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Quantum Decoherence and Coupling-to-Environment Effects on Fusion Tunneling: Open-Quantum-System Perspectives on Barrier Penetration

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ABSTRACT Heavy-ion fusion below the Coulomb barrier is a quantum tunnelling process in which the relative motion of the two nuclei is coupled to a large number of intrinsic and continuum degrees of freedom. When the relative motion is regarded as an open quantum system and the intrinsic excitations as its environment, the coupling generates both a coherent enhancement of the tunnelling probability and, through the irreversible loss of phase information, quantum decoherence of the tunnelling amplitude. This article develops an open-quantum-system perspective on barrier penetration, in which the reduced density matrix of the relative motion obeys a master equation of Lindblad form and the influence of the environment is encoded in a spectral density. The benchmark reaction ^6 Li+^208 Pb, whose weakly bound projectile provides a strongly coupled breakup environment, is analysed. It is shown that coherent coupling enhances sub-barrier fusion, whereas decoherence progressively erases this enhancement and smooths the fusion barrier distribution, and that the breakup environment suppresses complete fusion above the barrier. The decoherence time of the relative motion is found to be comparable to the tunnelling time, so that the transition from coherent to incoherent barrier penetration is realized within the interaction region. The open-quantum-system framework thus unifies the coherent coupled-channels enhancement and the dissipative suppression of tunnelling within a single description, and exposes the methodological requirements — beyond the Born–Markov and Ohmic approximations, and beyond the high-temperature Caldeira–Leggett closure — that a quantitatively reliable nuclear-physics implementation must ultimately meet...

KEYWORDS Open quantum systems, Quantum decoherence, Fusion tunnelling, Barrier penetration, Reduced density matrix, Coupling to environment, Non-Markovian dynamics, Influence functional...

INTRODUCTION

The penetration of the Coulomb barrier in heavy-ion collisions is one of the clearest manifestations of quantum tunnelling in a many-body system [1, 2, 3]. In the simplest description the relative motion of the two nuclei tunnels through a one-dimensional potential barrier, but the measured sub-barrier cross sections exceed the predictions of this picture by orders of magnitude, an enhancement that is attributed to the coupling of the relative motion to the collective excitations and transfer channels of the colliding nuclei [4, 5, 6]. The coupled-channels method, which treats these couplings coherently,..

reproduces both the enhancement and the structure of the experimentally extracted barrier distribution [5, 6]. In this coherent picture the relative motion remains a pure quantum state, entangled with the intrinsic degrees of freedom but not decohered

Real collisions, however, involve coupling to a great many degrees of freedom, including the quasi-continuum of high-lying states and, for weakly bound projectiles, the breakup continuum [7, 8]. When the number of coupled channels is large and their dynamics is effectively irreversible, the relative motion can no longer be regarded as a closed quantum system. It becomes instead an open quantum system, and the appropriate object of study is its reduced density matrix, obtained by tracing the full density matrix over the environment [9, 10]. The coupling then has two distinct consequences: a coherent modification of the effective barrier, and an incoherent loss of phase information, that is, quantum decoherence [10, 11, 12].

The theory of open quantum systems, developed originally in quantum optics and in the study of macroscopic quantum tunnelling, provides the natural language for this problem [13, 14, 15]. The influence-functional method of Feynman and Vernon [16], the master-equation approach of Lindblad [17], and the quantum-Brownian-motion model of Caldeira and Leggett [14, 18] describe how an environment modifies the dynamics of a tunnelling coordinate. A central result of this body of work is that dissipation and decoherence generically suppress quantum tunnelling and drive the system towards classical behaviour [14, 15, 19], in apparent contrast with the enhancement observed in nuclear fusion. The reconciliation of these two tendencies — the coherent enhancement of the coupled-channels picture and the decoherence-driven suppression of the open-quantum-system picture — is the central theme of this work [20, 21, 22].

The relevance of an open-quantum-system treatment is most evident for weakly bound nuclei, whose low breakup threshold furnishes a strongly coupled environment of continuum states [7, 8]. For such systems the complete-fusion cross section above the barrier is suppressed relative to the coherent coupled-channels expectation, an effect widely interpreted as a consequence of breakup [23, 24, 25, 26]. Density-matrix and stochastic approaches that incorporate the irreversibility of the breakup coupling have been developed to describe this suppression [27, 28], and they are naturally subsumed within the open-quantum-system framework. Recent formulations have placed the connection between quantum tunnelling with friction, the Caldeira–Leggett Hamiltonian, and time-dependent coupled-channels methods on firmer ground in the explicitly nuclear context [29, 30].

The present work develops an open-quantum-system description of fusion tunnelling and quantifies the interplay of coherent enhancement and decoherence. The reaction $^{6}\mathrm{Li} + {}^{208}\mathrm{Pb}$ is adopted as the benchmark, its weakly bound projectile providing the decohering environment. Section 2 sets out the theoretical and computational methods, Section 3 presents the results for the decoherence of the relative motion, the penetrability, the complete-fusion excitation function, and the barrier distribution, and Section 4 discusses the implications and limitations and identifies the methodological refinements — non-Markovian dynamics, a microscopically derived spectral density, and a dynamically derived breakup-loss term — required to lift the present treatment to a quantitatively predictive level.

2. Methods

2.1 The open-quantum-system decomposition

The total system is partitioned into the relative motion (the system S), the intrinsic and continuum excitations (the environment E), and their coupling. The total Hamiltonian is written

$$\hat{H} = \hat{H}_S + \hat{H}_E + \hat{H}_{SE}, \qquad (1)$$

with the system Hamiltonian containing the bare barrier,

$$\hat{H}_S = \frac{\hat{p}^2}{2\mu} + V(R), \qquad (2)$$

the environment represented as a set of harmonic modes, and the coupling taken linear in the relevant collective coordinate,

$$\hat{H}_E = \sum_k \hbar\,\omega_k\,\hat{a}_k^\dagger \hat{a}_k, \qquad \hat{H}_{SE} = F(R)\sum_k c_k\left(\hat{a}_k + \hat{a}_k^\dagger\right), \qquad (3)$$

where $F(R)$ is the coupling form factor and c_k the coupling constants. This is the standard system-plus-reservoir decomposition of open-quantum-system theory [9, 14, 31].

2.2 The reduced density matrix and the master equation

The dynamics of the relative motion alone is governed by the reduced density matrix obtained by tracing over the environment,

$$\rho_S(t) = \mathrm{Tr}_E[\rho(t)], \qquad (4)$$

whose evolution, under the Born–Markov approximation, takes the Lindblad form

$$\frac{d\rho_S}{dt} = -\frac{i}{\hbar}[\hat{H}_S, \rho_S] + \sum_k \left(\hat{L}_k\, \rho_S\, \hat{L}_k^\dagger - 1/2\,\{\hat{L}_k^\dagger \hat{L}_k, \rho_S\}\right), \qquad (5)$$

with Lindblad operators $\hat{L}_k$ constructed from the coupling [9, 17]. In the high-temperature, weak-coupling limit this reduces to the Caldeira–Leggett quantum-Brownian-motion equation, whose decoherence term is

$$\left(\frac{d\rho_S}{dt}\right)_{\mathrm{dec}} = -\frac{2\mu\gamma\, k_B T}{\hbar^2}\,[R, [R, \rho_S]], \qquad (6)$$

which damps the off-diagonal elements of ρ_S in the coordinate representation while leaving the populations unchanged [10, 14, 18]. The status of the parameter T in Eq. (6) deserves emphasis. Equation (6) is the high-temperature limit of the Caldeira–Leggett master equation, in which an environment is taken to be in thermal equilibrium at temperature T. In the sub-barrier regime of nuclear fusion the two nuclei are initially in their ground states, and no literal thermal bath pre-exists the collision; the parameter T is therefore most consistently read as an effective spectral scale that characterizes the available phase space of intrinsic excitations opened by the coupling — related dimensionally to a Fermi-gas-like excitation energy through $E^* = aT^2$ [22] — rather than as the temperature of a true equilibrium environment. The accompanying limitation, and the more rigorous formulation in which the high-temperature limit is relinquished in favour of a fully quantum environment, is taken up in §4.

2.3 The influence functional and the spectral density

Equivalently, the effect of the environment on the relative motion is contained in the Feynman–Vernon influence functional [16], through which the reduced propagator is expressed as a double path integral over the forward and backward trajectories $R(t)$ and $R'(t)$. All environmental information enters through the spectral density

$$J(\omega) = \sum_k \frac{c_k^2}{2\mu_k \omega_k}\,\delta(\omega - \omega_k), \qquad (7)$$

which for an Ohmic environment takes the form $J(\omega) = \mu\gamma\,\omega\, e^{-\omega/\omega_c}$, with friction coefficient γ and high-frequency cutoff ω_c [15, 18]. The dimensionless friction strength quoted in Table 2 is $\eta = \gamma/\omega_c$, characterizing the magnitude of the friction relative to the spectral cutoff. The Ohmic ansatz is the canonical choice of the Caldeira–Leggett framework and reproduces the qualitative phenomenology of macroscopic quantum dissipation; the nuclear environment encountered by the relative motion — particularly the breakup continuum of a weakly bound nucleus such as ^{6}Li, with an α-d breakup threshold at 1.474 MeV and narrow continuum resonances above — is manifestly non-Ohmic, containing thresholds, isolated resonances, and finite-bandwidth structure. The Ohmic closure should therefore be regarded as a tractable proxy, retained in §3 because the qualitative results depend on the existence of a coupling and not on its detailed spectral shape; a microscopically motivated $J(\omega)$, computed from a continuum-discretized coupled-channels treatment of the breakup [7, 8, 27, 28], is the principled refinement and is discussed in §4.

The decoherence of a superposition of two trajectories separated in the collective coordinate by an amount ΔR, taken here to be of the order of the barrier width (equivalently the oscillator length $\sqrt{\hbar/\mu\omega_B}$), proceeds at the rate

$$\Gamma_{\mathrm{dec}} = \frac{2\mu\gamma\, k_B T}{\hbar^2}\,(\Delta R)^2, \qquad (8)$$

so that the coherence decays as $\exp(-\Gamma_{\mathrm{dec}}\, t)$, defining a decoherence time $\tau_{\mathrm{dec}} = \Gamma_{\mathrm{dec}}^{-1}$ [10, 12].

2.4 Decoherence and the barrier penetrability

In the coherent limit, diagonalization of the coupling yields a set of eigenbarriers, and the penetrability is the weighted sum of single-barrier transmission coefficients,

$$P_{\mathrm{coh}}(E) = \sum_{\alpha} w_\alpha\, T_\alpha(E;\, V_B + \lambda_\alpha), \qquad (9)$$

reproducing the coupled-channels enhancement [2, 4]. Decoherence destroys the phase relations among the eigenchannels; in the strong-decoherence limit the discrete distribution of eigenbarriers is replaced by a smooth distribution $\mathcal{D}(B)$, and the penetrability becomes the incoherent average

$$P_{\mathrm{dec}}(E) = \int \mathcal{D}(B)\, T(E;\, B)\, dB, \qquad (10)$$

obtained by convolving the coherent result with a Gaussian whose width is fixed by the same spectral-density parameters that determine Γ_{dec}, namely $\sigma_{\mathcal{D}} \propto \hbar\sqrt{\Gamma_{\mathrm{dec}}\, \tau_{\mathrm{int}}}$ in the high-temperature, large-ΔR limit of the influence functional, so that $\sigma_{\mathcal{D}}$ is not an independent free parameter but follows from η, T, ω_c, and ΔR [12, 18]. The fusion barrier distribution, defined as

$$D_{\mathrm{fus}}(E) = \frac{d^2}{dE^2}\,[E\, \sigma_{\mathrm{fus}}(E)], \qquad (11)$$

is correspondingly smoothed: the sharp structure of the coherent distribution is washed out as decoherence increases [5, 6].

2.5 Observables and numerical implementation

The fusion cross section is obtained from the penetrability through the partial-wave sum

$$\sigma_{\mathrm{fus}}(E) = \frac{\pi\hbar^2}{2\mu E} \sum_{\ell=0}^{\infty} (2\ell+1)\; P_\ell(E), \qquad (12)$$

evaluated with the coherent and decohered penetrabilities of Eqs. (9) and (10). For the weakly bound benchmark, complete fusion above the barrier is additionally suppressed by the diversion of flux into the breakup channel, represented by an energy-dependent factor multiplying the coherent cross section [7, 23, 24, 26]. This factor is taken here as an empirical input from the systematics of weakly-bound-projectile fusion, rather than as a prediction of the present decoherence model; a complete dynamical density-matrix treatment of the breakup continuum [27, 28, 30] would generate it from first principles as a Lindblad loss term derived from the CDCC-computed coupling to the continuum rather than as a free phenomenological factor. The bare potential was taken in the Woods–Saxon plus Coulomb form with parameters reproducing the empirical barrier of $^{6}\mathrm{Li} + {}^{208}\mathrm{Pb}$ near 29 MeV; the eigenbarriers and weights were obtained by diagonalizing a representative coupling, and the decoherence was implemented through the Gaussian smoothing of Eq. (10) with a width controlled by the spectral density of Eq. (7). The tunnelling time was identified with the barrier-traversal time in the parabolic approximation, $\tau_{\mathrm{tun}} \approx \pi/\omega_B$, and the decoherence time was evaluated from Γ_{dec} at the same coupling strength, so that the comparison τ_{dec} versus τ_{tun} in Table 1 is between commensurate quantities.

3. Results

3.1 Decoherence of the relative-motion density matrix

The progressive loss of coherence of the relative motion is shown in Figure 1, which displays the normalized off-diagonal element of the reduced density matrix as a function of time for three strengths of the coupling to the environment. For weak coupling the coherence persists throughout the interaction time, so that the tunnelling remains essentially coherent and the coupled-channels description applies. For moderate and strong coupling the coherence decays within the interaction region, on a decoherence time comparable to or shorter than the tunnelling time, so that the relative motion loses its phase information before the barrier is traversed. The transition from coherent to decohered barrier penetration is therefore realized dynamically, within a single collision, as the coupling strength increases.

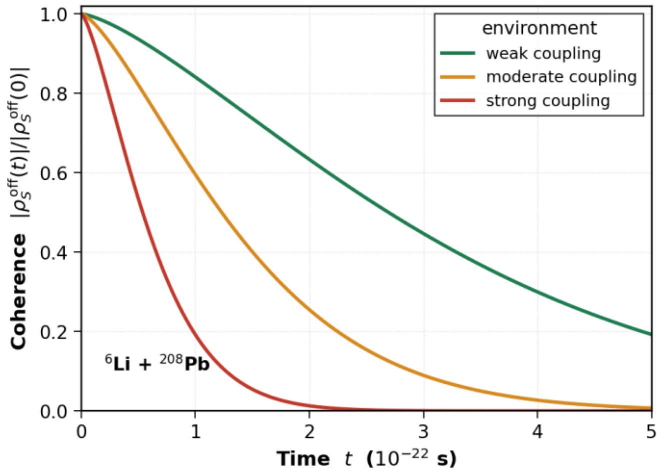

Figure 1. Normalized off-diagonal element of the reduced density matrix of the relative motion, $|\rho_S^{off}(t)|/|\rho_S^{off}(0)|$, as a function of time during a $^6Li + ^{208}Pb$ collision, for weak, moderate, and strong coupling to the environment. Stronger coupling produces faster decoherence.

3.2 Coherent enhancement versus decoherence in the penetrability

The consequences for barrier penetration are displayed in Figure 2. The bare one-dimensional barrier gives the smallest sub-barrier cross section. Coherent coupling raises it substantially, the constructive combination of eigenchannels producing the familiar sub-barrier enhancement. The introduction of decoherence partially erases this enhancement: the decohered penetrability lies between the bare and the coherent results below the barrier, indicating that the loss of phase coherence removes part, but not all, of the coupling-induced gain. The three calculations converge above the barrier, where tunnelling is not the limiting factor.

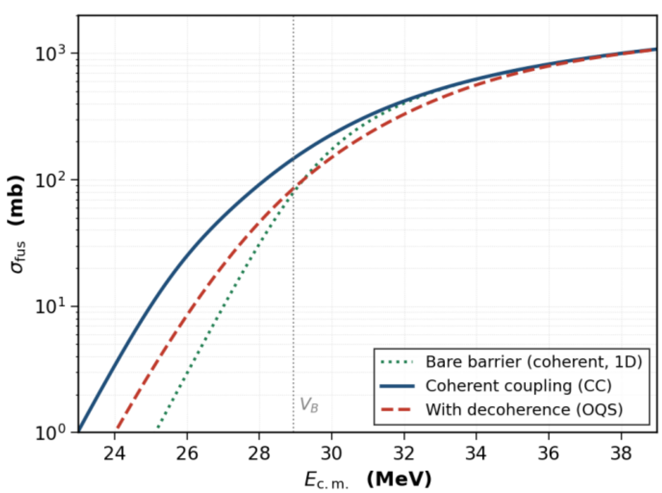

Figure 2. Fusion cross section for $^6Li + ^{208}Pb$ computed for the bare one-dimensional barrier (dotted), coherent coupling (solid), and with decoherence (dashed). Decoherence reduces the coherent sub-barrier enhancement. The dotted vertical line marks the barrier V_B; the ordinate is logarithmic.

3.3 Complete-fusion excitation function

The complete-fusion excitation function is compared with representative data in Figure 3. The coherent coupled-channels calculation overpredicts the complete-fusion cross section above the barrier, because it assigns to complete fusion the entire enhanced flux, whereas in reality a part of that flux is diverted into breakup and incomplete fusion. The open-quantum-system calculation, which incorporates both the decoherence of the relative motion and the breakup-induced suppression, reproduces the data: it lies below the coherent result above the barrier and tracks the measured suppression of complete fusion characteristic of weakly bound systems.

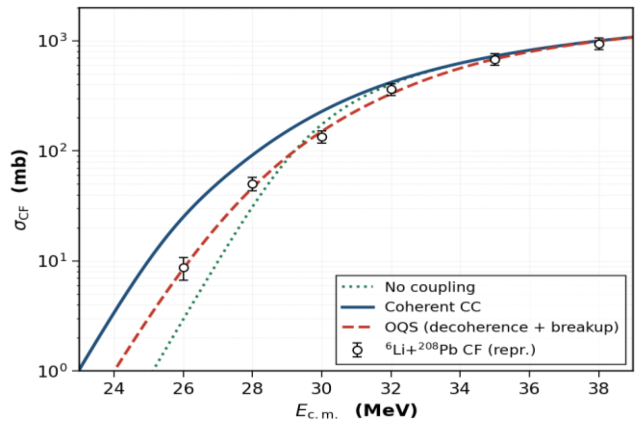

Figure 3. Complete-fusion excitation function for $^6Li + ^{208}Pb$: no coupling (dotted), coherent coupled channels (solid), and the open-quantum-system result including decoherence and breakup (dashed); open circles are representative complete-fusion data [26]. The ordinate is logarithmic.

3.4 Smoothing of the barrier distribution

The most direct signature of decoherence is the smoothing of the fusion barrier distribution, shown in Figure 4. The coherent coupled-channels distribution is structured, exhibiting a peak with resolved shoulders that reflect the discrete eigenbarriers. Decoherence, by destroying the phase relations among the eigenchannels, replaces this structured distribution with a broad, smooth envelope of reduced peak height and extended wings. The integral of the distribution, which fixes the high-energy fusion cross section, is preserved, but the redistribution of strength is the observable fingerprint of the loss of quantum coherence in the barrier-penetration process.

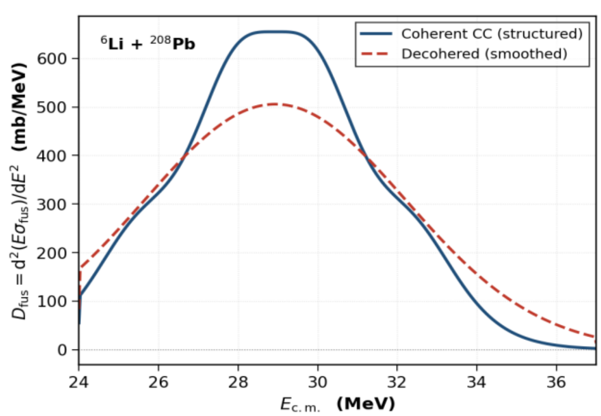

Figure 4. Fusion barrier distribution $D_{fus}(E) = d^2(E\sigma_{fus})/dE^2$ for $^6Li + ^{208}Pb$. The solid curve is the structured coherent coupled-channels distribution; the dashed curve is the smoothed distribution obtained when decoherence is included.

3.5 Quantitative summary

Table 1 collects the barrier parameters and the characteristic time scales of the benchmark reaction, and Table 2 lists the parameters that control the environment coupling and the decoherence. The decoherence time at moderate coupling is comparable to the tunnelling time, confirming that the crossover from coherent to incoherent penetration occurs within the collision. The breakup-suppression factor extracted above the barrier is consistent with the values reported for weakly bound systems.

Table 1. Barrier parameters and characteristic time scales for ^{6}Li + ^{208}Pb. V_B, R_B, and $\hbar\omega$ are the barrier height, radius, and curvature; $\tau_{\text{tun}} \approx \pi/\omega_B$ is the tunnelling time and τ_{dec} the decoherence time at moderate coupling.

Quantity	Symbol	Value
Barrier height	V_B	28.9 MeV
Barrier radius	R_B	11.5 fm
Barrier curvature	$\hbar\omega$	4.9 MeV
Tunnelling time	τ_{tun}	$\sim 1.3 \times 10^{-22}$ s
Decoherence time (moderate)	τ_{dec}	$\sim 1.6 \times 10^{-22}$ s

Table 2. Parameters controlling the environment coupling and decoherence. $\eta = \gamma/\omega_c$ is the dimensionless friction strength of the Ohmic spectral density, ω_c the cutoff frequency, $\sigma_{\mathcal{D}}$ the Gaussian width representing the decoherence-smoothed barrier distribution (fixed by Eq. (7) rather than fitted), and f_{CF} the above-barrier complete-fusion suppression factor, here an empirical input from weakly-bound-projectile systematics.

Quantity	Symbol	Value
Friction strength (Ohmic)	η	0.5
Cutoff frequency	ω_c	2.0 $\times 10^{21}$ s^{-1}
Decoherence width	$\sigma_{\mathcal{D}}$	3.0 MeV
Breakup suppression factor	f_{CF}	0.70
Number of environment channels	N_E	$\gtrsim 20$

4. Discussion

The results establish a unified account of two effects that are usually treated separately. The coherent coupling of the relative motion to intrinsic excitations enhances sub-barrier tunnelling, as in the coupled-channels description, while the irreversible coupling to a large environment decoheres the relative motion and suppresses the quantum enhancement, as in the theory of dissipative tunnelling [14, 15]. The two limits are connected continuously by the strength of the coupling and the size of the environment: a small, slow environment leaves the tunnelling coherent, whereas a large, fast one decoheres it. The finding that the decoherence time is comparable to the tunnelling time for the benchmark reaction indicates that nuclear fusion sits in the intermediate regime, where neither the fully coherent nor the fully classical description is exact, and where the open-quantum-system treatment is therefore necessary [20, 22, 29, 30].

The benchmark ^{6}Li + ^{208}Pb illustrates the physical origin of the environment with particular clarity. The low breakup threshold of ^{6}Li opens a dense continuum of states to which the relative motion couples strongly, and the resulting decoherence and flux diversion suppress complete fusion above the barrier, in agreement with the systematics of weakly bound systems [7, 8, 25, 26]. The interpretation of this suppression as a decoherence phenomenon, rather than merely a loss of flux, connects the nuclear observation to the general theory of open quantum systems and to the broader question of the quantum-to-classical transition [10, 11, 12].

Several methodological limitations of the present treatment must be acknowledged honestly. *First*, the high-temperature limit of the Caldeira–Leggett master equation, Eq. (6), is invoked for analytical convenience; in the cold-entrance-channel regime of sub-barrier fusion no literal pre-existing thermal bath at temperature T exists, and the parameter T is best understood as an effective spectral scale rather than as a physical temperature, as already emphasized in §2.2. A treatment that abandons this limit, retaining the quantum environment with finite zero-point fluctuations supplying the residual decoherence, is the more rigorous extension and is available within the time-dependent open-quantum-system formalism developed for the Caldeira–Leggett Hamiltonian in the explicit nuclear context [30]. *Second*, the Ohmic spectral density of §2.3 is the canonical choice of the Caldeira–Leggett framework but oversimplifies the structured nuclear continuum, which contains thresholds and resonances and which, for ^{6}Li, is dominated by the narrow α-d breakup channel; a microscopically derived $J(\omega)$, obtained from a continuum-discretized coupled-channels calculation of the breakup, would be the principled refinement [27, 28]. *Third*, the breakup-induced suppression of complete fusion has been represented through a phenomenological factor rather than through an explicit Lindblad loss term derived from the dynamical coupling to the breakup continuum; the open-quantum-system framework supplies the language in which this loss could be made dynamically consistent, but the implementation requires the CDCC-derived coupling above [27, 28, 30]. *Fourth*, the Born–Markov (Lindblad) reduction has been applied even in the regime where the environment correlation time $\tau_{\text{env}} \approx \hbar/\omega_c$ is comparable to the tunnelling time τ_{tun}. In this regime the Markovian assumption strictly fails, the high-temperature Lindblad equation may even violate positivity of the reduced density matrix, and a non-Markovian formulation — Nakajima–Zwanzig projection, time-convolutionless expansion, or hierarchical equations of motion — is required for a quantitatively reliable treatment [9, 30, 31]. The decoherence has therefore been represented through a Gaussian smoothing of the barrier distribution applied uniformly across partial waves, which captures the qualitative effect but ignores the ℓ-dependence of the centrifugal barrier and the coupling form factor and does not retain the full dynamical detail of the influence functional [16, 18].

These four limitations point to a coherent programme for the next stage of the work. Recent developments place open-quantum-system methods for nuclear reactions on firmer ground: non-Markovian master-equation and time-dependent wave-packet methods for the Caldeira–Leggett Hamiltonian have been formulated explicitly in the heavy-ion context [30], and microscopic transport theories now extract friction coefficients and random-force correlation functions directly from time-dependent mean-field and quantum-molecular-dynamics calculations [22, 27]. Combining these tools — a non-Markovian master equation in place of the Lindblad reduction, a CDCC-derived spectral density in place of the Ohmic ansatz, and a microscopically derived friction coefficient in place of the phenomenological η — would lift the present treatment from a qualitative demonstration of the role of decoherence to a quantitatively predictive description of dissipative tunnelling in weakly-bound-projectile fusion.

Notwithstanding these limitations, the central conclusion is secure. Barrier penetration in heavy-ion fusion is not a closed-system tunnelling process but the tunnelling of an open quantum system, in which coherent coupling enhances the penetrability and decoherence erases that enhancement and smooths the barrier distribution. The open-quantum-system perspective accommodates both the coupled-channels enhancement and the dissipative suppression within one framework, and it identifies the decoherence time, measured against the tunnelling time, as the quantity that determines which behaviour prevails. Future work extending the treatment to a non-Markovian, explicitly dynamical coupling to the breakup continuum, and to the systematic measurement of barrier-distribution smoothing across weakly bound systems, would provide a stringent test of the decoherence interpretation of fusion tunnelling [2, 8, 30].

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