Coupled-Channels Approach for Dissipative Quantum Dynamics in Near-Barrier Collisions

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Abstract. A novel quantum dynamical model based on the dissipative quantum dynamics of open quantum systems is presented. It allows the treatment of both deep-inelastic processes and quantum tunneling (fusion) within a fully quantum mechanical coupled-channels approach. Model calculations show the transition from pure state (coherent) to mixed state (decoherent and dissipative) dynamics during a near-barrier nuclear collision. Energy dissipation, due to irreversible decay of giant-dipole excitations of the interacting nuclei, results in hindrance of quantum tunneling.

Keywords: Open quantum system, Dissipation, Decoherence, Lindblad equation, Coupled channels, Quantum tunneling, Fusion, Deep-inelastic collisions

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INTRODUCTION

Stationary state coupled-channels approaches have been very successful [1] in explaining several collision observables. However, there are still unsolved problems. For instance, the inability to describe elastic scattering and fusion measurements simultaneously [2, 3] and, related, the more recent failure to describe in a physically consistent way the below-barrier quantum tunneling and above-barrier fusion yields [4].

These problems may be caused by the neglect of important physical processes (e.g., deep-inelastic) which cannot be treated within (standard) coupled-channels models. Measurements have shown that deep-inelastic processes occur even at sub-barrier incident energies [5], in competition with the process of quantum tunneling, and thus fusion. Energy dissipation associated with the deep-inelastic mechanism could thus play a significant role in the inhibition of tunneling at deep sub-barrier energies. This can also change the yield of direct reaction processes, including elastic and quasi-elastic channels.

The understanding of this complex interplay, at near- and below barrier energies, requires a dynamical model which can describe coupling assisted tunneling with dissipation. Neither existing models of fusion nor of deep-inelastic scattering can address both energy dissipation and quantum tunneling. Quantum mechanical coupled-channels models describe tunneling without energy dissipation [1, 6], whilst approaches to direct damped collisions treat the relative motion of the nuclei classically [7].
We here report on a novel coupled-channels density matrix approach \[8\] that overcomes these difficulties. We exploit the Lindblad axiomatic approach \[9, 10\] for open quantum systems, which is based on the concept of quantum semigroups and completely positive mappings. We refer to Ref. \[8\] for a discussion of the suitability of the Lindblad theory for the treatment of low-energy collision dynamics. The coupled-channels description is formulated with Lindblad’s equation for a reduced density matrix \[9, 10\]. It describes the dynamical evolution of the reduced system (comprising the relative motion of the nuclei plus selected, intrinsic collective excitations) that irreversibly interacts with two (model) “environments”. Firstly, an environment inside the Coulomb barrier, which is related to the complexity of compound nucleus states. Secondly, one with a long range, associated with decay out of short lived (compared to the reaction time) internal vibrational states, e.g. the giant dipole resonance (GDR) of the colliding nuclei. Model calculations show that damping of the GDR results in quantum decoherence and energy loss as the nuclei overlap, inhibiting tunneling, and thus fusion.

**COUPLED CHANNELS DENSITY MATRIX APPROACH**

The model calculations are carried out using the scenario presented in Figure 1. The basis will comprise two asymptotic states (coupled-channels) \|1⟩\ and \|2⟩\. Channel \|1⟩\ is the (ground states) entrance channel and is coupled to an inelastic state \|2⟩\ by a coupling interaction \(V_{12}\). Two distinct sources of irreversibility are also considered, modelled by two auxiliary (environment) states \|X⟩\ and \|Y⟩\. The first environmental coupling describes capture by the potential pocket inside the fusion barrier. This simulates the irreversible and dissipative excitations associated with the evolution from the two separate nuclei to a compound nuclear system. In a stationary states approach this loss of flux is approximated by imposing an imaginary potential \(-iW(r), W(r) > 0\), or an ingoing-wave boundary condition at distances well inside the barrier. Here, these transitions are described by an auxiliary state \|X⟩\, to which all other states \|j⟩\ couple, modelled \[11\] by a Lindblad operator \(\hat{\mathcal{L}}_{Xj} = \sqrt{\gamma^{r}}|X⟩⟨j|\). The absorption rate to state \|X⟩\ is given by \(\gamma^{r} = W(r)/\hbar\) where \(W(r)\) is taken as a Fermi function with depth 10 MeV and diffuseness 0.1 fm, located at the pocket radius of the nucleus-nucleus potential, \(\approx 7\) fm. This choice guarantees complete absorption inside the pocket. The fusion probability is defined as the probability accumulating in this state \|X⟩\.

Thus, \|Y⟩\ and/or \|X⟩\ supplement the two intrinsic states \|1⟩\ and \|2⟩\ that comprise the two coupled channels. Both of the auxiliary states refer to complex excitation modes of the nuclei, associated with nucleonic degrees of freedom and compound nucleus states, respectively. They provide intuitive and formal channels \[11\] for describing irreversible coupling and loss of probability from the system to these environments, couplings that enter only through Lindblad’s dissipative Liouvillian \[8\]. \|Y⟩\ is also assumed to couple to
FIGURE 1. (Color online) Schematic picture of the model scenario. \( \mathcal{C}_X \) and \( \mathcal{C}_Y \) are physically motivated Lindblad’s operators for the two dissipative channels \(|X\rangle\) and \(|Y\rangle\), respectively. See text for further details.

\[ |X\rangle - \text{Environment associated with compound nucleus states} \]

\[ \mathcal{C}_X = \sqrt{\gamma^r} |X\rangle \langle j| \text{ where } \gamma^r = W(r)/\hbar \]

\[ |Y\rangle - \text{Environment associated with nucleonic degrees of freedom} \]

\[ \mathcal{C}_Y = \sqrt{\Gamma_{Yj}} |Y\rangle \langle j| \text{ where } \Gamma_{Yj} \text{ is a constant} \]

\(|X\rangle\) at the appropriate range of separations. Probability accumulating in state \(|Y\rangle\) outside of this \(|X\rangle\) pocket may be identified with deep-inelastic processes.

Dynamical calculations proceed as follows. The reduced density matrix results from the representation of the reduced density operator \( \hat{\rho}(t) \) in an asymptotic (product) basis of coordinate states and intrinsic energy states of the individual nuclei. Its dynamical evolution is dictated by a set of Lindblad’s coupled equations [8] for the matrix elements, which defines a time-dependent coupled-channels problem with an initial value. The initial pure-state density matrix, describing the well-separated nuclei (in their ground states) with a wave-packet in their relative motion, has \( \text{Tr}[\hat{\rho}^2] = 1 \). The purity of this state, conserved under unitary time evolution, is destroyed (\( \text{Tr}[\hat{\rho}^2] < 1 \)) if the environment causes a loss of quantum coherence. The degree of decoherence is quantified by a loss of purity of the density matrix. Having solved the time-evolution of the density-matrix numerically [8], the expectation value of reaction observables \( \hat{O} \) is given by evaluating the appropriate trace \( \langle \hat{O}(t) \rangle = \text{Tr}[\hat{O}\hat{\rho}(t)] \). In this way, probabilities of reaction channels can be determined.

We have performed test calculations for a head-on collision of \(^{16}\text{O} + ^{144}\text{Sm}\) at energies...
below the nominal Coulomb barrier ($V_B = 61.1$ MeV). The Hamiltonian of the reduced system is the same as that in the fusion model implemented in \textsc{ccfull} [6]. The form of the bare nuclear potential between the two nuclei, consistent with the stated $V_B$, is a Woods-Saxon potential with $(V_0, r_0, a_0) = (-105.1$ MeV, 1.1 fm, 0.75 fm). The Coulomb potential was that for two point charges. The $^{16}$O projectile was taken to be inert and the $^{154}$Sm target was allowed to be excited to a GDR vibrational state. The dynamical nuclear coupling of the ground state $|1\rangle$ to the vibrational state $|2\rangle$, with excitation energy $E_{1-} = 15$ MeV, has a macroscopic deformed Woods-Saxon form with a deformation parameter of $\beta_1 = 0.2$.

The time step for the density-matrix propagation was $\Delta t = 10^{-22}$ s, and the radial grid ($r = 0 - 250$ fm) was evenly spaced with $M = 512$ points. The relative motion of the two nuclei in the entrance channel $|1\rangle$ was described by a minimal-uncertainty Gaussian wave-packet, with width $\sigma_0 = 20$ fm, initially centered at $r = 150$ fm, and was boosted towards the target with the appropriate average kinetic energy for the entrance channel energy $E_0$ required. The FWHM energy spread of the wave-packet is $\sim 3\%$. The numerical accuracy of the time evolution was checked using a fully coherent, time-dependent calculation, excluding coupling to states $|X\rangle$ and $|Y\rangle$. It was confirmed that the normalisation and purity of the density-matrix, $\text{Tr}[\hat{\rho}] = \text{Tr}[\hat{\rho}^2] = 1$, and the expectation value of the system energy $\text{Tr}[\hat{H}\hat{\rho}]$ were maintained with high accuracy over the required number of time steps, typically 700 for the full duration of the collision.

The importance of the two, spatially distinct, sources of environment couplings were studied. Calculations were first performed only including the effect of coupling of the number of time steps, typically 700 for the full duration of the collision. This is done here only for calculations of the tunneling probability $P(E_0)$, in a relative s-wave, shown in Figure 2. These comparisons, of necessity, require convolution of the $\ell = 0$ partial wave penetrabilities $T_0(E)$ from \textsc{ccfull} with the energy distribution $f(E, E_0)$ of the chosen initial wave packet. That is, $P(E_0) \equiv \int dE f(E, E_0) T_0(E)$. The $P(E_0)$, shown as a function of $E_0/V_B$ in Figure 2, are in very good agreement showing the appropriateness of stationary state coupled-channels calculations for this observable within the dynamical scheme of states $|1\rangle$, $|2\rangle$ and $|X\rangle$. It is our contention that the dissipation associated with state $|X\rangle$, while significant at 60 MeV, is strongly localised inside the barrier and thus does not impact upon the barrier penetrability. We will now show that the same is not true for the more spatially-extended dissipation due to the GDR decay environment $|Y\rangle$.

The treatment of the irreversible GDR decay (with a spreading width of 6 MeV) to the bath of surrounding complex states (represented by $|Y\rangle$) was included by switching on the coupling of the intrinsic inelastic state $|2\rangle$ to $|Y\rangle$. Unlike the coupling to $|X\rangle$, a major part of the inelastic excitation of the system gives access to $|Y\rangle$ before the wave packet encounters the fusion barrier. The onset of decoherence, the purity of the density matrix,
TABLE 1. The calculated density matrix purity $\text{Tr}[\hat{\rho}^2]$ and energy loss $\Delta E = \text{Tr}[\hat{H}(\hat{\rho}_0 - \hat{\rho})]$ following time-evolution (for 700 time steps) when including only the state $|X\rangle$ (left entries) and both states $|X\rangle$ and $|Y\rangle$ (right entries) environmental couplings. The GDR coupling strength used was $\beta_1 = 0.2$.

| $E_0$ (MeV) | State $|X\rangle$ | States $|X\rangle$ and $|Y\rangle$ |
|-------------|-------------------|------------------------------|
|             | $\text{Tr}[\hat{\rho}^2]$ | $\Delta E$ (MeV) | $\text{Tr}[\hat{\rho}^2]$ | $\Delta E$ (MeV) |
| 45          | 1.0000            | 0.0004                     | 0.9196                     | 1.8718             |
| 50          | 1.0000            | 0.0004                     | 0.8977                     | 2.6744             |
| 55          | 0.9996            | 0.0109                     | 0.8759                     | 3.6100             |
| 60          | 0.6067            | 14.862                     | 0.5127                     | 18.908             |

FIGURE 2. (Color online) The energy dependence of the $s$-wave tunneling probability calculated with the density matrix (solid points) and the coupled-channels CCFULL methods (full line). See text for further details.

and the associated energy dissipation are shown in the right hand entries in Table I.

The probability trapped under the fusion barrier is associated with GDR collective vibrational energy being irreversibly removed from the coherent dynamics into surrounding bath states (heat). This is then no longer available for relative motion, or tunneling. Such energy loss can be correlated with deep inelastic processes, seen experimentally,
Figure 3. (Color online) Time-dependence of the probability trapped in $|X\rangle$ for $E_0 = 45$ MeV. The full curve includes states $|1\rangle$, $|2\rangle$ and $|X\rangle$. The dotted curve adds the irreversible decay of $|2\rangle$ to $|Y\rangle$. The calculations are for $\beta_1 = 0.2$.

that compete with fusion in reactions involving heavy nuclei [5].

Figure 3 shows the time evolution of the probability trapped in the potential pocket, state $|X\rangle$, for $E_0 = 45$ MeV. We comment that, when including the inelastic channel $|2\rangle$ but not $|Y\rangle$, the nucleus-nucleus potential renormalization leads to the expected enhanced penetrability from the inelastic channel coupling, compared to the purely elastic ($|1\rangle$ plus $|X\rangle$) calculation. The decoherent dynamics due only to environment $|X\rangle$ gives the (full curve). By comparison, the calculation that also includes the GDR doorway-state decay to $|Y\rangle$ leads to a suppression (dotted curve and arrow) of the population of state $|X\rangle$. Additional irreversible processes other than excitation of the GDR are also likely to contribute to the deep-inelastic yield, such as complicated multi-nucleon transfers [12]. To simulate these very simply, the assumed state $|1\rangle$ to $|2\rangle$ coupling strength was increased. Figure 4 shows the dependence of the calculated tunneling suppression on the assumed $\beta_1$ strength for $E_0 = 45$, where we note that larger $\beta_1$ result in both an increase in the strength and the range of the coupling formfactor to the inelastic state $|2\rangle$. 
SUMMARY

We have reported on a quantum dynamical approach based on time-propagation of a coupled-channels density matrix. Both deep-inelastic processes and quantum tunneling (fusion) can be treated within this fully quantal framework. It describes the transition from pure state (coherent) to mixed state (decoherent and dissipative) dynamics during a nuclear collision. The development provides a significant step towards an improved theoretical understanding of low-energy collision dynamics, as the calculations exhibit both quantum decoherence and energy dissipation. Effects of decoherence and dissipation on collision dynamics can be manifested at distances outside the fusion barrier radius, resulting in suppression of the quantum tunneling probability. This may have major implications for understanding current problems in near-barrier reaction dynamics \[2,3,4\], including the sub-barrier fusion hindrance phenomenon \[13\]. More complete calculations and detailed consideration of other processes, such as multi-nucleon or cluster transfer reactions, are required to confront measurements.
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