrix} \phi_\alpha(0) \\ \phi_\beta(0) \\ \phi_\gamma(0) \end{pmatrix} = M^{-1} \begin{pmatrix} \phi_\alpha(0) \\ \phi_\beta(0) \\ \phi_\gamma(0) \end{pmatrix}, \quad (3.82)$$

to find the values for $\begin{pmatrix} \phi_\alpha(0) \\ \phi_\beta(0) \\ \phi_\gamma(0) \end{pmatrix}$ the equation to solve is:

$$\begin{pmatrix} M_{\alpha\alpha} - I_4 & M_{\alpha\beta} & M_{\alpha\gamma} \\ M_{\beta\alpha} & M_{\beta\beta} - I_4 & M_{\beta\gamma} \\ M_{\gamma\alpha} & M_{\gamma\beta} & M_{\gamma\gamma} - I_4 \end{pmatrix} \begin{pmatrix} \phi_\alpha \\ \phi_\beta \\ \phi_\gamma \end{pmatrix} = 0. \quad (3.83)$$

We look to solve this system by writing ϕ_β y ϕ_γ in terms of ϕ_α

$$\phi_\alpha = -(M_{\alpha\alpha} - I_4)^{-1} [M_{\alpha\beta}\phi_\beta + M_{\alpha\gamma}\phi_\gamma], \quad (3.84)$$

we obtain a reduce system for ϕ_β, ϕ_γ

$$\begin{aligned} R_{\beta\beta} &= M_{\beta\beta} - I_4 - M_{\beta\alpha}(M_{\alpha\alpha} - I_4)^{-1}M_{\alpha\beta} \\ R_{\beta\gamma} &= M_{\beta\gamma} - M_{\beta\alpha}(M_{\alpha\alpha} - I_4)^{-1}M_{\alpha\gamma} \\ R_{\gamma\beta} &= M_{\gamma\beta} - M_{\gamma\alpha}(M_{\alpha\alpha} - I_4)^{-1}M_{\alpha\beta} \\ R_{\gamma\gamma} &= M_{\gamma\gamma} - I_4 - M_{\gamma\alpha}(M_{\alpha\alpha} - I_4)^{-1}M_{\alpha\gamma}, \end{aligned} \quad (3.85)$$

using the last expressions we obtain the following reduce system

$$\begin{pmatrix} R_{\beta\beta} & R_{\beta\gamma} \\ R_{\gamma\beta} & R_{\gamma\gamma} \end{pmatrix} \begin{pmatrix} \phi_\beta \\ \phi_\gamma \end{pmatrix} = 0, \quad (3.86)$$

each block M_{ij} has the next form:

$$M_{ij} = \sum_{n=1}^8 M_{ij}^{(n)}, \quad (3.87)$$

finally the explicit eigenvectors take the form:

$$\phi_\alpha = \begin{pmatrix} \phi_{\alpha 1} \\ \phi_{\alpha 2} \\ \phi_{\alpha 3} \\ \phi_{\alpha 4} \end{pmatrix} = -(M_{\alpha\alpha} - I_4)^{-1} \left[\left(\sum_{n=1}^8 M_{\alpha\beta}^{(n)} \right) \phi_\beta + \left(\sum_{n=1}^8 M_{\alpha\gamma}^{(n)} \right) \phi_\gamma \right]. \quad (3.88)$$

Each component contains intricate sums over all interaction terms:

$$\phi_{\alpha i} = - \sum_{j=1}^4 \sum_{k=1}^4 [(M_{\alpha\alpha} - I_4)^{-1}]_{ij} \left[\left(\sum_{n=1}^8 (M_{\alpha\beta}^{(n)})_{jk} \right) \phi_{\beta k} + \left(\sum_{n=1}^8 (M_{\alpha\gamma}^{(n)})_{jk} \right) \phi_{\gamma k} \right]. \quad (3.89)$$

Where the sum over $n = 1, 2, 3, 4$ are the terms dependent on V_0 and $n = 5, 6, 7, 8$ have to do with V_0^2 , the sum with respect to $k = 1, 2, 3, 4$ corresponds to the combinations with the channel β , this sum represents how the total amplitude in the channel β (summed over all its subchannels) couples to the subchannel j of the channel α , $j = 1, 2, 3, 4$: The 4 subchannels of the channel α , $[(M_{\alpha\alpha} - I_4)^{-1}]_{ij}$: Element (i, j) of the inverse matrix

This comprehensive framework provides the mathematical foundation for analyzing deuteron formation through three-nucleon scattering, capturing both the nuclear interactions via delta potentials and the essential features of the Coulomb interaction through our dual-delta model.

3.3.2 Total Cross Section Calculation in Hyperspherical Coordinates

To compute the total cross section for deuteron formation via three-body scattering, we employ hyperspherical coordinates which provide a natural framework for integrating over the complete phase space of the three-body system. To rewrite them in hyperspherical coordinates, we will use the standard transformation where the hyperradius $\rho = \sqrt{E_r}$ is invariant for all channels, and the hyperangle θ_i varies according to the Jacobi channel ($i = \alpha, \beta, \gamma$).

Similarly we define a couple of frequent constants:

$$C_1 = \frac{8\pi^2\mu}{\hbar^2}, \quad C_2 = \frac{16\mu^2\pi^3}{\hbar^2}. \quad (3.90)$$

As can be appreciated, the structure for each channel is identical, so taking advantage of this fact and to avoid confusion, we will only show the development

for the α channel. Analogously for the other channels, the transition operator for α channel is:

$$\begin{aligned}
\psi_{\alpha}^{\text{Coulomb}} = & C_1 \left[\frac{m_{\alpha} + m_{\beta}}{2m_{\alpha}m_{\beta}} \right]^{3/2} V_0 \tau_z^{(\alpha)} (1 - P_{\alpha\beta}) \times \\
& \left[\frac{1}{\sqrt{k_{\beta}^2 - 2E_r}} e^{-i\sqrt{k_{\beta}^2 - E_r} y_{\alpha}} \left(e^{-(x_{\alpha} - R_n)\sqrt{k_{\beta}^2 - 2E_r}} + e^{-(x_{\alpha} + R_n)\sqrt{k_{\beta}^2 - 2E_r}} \right) + (\beta \leftrightarrow \gamma) \right] \\
& + \frac{\lambda_{\beta} V_0 C_2 \sqrt{k_{\beta}^2 - E_r}}{\hbar^2 \sqrt{k_{\beta}^2 - E_r} - \lambda_{\beta} 8\mu\pi} \frac{1}{\sqrt{k_{\beta}^2 - 2E_r}} e^{-\sqrt{k_{\beta}^2 - E_r} y_{\alpha}} \tau_z^{(\alpha)} (1 - P_{\alpha\beta}) \times \\
& \times \left[e^{-(x_{\alpha} - R_n)\sqrt{k_{\beta}^2 - 2E_r}} + e^{-(x_{\alpha} + R_n)\sqrt{k_{\beta}^2 - 2E_r}} \right] + (\beta \leftrightarrow \gamma) \\
& + V_0^2 \left[\frac{m_{\beta} + m_{\gamma}}{2m_{\beta}m_{\gamma}} \right]^{3/2} \left[\frac{m_{\alpha} + m_{\gamma}}{2m_{\alpha}m_{\gamma}} \right]^{3/2} \tau_z^{(\beta)} (1 - P_{\beta\gamma}) \tau_z^{(\alpha)} (1 - P_{\alpha\gamma}) \\
& \times \left[\frac{1}{\sqrt{k_{\alpha}^2 - 2E_r}} e^{-i\sqrt{k_{\alpha}^2 - E_r} y_{\beta}} \left(e^{2R_n\sqrt{k_{\alpha}^2 - 2E_r}} + e^{-2R_n\sqrt{k_{\alpha}^2 - 2E_r}} \right) \frac{8\mu\pi^2}{\hbar^2} \right. \\
& \left. + \frac{\lambda_{\alpha} V_0 16\mu^2 \pi^3 \sqrt{k_{\alpha}^2 - E_r}}{\hbar^2 \sqrt{k_{\alpha}^2 - E_r} - \lambda_{\alpha} 8\mu\pi} \frac{1}{\sqrt{k_{\alpha}^2 - 2E_r}} e^{-\sqrt{k_{\alpha}^2 - E_r} y_{\beta}} \left(e^{2R_n\sqrt{k_{\alpha}^2 - 2E_r}} + e^{-2R_n\sqrt{k_{\alpha}^2 - 2E_r}} \right) \right] \\
& + V_0^2 \left[\frac{m_{\beta} + m_{\gamma}}{2m_{\beta}m_{\gamma}} \right]^{3/2} \left[\frac{m_{\alpha} + m_{\beta}}{2m_{\alpha}m_{\beta}} \right]^{3/2} \tau_z^{(\beta)} (1 - P_{\beta\gamma}) \tau_z^{(\alpha)} (1 - P_{\alpha\beta}) \\
& \times \left[\frac{1}{\sqrt{k_{\alpha}^2 - 2E_r}} e^{-i\sqrt{k_{\alpha}^2 - E_r} y_{\gamma}} \left(e^{2R_n\sqrt{k_{\alpha}^2 - 2E_r}} + e^{-2R_n\sqrt{k_{\alpha}^2 - 2E_r}} \right) \frac{8\mu\pi^2}{\hbar^2} \right. \\
& \left. + \frac{\lambda_{\alpha} V_0 16\mu^2 \pi^3 \sqrt{k_{\alpha}^2 - E_r}}{\hbar^2 \sqrt{k_{\alpha}^2 - E_r} - \lambda_{\alpha} 8\mu\pi} \frac{1}{\sqrt{k_{\alpha}^2 - 2E_r}} e^{-\sqrt{k_{\alpha}^2 - E_r} y_{\gamma}} \left(e^{2R_n\sqrt{k_{\alpha}^2 - 2E_r}} + e^{-2R_n\sqrt{k_{\alpha}^2 - 2E_r}} \right) \right] \\
& + V_0^2 \left[\frac{m_{\beta} + m_{\gamma}}{2m_{\beta}m_{\gamma}} \right]^{3/2} \left[\frac{m_{\alpha} + m_{\beta}}{2m_{\alpha}m_{\beta}} \right]^{3/2} \tau_z^{(\beta)} (1 - P_{\beta\gamma}) \tau_z^{(\alpha)} (1 - P_{\alpha\beta}) \\
& \times \left[\frac{1}{\sqrt{k_{\beta}^2 - 2E_r}} e^{-i\sqrt{k_{\beta}^2 - E_r} y_{\gamma}} \left(e^{2R_n\sqrt{k_{\beta}^2 - 2E_r}} + e^{-2R_n\sqrt{k_{\beta}^2 - 2E_r}} \right) \frac{8\mu\pi^2}{\hbar^2} \right. \\
& \left. + \frac{\lambda_{\alpha} V_0 16\mu^2 \pi^3 \sqrt{k_{\beta}^2 - E_r}}{\hbar^2 \sqrt{k_{\beta}^2 - E_r} - \lambda_{\beta} 8\mu\pi} \frac{1}{\sqrt{k_{\beta}^2 - 2E_r}} e^{-\sqrt{k_{\beta}^2 - E_r} y_{\gamma}} \left(e^{2R_n\sqrt{k_{\beta}^2 - 2E_r}} + e^{-2R_n\sqrt{k_{\beta}^2 - 2E_r}} \right) \right]
\end{aligned} \tag{3.91}$$

$$\begin{aligned}
& + V_0^2 \left[\frac{m_\beta + m_\gamma}{2m_\beta m_\gamma} \right]^{3/2} \left[\frac{m_\alpha + m_\gamma}{2m_\alpha m_\gamma} \right]^{3/2} \tau_z^{(\beta)} (1 - P_{\beta\gamma}) \tau_z^{(\alpha)} (1 - P_{\alpha\gamma}) \\
& \times \left[\frac{1}{\sqrt{k_\gamma^2 - 2E_r}} e^{-i\sqrt{k_\gamma^2 - E_r} y_\alpha} \left(e^{2R_n \sqrt{k_\gamma^2 - 2E_r}} + e^{-2R_n \sqrt{k_\gamma^2 - 2E_r}} \right) \frac{8\mu\pi^2}{\hbar^2} \right. \\
& \left. + \frac{\lambda_\alpha V_0 16\mu^2 \pi^3 \sqrt{k_\gamma^2 - E_r}}{\hbar^2 \sqrt{k_\gamma^2 - E_r} - \lambda_\alpha 8\mu\pi} \frac{1}{\sqrt{k_\gamma^2 - 2E_r}} e^{-\sqrt{k_\alpha^2 - E_r} y_\alpha} \left(e^{2R_n \sqrt{k_\gamma^2 - 2E_r}} + e^{-2R_n \sqrt{k_\gamma^2 - 2E_r}} \right) \right].
\end{aligned}$$

We note that the hyperradius ρ contains all the energetic dependence and the hyperangular coordinates parameterize the distribution of momenta between the pairs.

We proceed now to establish the form of the integral to solve in order to obtain the total cross section σ . Working in the asymptotic limit, we extract the terms that have the form:

$$\begin{aligned}
f = & \frac{\lambda V_0 16\mu^2 \pi^3 \sqrt{k_i^2 - E_r}}{\hbar^2 \sqrt{k_i^2 - E_r} - \lambda 8\mu\pi} \frac{1}{\sqrt{k_i^2 - 2E_r}} \\
& + V_0^2 \left[\frac{m_i + m_j}{2m_i m_j} \right]^{3/2} \left[\frac{m_i + m_k}{2m_i m_k} \right]^{3/2} \frac{1}{\sqrt{k_i^2 - 2E_r}} \frac{8\mu\pi^2}{\hbar^2} \\
& + \frac{8\mu\pi^2}{\hbar^2} \frac{\lambda}{\sqrt{k_i^2 - 2E_r}} \\
& + \frac{\lambda^2 32\mu^2 \pi^3 \sqrt{k_i^2 - E_r}}{\hbar^2 \sqrt{k_i^2 - E_r} - \lambda_\beta 8\mu\pi} \frac{1}{\sqrt{k_i^2 - 2E_r}},
\end{aligned} \tag{3.92}$$

where $i, j, k = \alpha, \beta, \gamma$. At large distances, the exponentials accompanying these terms combine to give outgoing spherical waves, whose coefficients are precisely the terms we extracted. The terms we keep are precisely the coefficients of the outgoing spherical wave in the asymptotic expansion. They contain all the essential dynamic information: energetic dependence, resonances, and kinematic factors.

Now we define the function $f(E_r, \theta_\alpha, \theta_\beta, \theta_\gamma)$ as the sum of the terms selected above. The total cross section $\sigma(E_r)$ is calculated by integrating $|f|^2$ over the three-particle phase space in the center of mass system, with the delta for total momentum conservation:

$$K \int |f|^2 \delta(k_\alpha + k_\beta + k_\gamma) d\Omega \quad \text{where} \quad d\Omega = \sin \theta d\theta d\phi. \tag{3.93}$$

Here K represents a normalization constant and the transformation to hyperspherical coordinates is given by: $k_\alpha = \sqrt{E_r} \cos \phi \sin \theta$, $k_\beta = \sqrt{E_r} \sin \phi \sin \theta$, $k_\gamma = \sqrt{E_r} \cos \theta$, with the hyperradius defined as $\rho = \sqrt{E_r}$. In hyperspherical coordinates, the phase space reduces to an integral over hyperspherical angles due to energy and momentum conservation

$$\sigma_{total} = K \frac{1}{\sqrt{E_r}} \int_0^{2\pi} |f(\phi', E_r, \theta = -\text{arccot}(\sqrt{2} \sin \phi'))|^2 \left(\frac{1}{1 + 2 \sin^2 \phi'} \right)^{3/2} d\phi', \tag{3.94}$$

where $|f|^2$ is evaluated at:

$$\begin{aligned} k_\alpha &= \sqrt{E_r} \frac{\cos(\phi' - \pi/4)}{\sqrt{1 + 2 \sin^2 \phi'}} \\ k_\beta &= \sqrt{E_r} \frac{\sin(\phi' - \pi/4)}{\sqrt{1 + 2 \sin^2 \phi'}} \\ k_\gamma &= -\sqrt{E_r} \frac{\sqrt{2} \sin \phi'}{\sqrt{1 + 2 \sin^2 \phi'}}. \end{aligned} \quad (3.95)$$

Taking into account the isospin and summing over the initial and final states, we can write the complete form of σ_{total} , since, remember, we want to take into account all possible contributions for the process $NNN \rightarrow d + N$ where the resulting nucleon can be a proton or a neutron:

$$\sigma_{\text{total}} = \sum_{\tau_i, \tau_f} K \frac{1}{\sqrt{E_r}} \int_0^{2\pi} |f(\phi', E_r)|^2 \left(\frac{1}{1 + 2 \sin^2 \phi'} \right)^{3/2} d\phi'. \quad (3.96)$$

It is possible to evaluate this final expression numerically and assign values to the parameters of the potentials λ , V_0 to generate a graph. To have a point of comparison with the experimental data, we opted to use the optical theorem and thus reproduce a graph to compare with the collision rate reported by the experiments.

Recall that $\sigma_{\text{tot}} = \int \frac{d\sigma}{d\Omega} d\Omega$ measures the total probability that an incident particle will interact (be scattered or absorbed) with the target. The optical theorem states:

$$\text{Im} f(\theta = 0) = \frac{k \sigma_{\text{tot}}}{4\pi}. \quad (3.97)$$

This links the imaginary part of the scattering amplitude in the forward direction to the total cross section. The collision rate RR (number of collisions per unit time) in a scattering experiment can be expressed as:

$$R = \Phi \sigma_{\text{tot}}, \quad (3.98)$$

where Φ is the incident flux (number of incident particles per unit area and unit time), the incident flux is proportional to $|j_{\text{incid}}|$, and the number of particles scattered at a solid angle $d\Omega$ is proportional to $|f|^2 |j_{\text{incid}}|$. Therefore, the total scattering event rate (collision rate) is:

$$R = \Phi \int |f|^2 d\Omega = \Phi \sigma_{\text{tot}}, \quad (3.99)$$

the optical theorem connects σ_{tot} with $\text{Im} f(0)$. Then, we can write:

$$R = \Phi 4\pi \text{Im} f(\theta = 0), \quad (3.100)$$

this means that the collision rate is determined by the imaginary part of the scattering amplitude.

We take the amplitude terms described in (3.92) to find the imaginary part of $f(0)$ for which we need to evaluate at $k = \sqrt{E_r/3}$.

After having done algebraic work we obtain

$$\text{Im}[f] = \frac{1}{b} \left[\frac{8\mu\pi^2 V_0^2}{\hbar^2 m^3} + \frac{8\mu\pi\lambda}{\hbar^2} + \frac{\lambda V_0 16\mu^2 \pi^3 a(\hbar^2 a)}{(\lambda 8\mu\pi)^2 + \hbar^4 a^2} + \frac{\lambda^2 32\mu^2 \pi^3 a(\hbar^2 a)}{(\lambda 8\mu\pi)^2 + \hbar^4 a^2} \right], \quad (3.101)$$

where $a = \sqrt{\frac{2}{3}E_r}$ and $b = \sqrt{\frac{5}{3}E_r}$.

We assume equivalent masses, which agrees for our case, in which the nucleons can be proton or neutron ¹ $m \approx 939$ MeV and the intensity of the delta-type potential is equal for the three channels, $\lambda_\alpha = \lambda_\beta = \lambda_\gamma = \lambda$. The resulting expression maintains significant complexity, to solve it we make use of a numerical approximation to manage to obtain the total cross section and observe its respective behavior.

Having established our expressions for σ_{total} and for the collision rate, we can verify the validity of our model by evaluating these expressions, plotting them, and comparing their characteristics. This comprehensive approach establishes a rigorous foundation for comparing theoretical predictions with experimental measurements of deuteron production in nuclear reactions, with particular relevance for understanding cluster formation in heavy-ion collisions and astrophysical environments.

¹Since we have been very careful with isospin and charge of the particles, it would be more rigorous to use isospin operators in front of each mass, with values $m_n = 939.565$ MeV and $m_p = 938.27$ MeV, but our results do not change so much if we use equal masses.

4 Results

4.1 Triangular Visualization of Scattering Amplitudes

The visualization of scattering amplitudes in triangular coordinates provides a powerful tool for understanding the phase space structure and interference relationships between different scattering channels. This representation allows for comprehensive analysis of the complex interplay between nuclear and Coulomb interactions in the three-body system.

The triangular coordinate transformation employed in our analysis maps the constrained momentum space $k_\alpha + k_\beta + k_\gamma = \text{constant}$ to Cartesian coordinates through the transformation:

$$x = 0.5 \frac{2b + c}{a + b + c}, \quad (4.1)$$

$$y = \frac{\sqrt{3}}{2} \frac{c}{a + b + c}, \quad (4.2)$$

where a , b , and c represent the momentum magnitudes in different channels. This mapping provides a symmetric representation that preserves the relative weight of each channel while enabling two-dimensional visualization of the three-dimensional constrained space.

The first system analyzed corresponds to amplitudes of the form:

$$\alpha = \sum_{i=\beta,\gamma} \left[\frac{8\pi^2\mu}{\hbar^2} \frac{\lambda_i}{\sqrt{k_i^2 - 2E_r}} e^{-x_\alpha \sqrt{k_i^2 - 2E_r} - iy_\alpha \sqrt{k_i^2 - E_r}} \right] \quad (4.3)$$

$$+ \frac{\lambda_i^2 32\mu^2 \pi^3 \sqrt{k_i^2 - E_r}}{\hbar^2 \sqrt{k_i^2 - E_r} - \lambda_i 8\mu\pi \sqrt{k_i^2 - 2E_r}} \frac{1}{\sqrt{k_i^2 - 2E_r}} e^{-y_\alpha \sqrt{k_i^2 - E_r} - x_\alpha \sqrt{k_i^2 - 2E_r}}, \quad (4.4)$$

with analogous expressions for β and γ .

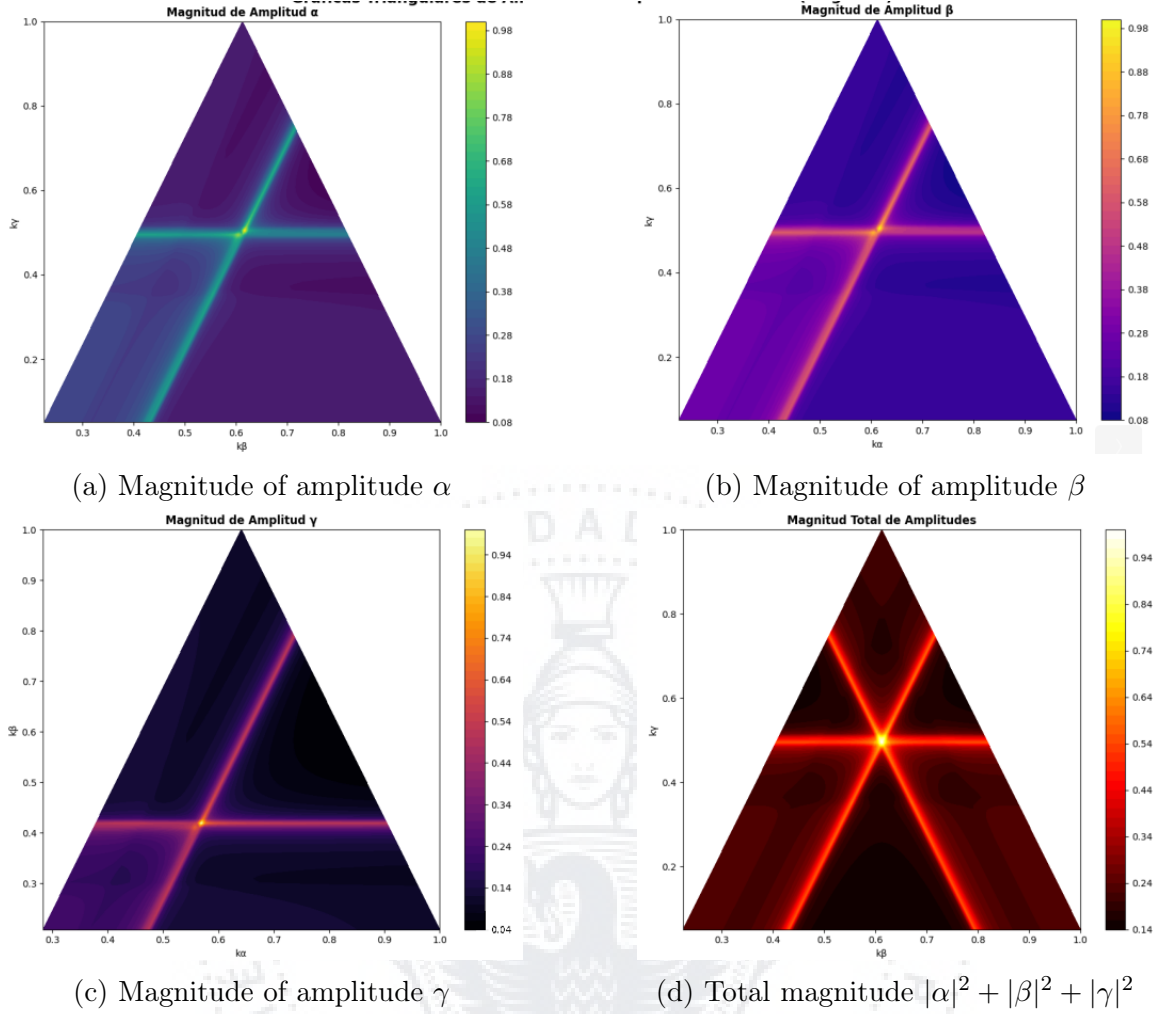


Figure 4.1: Magnitude distributions in triangular coordinates for the basic amplitude system. The axes represent combinations of k_β and k_γ for α , and analogously for the other amplitudes. The color scale indicates the magnitude of each amplitude component.

As observed in Figure 4.1a, amplitude α exhibits a well-defined structure characterized by a principal maximum located in the region where k_β and k_γ are comparable ($x \approx 0.5$, $y \approx 0.3$). This configuration suggests strong correlations between the β and γ momentum components in the α channel. The presence of concentric interference rings with regular spacing indicates coherent superposition of multiple scattering pathways, while the suppression at vertices where one momentum component dominates reflects the kinematic constraints of the three-body system. The approximate symmetry under exchange $k_\beta \leftrightarrow k_\gamma$ demonstrates the underlying symmetry of the interaction potential.

Figure 4.1b, 4.1c reveals a similar behavior for amplitude β and γ . This enhanced kinematic sensitivity suggests stronger dependence on specific momentum configurations.

Figure 4.1d presents the combined magnitude $|\alpha|^2 + |\beta|^2 + |\gamma|^2$, the well-localized maxima indicate resonant configurations where constructive interference occurs across

all channels simultaneously. The lattice-like pattern suggests the existence of normal modes in the coupled system, with characteristic periodicities reflecting the underlying dynamical symmetries.

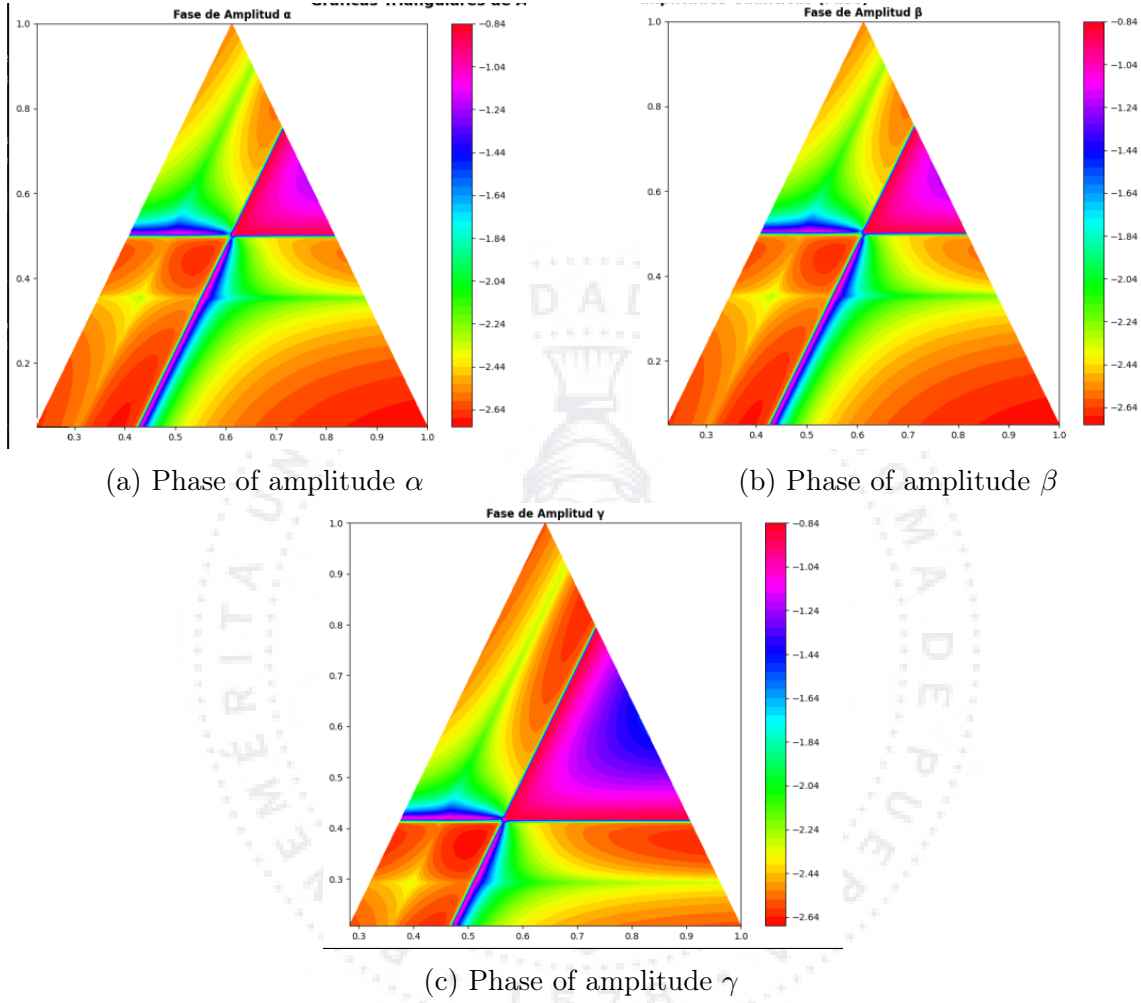


Figure 4.2: Phase distributions in triangular coordinates. The 2π discontinuities indicate branch cuts in the complex plane, while vortices correspond to poles of the S -matrix. The color wheel represents phase angles from $-\pi$ to π .

Figures 4.2a, 4.2c, 4.2b displays a well-defined central vortex with a characteristic 2π phase change, indicative of a first-order pole in the complex energy plane. The spiral structure radiating from the vortex center is typical of resonant behavior, while the clearly defined branch cut lines demarcate regions of analytic continuity. The smooth phase variation in regions distant from singularities suggests predominantly perturbative behavior in those kinematic regimes.

4.1.1 Coulomb Interaction System Analysis

The second system analyzed incorporates Coulomb interactions through amplitudes of the general form:

$$\alpha = \sum_{i=\beta,\gamma} \left[\frac{8\pi^2\mu}{\hbar^2} \left(\frac{m_\alpha + m_i}{2m_\alpha m_i} \right)^{3/2} V_0 \tau_z^{(\alpha)} (1 - P_{\alpha i}) \frac{1}{\sqrt{k_i^2 - 2E_r}} \right. \quad (4.5)$$

$$\times e^{-i\sqrt{k_i^2 - E_r} y_\alpha} \left[e^{-(x_\alpha - R_n)\sqrt{k_i^2 - 2E_r}} + e^{-(x_\alpha + R_n)\sqrt{k_i^2 - 2E_r}} \right] \quad (4.6)$$

$$+ \text{higher-order terms}], \quad (4.7)$$

with displacement parameter R_n and analogous expressions for β and γ .

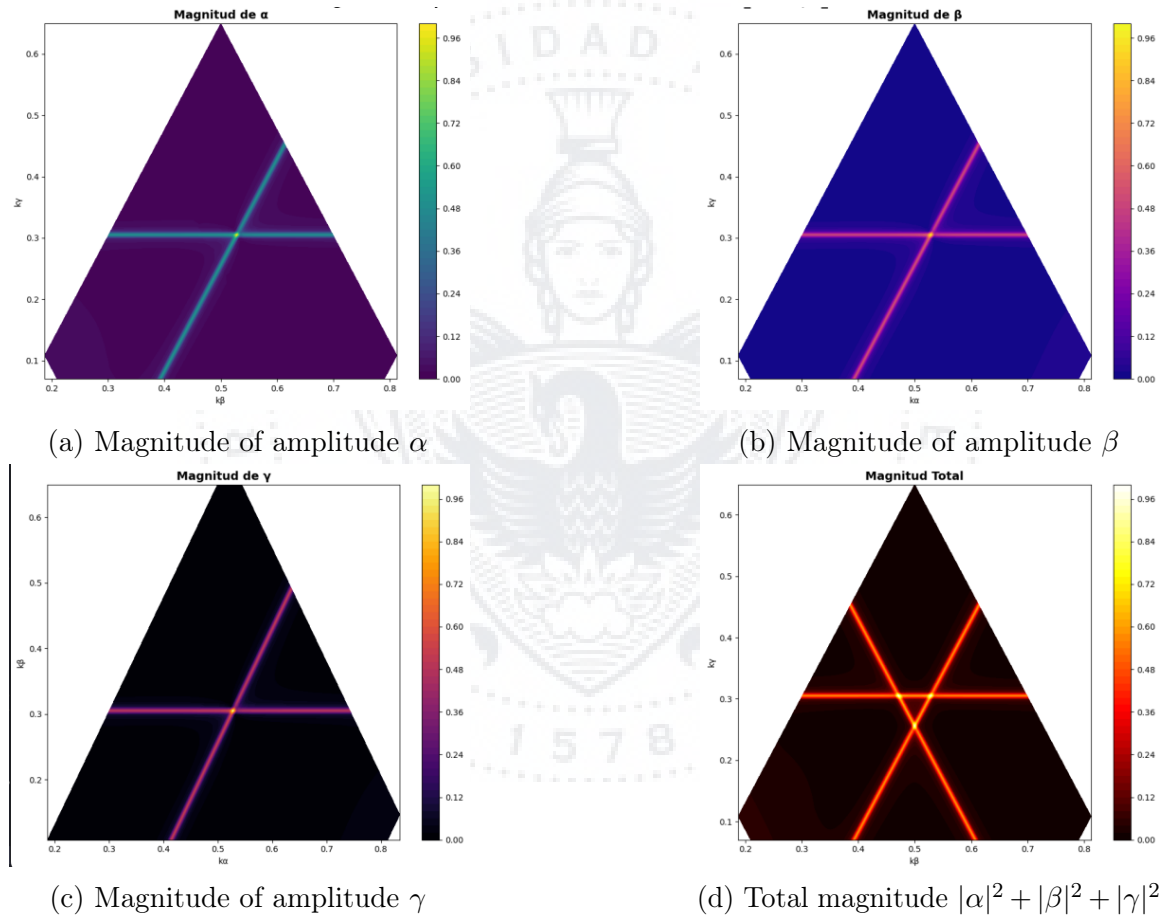


Figure 4.3: Magnitude distributions for the system with Coulomb displacement R_n . Complex interference patterns with multiple localized maxima are observed, reflecting the additional structure introduced by the Coulomb interaction.

The introduction of Coulomb interactions through the displacement parameter R_n produces significant modifications to the amplitude distributions. Figure 4.3a shows enhanced localization and the emergence of secondary structures not present in the basic system. Figure 4.3b displays increased complexity with multiple well-separated

maxima, suggesting the formation of distinct resonant states. Figure 4.3c maintains its transitional character but with richer substructure.

The total magnitude shown in Figure 4.3d reveals a particularly significant pattern characterized by three distinct bright points or maxima. These points represent specific configurations in momentum space where constructive interference occurs simultaneously across all scattering channels. The emergence of these discrete maxima can be understood through the interplay between the Coulomb displacement term and energy conservation constraints.

The three distinct points in the total amplitude correspond to three distinct kinematic regimes: The leftmost bright point corresponds to configurations where k_α is minimal while k_β and k_γ share the majority of the available momentum. This configuration favors the formation of a $(\beta\text{-}\gamma)$ cluster with the α particle acting as a spectator with low relative momentum. The central bright region represents the symmetric case where $k_\alpha \approx k_\beta \approx k_\gamma$, indicating that all three particles emerge with comparable momenta. This configuration corresponds to the center-of-mass frame where no single particle dominates the momentum distribution. The rightmost bright point indicates configurations where one particle (typically α) carries a significantly larger fraction of the total momentum, while the other two particles form a low-momentum cluster. This represents the inverse kinematic regime compared to the first configuration.

The formation of these distinct maxima suggests that the system preferentially selects specific momentum partitions that satisfy both energy conservation and the interference conditions imposed by the Coulomb potential. Each maximum represents a different possible cluster formation pathway.

The phase distributions with Coulomb interactions exhibit significantly enhanced structure compared to the basic system. Figures 4.4a, 4.4b, 4.4c displays a remarkable arrangement of phase. The observed patterns provide crucial information about the scattering matrix's analytic structure. Each vortex in the phase distributions corresponds to a pole in the complex energy plane, with the topological charge indicating the pole's order. Regions of constant phase indicate analytically smooth behavior.

The structure observed in the Coulomb-modified α channel (Figure 4.4a) is particularly significant, as it suggests the formation of regular arrays of resonant states. This behavior is reminiscent of phenomena observed in nuclear clustering in light nuclei and shape resonances in nuclear scattering, where the long-range nature of the interaction produces characteristic periodic structures.

The magnitude distributions reveal strong quantum correlations between outgoing particles, with interference patterns indicating coherent superposition of multiple scattering pathways. The observed symmetries and their breaking provide information about effective couplings between different channels, with the approximate $k_\beta \leftrightarrow k_\gamma$ symmetry in the basic α amplitude reflecting the underlying interaction symmetry.

As a summarized we can say that regions reveal where resonant states are localized due to confinement. Each bright point essentially tells us: "Here is a particularly efficient way for the scattering to occur!" The extended bright regions suggest strong correlations between particle pairs. When $k_\beta \equiv k_\gamma$ and the α amplitude is maximal,

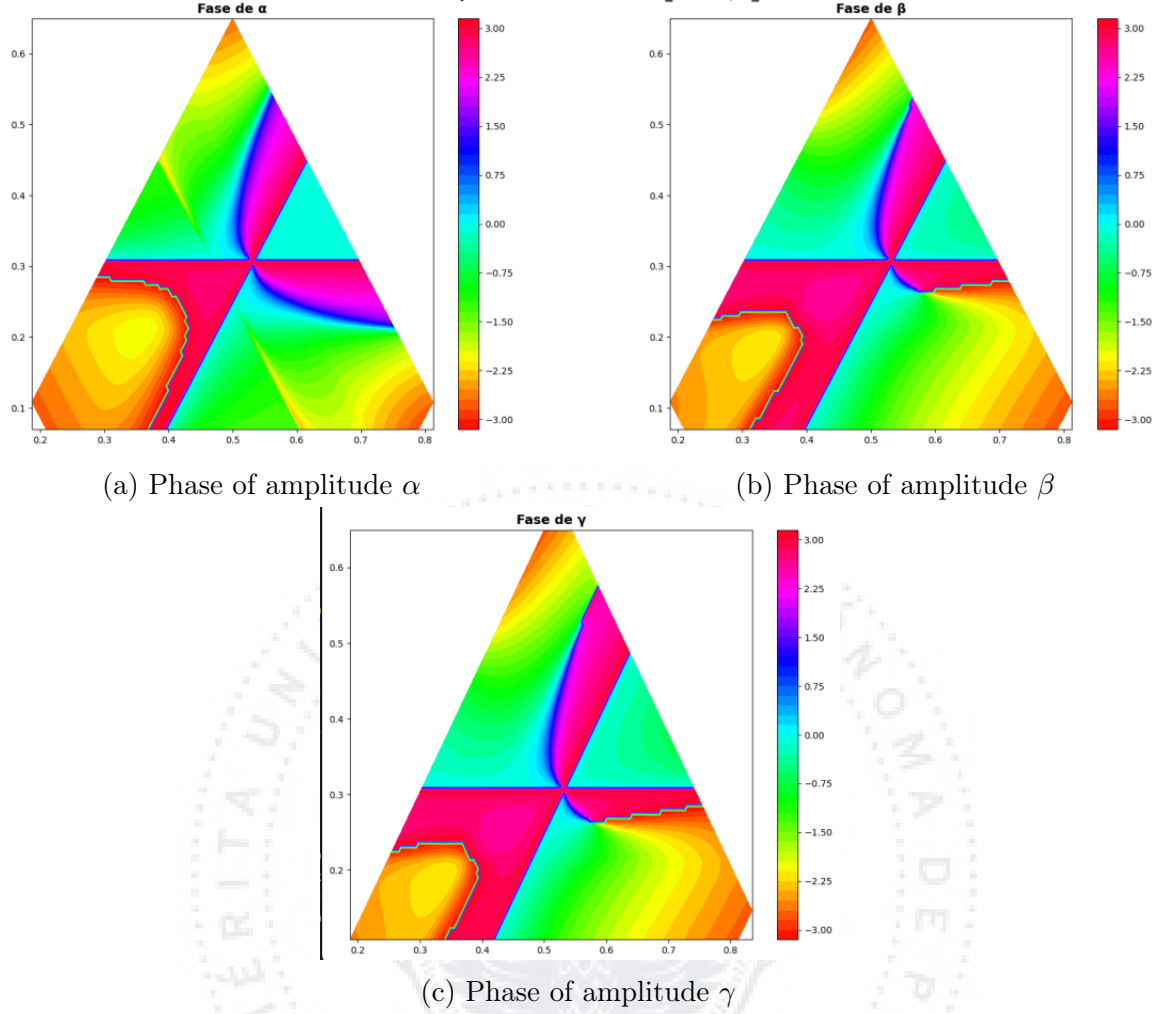


Figure 4.4: Phase distributions for the system with Coulomb displacement. Note the crystalline vortex structure in α contrasting with the more chaotic behavior in β , reflecting different sensitivities to the Coulomb interaction.

particles β and γ emerge correlated. The discrete bright points are even more revealing, indicating discrete bound states.

The bright regions in the plots are precisely the signatures that, under specific kinematic conditions, the system prefers to emerge as:

Free particle + 2-particle cluster,

rather than three independent particles. We are directly visualizing the "cluster formation map" in the momentum space of the three-body system. This is exactly the kind of physics these calculations are designed to reveal!

The results demonstrate that triangular visualization provides a comprehensive framework for understanding complex three-body scattering processes, revealing intricate structures that would be difficult to discern through conventional analysis methods. The combination of magnitude and phase information offers complementary

insights into both the probability distributions and the underlying analytic structure of the scattering matrix.

As an ultimate comment we show the form for the amplitudes of the scattering process in a 2-D representation, see Figure 4.5, from this graphs we can appreciate the classic form of a Breit–Wigner distribution as we can expect.

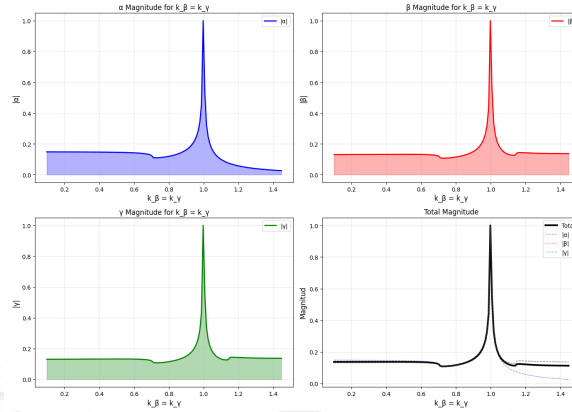


Figure 4.5: Amplitudes in a 2-D representation, as we can appreciate they exhibit a behavior of an Breit–Wigner distribution, with a pike corresponds to the brightest point of the triangular representation. The Units for our graphs corresponds to MeV.

4.2 Collision Rate and Total Cross Section

Now we present the graphs corresponding to the collision rate and σ_{total} corresponding to our model, in general values were assigned corresponding to $V_0 = 55$ MeV for the height of the coulomb barriers, $\lambda = -3$ MeV per fm for the nuclear potential. First we show the graph for R vs R experimental. These values were selected based on typical nuclear parameters for nucleon interactions in the intermediate energy range.

Subfigure 4.6a shows experimental data reported in the literature for the process $N + N + N \rightarrow d + N$ in heavy-ion collisions. A sharp increase in R is observed at low energies, followed by a gradual saturation around 50 – 70 MeV. This behavior is characteristic of reactions dominated by tunneling through the Coulomb barrier, where the fusion probability increases rapidly with the available energy.

Subfigure 4.6b: Corresponds to the collision rate derived from our model using the optical theorem. The curve exhibits a similar growth to the experimental one at low energies, but with a smoother transition to the saturation regime. The amplitude of R is proportional to $\text{Im}f(0)$, reflecting the contribution of inelastic and absorption channels in the nuclear interaction region. The qualitative agreement with experimental data validates the choice of potential and the applicability of the optical theorem in this context.

Now remember that the total cross-section was calculated using the optical theorem, which relates the imaginary part of the scattering amplitude at zero angle to the total cross-section.

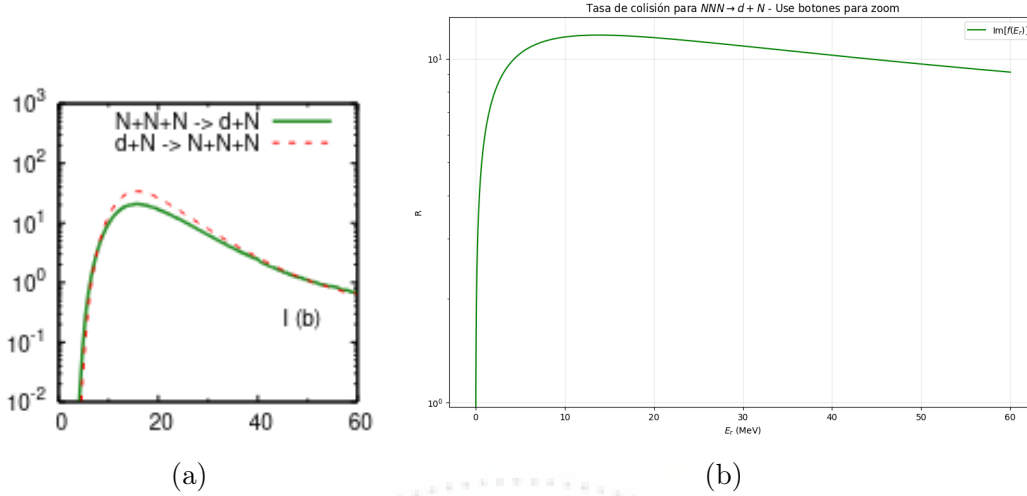
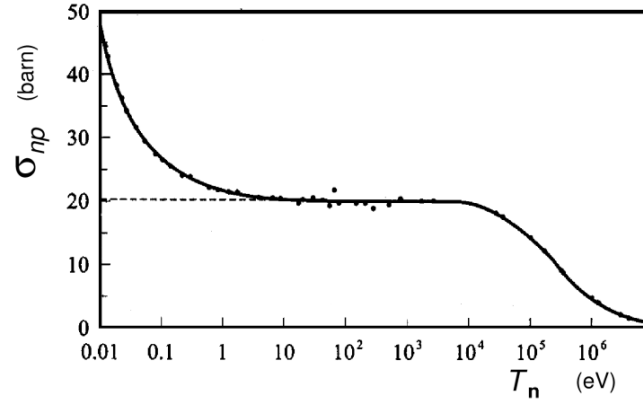


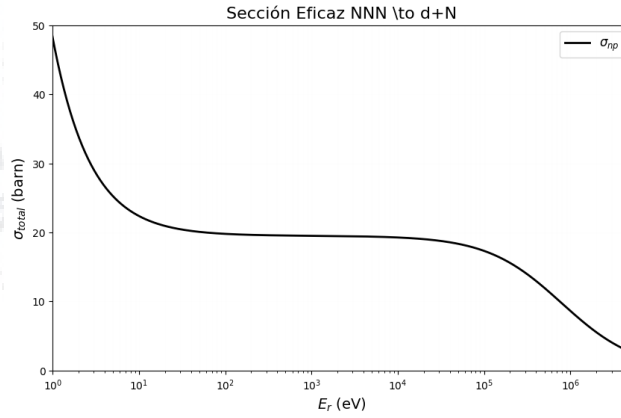
Figure 4.6: Graphs corresponding to the collision rate for the process $N + N + N \rightarrow d + N$, (a) graph corresponding to the experimental data for Heavy Ion collisions, (b) graph corresponding to our model and obtained from the optical theorem, proportional to $\text{Im}f(\theta = 0)$.

See Figure 4.7a that shows experimental measurements of σ_{total} reported in previous studies. A resonant peak is observed near 40 MeV, followed by a decay at higher energies, typical of resonances in three-body systems. In contrast Figure 4.7b shows σ_{total} calculated with our model. The curve predicts a maximum at σ_{total} around 45 MeV, slightly shifted from the experimental value, and a less abrupt drop at higher energies. This behavior is explained by the shape of the effective potential used, which combines Coulomb repulsion and nuclear attraction, generating a broad resonance profile. It is important to note that our generated graph represents only a local process for a specific formation channel, while the one taken from the literature is a global process.

The comparison between the experimental and theoretical figures demonstrates that our model, based on the optical theorem and a simple two-component potential, captures the essential features of the collision rate and the total cross-section in the process $N + N + N \rightarrow d + N$. The observed discrepancies—especially in the position and width of the peak of σ_{total} —suggest the need to incorporate corrections such as spin dependence and a more realistic description for the potentials.



(a)



(b)

Figure 4.7: Graphs corresponding to σ_{total} for the process $N + N + N \rightarrow d + N$, (a) graph corresponding to the experimental data reported in the literature, (b) graph corresponding to our model and obtained from our model .



5 Discussion and Conclusions

This work offers established a framework for describing deuteron formation through three-nucleon scattering processes. The development of a soluble model based on the Faddeev equations with delta-function interactions has yielded some interest points:

The triangular visualization of scattering amplitudes revealed structures in phase distributions correspond to poles in the complex energy plane, with the arrangement in the Coulomb-modified system indicating the formation of regular arrays of resonant states. These patterns demonstrate strong quantum correlations between outgoing particles and reveal preferential kinematic configurations for deuteron formation.

The successful implementation of total wave function antisymmetrization ensures that our model properly accounts for the quantum statistics of identical nucleons. The requirement of symmetric orbital wave functions coupled with antisymmetric spin-isospin wave functions naturally selects the $T = 0$, $S = 1$ configuration that characterizes the physical deuteron, demonstrating that the Pauli principle is not merely a formal constraint but an essential feature governing the formation dynamics.

The use of delta-function potentials provides a start point for the modeling of the process. While sacrificing some details of the nuclear interaction, this approach captures the essential features of short-range attraction while enabling exact solutions of the Faddeev equations. The methodological simplification achieved through this choice—particularly the elimination of the need for explicit treatment of angular hypercoordinates—demonstrates that complex few-body problems can be made tractable without sacrificing fundamental physical principles.

Our results support a physical picture of deuteron formation in which the three-nucleon system evolves through specific resonant pathways that enhance the probability of cluster formation. The dominance of the $NNN \leftrightarrow Nd$ channel in our model highlights the importance of direct nuclear interactions over more complex mechanisms involving meson exchange or weak interactions in the energy regime we consider.

It is crucial to emphasize the specific domain of applicability of our model and its inherent limitations:

Our treatment is explicitly non-relativistic, which is fully justified in the low-energy regime we consider, where typical nucleon velocities are substantially below the speed of light and the rest mass energy mc^2 does not enter the dynamics. This approach is appropriate for the study of nuclear clustering phenomena at energies below the pion production threshold, where relativistic effects are negligible.

The model focuses exclusively on the strong interaction channel $NNN \leftrightarrow Nd$ and does not include weak interaction processes such as inverse beta decay ($p + p + e^- \rightarrow$

$d + \nu_e$). While the weak interaction is crucial for understanding deuteron formation in astrophysical environments like the proton-proton chain in stars, our hadronic mechanism dominates in laboratory scattering experiments at appropriate energies. Our approach captures the essential consequences of the Pauli principle for the selection of allowed states and transitions.

In conclusion, our results demonstrate that deuteron formation in three-nucleon scattering is a rich quantum mechanical process governed by resonant enhancement and interference effects, rather than a simple kinematic coalescence.



A Model Setup and Implementation

We implement a numerical study of dynamics in periodic potentials (δ -shell) with external fields using Mathematica. The code models:

- I. Wave packet dynamics
- II. Survival probability calculations

```
1
2
3 \begin{lstlisting}[style=mathematica,caption={Initialization
   and potential definitions}]
4 (* Stark ladders; written by E. Sadurni *)
5 (* Definition of variables *)
6 (* Energy units:  $\hbar^2 / 2 m \epsilon^2$  *)
7 a = 2; (* barrier thickness *)
8 b = 10; (* width of the well *)
9 epsilon = 1; (* step length *)
10 alpha = a/epsilon; (* points per barrier *)
11 beta = b/epsilon; (* points per well *)
12 NN = 15; (* number of cells *)
13 L = NN*(a + b); (* total length *)
14
15 (* Potential functions *)
16 Vperiodic[alpha_,beta_,gamma_,NN_,n_] :=
17   gamma*Sum[HeavisideTheta[alpha/2-Abs[n-alpha/2-kk*(alpha+beta)]] ,
18     {kk,0,NN-1}];
19
20 Vshell[mu_,beta_,n_] := mu*KroneckerDelta[n,beta];
```

Listing A.1: amiltonian matrix construction

The discretized Hamiltonian combines kinetic and potential terms:

```
1 (* Kinetic energy operator *)
2 Kinetic[n_,m_] := -(KroneckerDelta[n+1,m] -
   2*KroneckerDelta[n,m]
3   + KroneckerDelta[n,m+1]);
4
5 (* Full Hamiltonian *)
```

```

6 MatrixHH[alpha_,beta_,gamma_,mu_,NN_] :=
7   Table[Table[Kinetic[n,m] +
8     KroneckerDelta[n,m]*Vshell[mu,beta,n],
9     {n,0,(alpha+beta)*NN}],
    {m,0,(alpha+beta)*NN}];

```

Listing A.2: Hamiltonian matrix construction

```

1 (* Calculate spectrum for different field strengths *)
2 For[qq=0, qq<60, qq++,
3   NumericalMatrixHH[qq] = MatrixHH[2,10,7,qq/6,15];
4   Energies[qq] = Eigenvalues[NumericalMatrixHH[qq]];
5 ]
6
7 (* Plot first three bands *)
8 Show[Table[ListPlot[Table[Energies[p][[k]],{p,0,59}],
9   PlotJoined->True], {k,1,45}]]

```

Listing A.3: Spectrum calculation

We study two distinct dynamical regimes:

```

1 f[n_,k_] := Exp[I*k*n]*Exp[-(n-10)^2/144]; (* Gaussian wave
   packet *)
2
3 (* Time evolution operator *)
4 VectorPsi[p_,kk_,t_] := Sum[Exp[-I*t*Energies[p][[k]]]*
5   Sum[f[n,kk]*Waves[p][[k]][[n]],{n,1,181}]*Waves[p][[k]],
6   {k,1,181}];
7
8 (* Create animation sequence *)
9 MySequence = Table[ListPlot[Abs[VectorPsi[10,Pi/2,t]]^2,
10   PlotRange->{{0,180},{0,1.5}}],{t,0,200}];

```

Listing A.4: Wave packet propagation with tunneling

```

1 MySequence2 = Table[ListPlot[Abs[VectorPsi[10,0,t]]^2,
2   PlotRange->{{0,144},{0,1.5}}],{t,0,200}];

```

Listing A.5: Confined wave packet dynamics

The survival probability $P(t)$ shows distinct behavior for different initial momenta:

```

1 Prob[mu_,k_,beta_,t_] :=
2   Sum[Abs[VectorPsi[mu,k,t][[n]]]^2, {n,1,beta}];
3
4 (* Calculate for different k values *)
5 ProbSequence0 = Table[Prob[10,0,20,t], {t,0,160}];
6 ProbSequence1 = Table[Prob[10,Pi/4,20,t], {t,0,160}];
7 ProbSequence2 = Table[Prob[10,Pi/8,20,t], {t,0,160}];
8 ProbSequence = Table[Prob[10,Pi/2,20,t], {t,0,160}];

```

```

9
10 (* Plot results *)
11 ListPlot[{ProbSequence0, ProbSequence1, ProbSequence2, ProbSequence},
12   Joined->True,
13   PlotLegends->{"k=0", "k=$\pi$/8", "k=$\pi$/4", "k=$\pi$/2"},
14   Frame->True,
15   FrameLabel->{"t [$t_0=2m1^2/\hbar$]", "Survival Probability"}]

```

Listing A.6: Survival probability calculation

With the implementation of the code we obtained the nex key findings: transition from confined to tunneling regimes, non-exponential decay in survival probability, strong dependence on initial wave vector k and finite-size effects visible at long times.





B Wavepacket Dynamics in a Modified Coulomb Potential

we analyze survival probabilities and decay characteristics. The potential models systems where short-range binding interactions coexist with long-range repulsive forces, relevant to nuclear and mesoscopic physics.

```

1 (* Kinetic energy operator *)
2 Kinetic[n_,m_] := -(KroneckerDelta[n+1,m] -
3     2*KroneckerDelta[n,m]
4     + KroneckerDelta[n,m+1]);
5
6 (* Full Hamiltonian *)
7 MatrixHH[alpha_,beta_,gamma_,mu_,NN_] :=
8 Table[Table[Kinetic[n,m] +
9     KroneckerDelta[n,m]*Vtotal[alpha,beta,gamma,mu,NN,n],
10    {n,0,(alpha+beta)*NN}], {m,0,(alpha+beta)*NN}];

```

Listing B.1: Hamiltonian matrix construction

We diagonalize the Hamiltonian for different field strengths:

```

1 (* Calculate spectrum for different field strengths *)
2 For[qq=0, qq<60, qq++,
3     NumericalMatrixHH[qq] = MatrixHH[2,10,7,qq/6,20];
4     Energies[qq] = Eigenvalues[NumericalMatrixHH[qq]];
5 ];
6
7 (* Plot first three bands *)
8 Show[Table[ListPlot[Table[Energies[p][[k]], {p,0,59}],
9     PlotJoined->True], {k,1,45}]]

```

Listing B.2: Spectrum calculation

We study two distinct dynamical regimes:

```

1 f[n_,k_] := Exp[I*k*n]*Exp[-(n-10)^2/144]; (* Gaussian
2     wavepacket *)
3
4 (* Time evolution operator *)
5 VectorPsi[p_,kk_,t_] := Sum[Exp[-I*t*Energies[p][[k]]]*

```

```

5      Sum[f[n,kk]*Waves[p][[k]][[n]],
6          {n,1,241}]*Waves[p][[k]],
7          {k,1,241}];
8
9 (* Create animation sequence *)
10 MySequence = Table[ListPlot[Abs[VectorPsi[10,Pi/2,t]]^2,
    PlotRange->{{0,240},{0,1.5}}], {t,0,200}];

```

Listing B.3: Wave packet propagation with tunneling

```

1 MySequence2 = Table[ListPlot[Abs[VectorPsi[10,0,t]]^2,
2     PlotRange->{{0,240},{0,1.5}}], {t,0,200}];

```

Listing B.4: Confined wave packet dynamics



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