Quantum friction

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We introduce a type of quantum dissipation – local quantum friction – by adding to the Hamiltonian a local potential that breaks time-reversal invariance so as to cool the system. Unlike the Kossakowski-Lindblad master equation, local quantum friction directly affects unitary evolution of the wavefunctions rather than the density matrix: it may thus be used to cool fermionic many-body systems with thousands of wavefunctions that must remain orthogonal. In addition to providing an efficient way to simulate quantum dissipation and non-equilibrium dynamics, local quantum friction coupled with adiabatic state preparation significantly speeds up many-body simulations, making the solution of the time-dependent Schrödinger equation significantly simpler than the solution of its stationary counterpart.

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Quantum dissipation in strongly coupled systems – where a subsystem irreversibly loses energy to the surrounding environment – has been studied for over half a century, but progress beyond simple systems has been slow due to its cumbersome theoretical framework. In addition to the formal difficulties of deriving accurate descriptions for interesting strongly interacting systems that lack a small expansion parameter – nuclear and chemical reactions, transport phenomena, response to very intense external fields, etc. – the evolution equations for the reduced density matrix of the subsystem of interest have strong memory effects [1–4]. This makes even numerical implementations of the derived master equations prohibitive in three dimensions (3D) because of the memory required to store the density matrix with a long history. In this letter, we propose a simple and efficient technique for quantum dissipation via unitary evolution with a local quantum friction potential which has no memory effects. Unlike the Kossakowski-Lindblad (KL) master equation [5] the local quantum friction effects strictly unitary evolution of wavefunctions. We apply this to efficiently generate initial configurations for density functional theories (DFTs) [6], thereby solving a long-standing problem in applying time-dependent DFT (TDDFT) [7] to large scale systems (N ∼ 10^5 to 10^6 single particle states on a three-dimensional (3D) lattice). Traditional methods require diagonalizing the single-particle Hamiltonian which takes O(N^3) operations per iteration with significant communication requirements on parallel computers. In contrast, real-time evolution scales as O(N^2 log N). The use of local quantum friction makes solving the time-dependent Schrödinger equation significantly simpler than the solving its stationary counterpart. Thus, the procedure we describe may advance several fields of physics where fermionic systems can be studied with TDDFT, including nuclear physics (nuclei and neutron stars), trapped cold fermionic atoms, and electronic structure.

Modern approaches to the nuclear structure of medium to heavy nuclei rely on density functional theory (DFT): an in principle exact approach [6] that includes and extends mean-field techniques. DFT and its time-dependent extension TDDFT, see e.g. [7–10], provide a unified approach to study both structure and reactions (dynamics). With more than two decades of success describing normal electronic systems, TDDFT and the formally related time-dependent Hartree-Fock approach have been used extensively in nuclear physics (see, for example, [11]). Including pairing correlations extends the application to cold atomic gases (via the superfluid local density approximation (SLDA) [12–16]) and additional nuclear systems (via the Hartee-Fock-Bogoliubov (HFB) and Skyrme functionals [12–17]): Pairing correlations are essential to describe low-energy induced fission of medium and heavy nuclei, for example.

The implementation of TDDFT in 3D without symmetry restrictions has remained an outstanding problem due to the numerical complexity of the problem. For example, consider the fission of a heavy nucleus into two spatially separated fragments: at a minimum, one requires a volume of 40 × 40 × 60 fm^3 with a resolution of at least 1 fm (corresponding to an energy cutoff of ∼ 200 MeV). A single particle wavefunction thus requires N ∼ 400 000 components including pairing and spin degrees of freedom. Correctly describing time-dependent pairing correlations requires essentially the full single-particle spectrum, so the construction of an initial state with conventional iterative techniques requires repeatedly diagonalizing the N × N single-particle Hamiltonian (an O(N^3) operation) for the hundreds of iterations required to converge to the self-consistent ground state with sufficient accuracy for starting numerically stable TDDFT time-integration al-
Nonlinear optimization methods help, see Broyden’s method [19], but still require hundreds of iterations, and convergence can remain elusive when the $N \gtrsim 10^5$.

To put this in perspective, a single diagonalization for both proton and neutron single-particle Hamiltonians took essentially the entire (now retired) JaguarPF computer – 217 800 of the 224 256 processor cores – about 6 hours of wall-time (about one million CPU hours), or about a month to determine just the initial state. Extending this approach to study nuclear matter in the crust of neutron stars requires approximately an order of magnitude more states, and hence will take hundreds to thousands of times longer which is prohibitively expensive, even with exascale computing. In contrast, the cooling thus removes any excess energy introduced as currents by the state preparation $H_s$ in a manner similar to classical friction – the faster the system moves, the more currents are generated, and the faster $U_t$ will cool the system.

The local density $\rho_t$ provides a natural way to normalize the potential (2) that works well in practice:

$$U_t = -\beta \frac{\mathbf{j}_t}{\rho_t} = -\beta \frac{\mathbf{\hat{\rho}}_t}{\rho_t},$$

where $\beta$ is a dimensionless constant of order unity. Thus, we have an efficient and practical method for preparing arbitrary initial states in quantum systems: Proceed as with adiabatic state preparation, but evolve with the Hamiltonian $H_t + U_t$ including the local quantum friction potential (3), which explicitly breaks time-reversal invariance, and removes any irrotational currents generated by faster-than-adiabatic evolution. After sufficient evolution – generally much shorter than required by pure adiabatic state preparation – the system will cool to a state without irrotational currents. In principle, this final state may be some excited eigenstate of the system, but evolving from the ground state of $H_0$ generally ensures convergence to the ground state of $H_1$.

The beauty of local quantum friction is its implementation. $U_t$ can be applied in exactly the same way as any local external potential contained in $H_t$, and manifestly preserves unitary evolution; all evolved wavefunctions remain normalized and orthogonal. It can thus be applied directly to fermionic TDDFTs which must evolve hundreds of thousands of single-particle wave functions $\psi_n(t)$ while preserving orthonormality $\langle \psi_m(t) | \psi_n(t) \rangle = \delta_{mn}$. Each wavefunction evolves with the same single-particle Hamiltonian $H_t + U_t$, but the density $\rho_t$ and current density $\mathbf{j}_t$ are now traces over the Slater determinant of states:

$$\mathbf{j}_t = \frac{\hbar}{m} \text{Im} \sum_{n=1}^{N} \psi_n^*(t) \nabla \psi_n(t), \quad \rho_t = \sum_{n=1}^{N} \psi_n^*(t) \psi_n(t).$$

In this manner, a set of orthogonal single-particle wave functions constructed for the trivial initial Hamiltonian $H_0$ is continuously transformed into another set of orthogonal single-particle wave functions finally describing
the self-consistent ground state of the non-trivial Hamiltonian \( H_1 \). In other words, the evolution evolves one Slater determinant into another Slater determinant. This is not complicated by the fact that for TDDFT, the single-particle Hamiltonian \( H_0 \) depends non-linearly on the single-particle wavefunctions – the evolution remains unitary.

Note that one need not start with eigenstates of \( H_0 \). In principle, any set of orthogonal wavefunctions can be used to start the process and local quantum friction \( (1) \) will eventually bring the system to a self-consistent state devoid of irrotational currents. In practice, starting with a poor choice of initial wavefunctions may stall or terminate the process near stationary excited states of \( H_1 \): the use of quasi-adiabatic state preparation from the ground state of \( H_0 \) generally ensures a more rapid cooling to the ground state of \( H_1 \).

We shall now illustrate the power of this approach with three examples of increasing numerical complexity. In the first example (Fig. 1), we prepare the ground state of a Bose gas in a quartic trap with and without a vortex. The ground state and first Landau-level for a non-interacting gas in a harmonic trap \( H_0 \) evolve into the ground state and single vortex state of the interacting gas in a quartic trap \( H_1 \). With only a single wavefunction, one does not typically observe stalling near states with no irrotational currents, so adiabatic state preparation is neither needed nor helpful – instead the system is cooled directly from the ground-state of \( H_0 \) after rapidly quenching the system to \( H_1 \). In this case only, one may compare with imaginary time evolution finding that local quantum friction is somewhat slower, but still exhibits the near exponential convergence.

In the second example, we determine the lowest 20 eigenstates of a symmetrized Woods-Saxon potential in three dimensions. We discretize the Schrödinger equation using the discrete variable representation (DVR) technique described in Ref. [22] on a \( 32^3 \) spatial lattice. The Hamiltonian matrix has \( 32^768^2 \) entries and is cumbersome to diagonalized on a laptop. Evolving with local quantum friction, however, the 20 lowest bound states can be found in under half an hour. We solve the problem with and without quasi-adiabatic switching and, although direct cooling works, quasi-adiabatic switching improves the efficiency allowing one to evolve for shorter periods \( T \).

In the final example, we demonstrate local quantum friction applied to a large-scale TDDFT simulation modeling the unitary Fermi gas with the TDSLDA [12–16]. We start with a self-consistent solution in an axially symmetric trap \( V_0(x,y) = m\omega_z^2(x^2 + y^2)/2 \) with periodic boundary conditions along \( z \). Note that translational invariance in \( z \) renders this an effectively two-dimensional problem that can be solved using traditional approaches. Using the combination of adiabatic switching and local quantum friction, we evolve to the ground

![FIG. 1. (Color online) Preparation of the ground state (GS) (left) and the single vortex state (right) with the Gross-Pitaevskii equation (GPE) (density profiles shown inset). Dotted lines show adiabatic state preparation from exact HO eigenstates: slower preparations have lower final energy. Solid lines show the local cooling algorithm from the HO initial state. The thin grey line shows imaginary time evolution which is not practical for fermionic DFTs. The lower subplots demonstrate the convergence on a logarithmic scale: like imaginary time evolution, quantum friction can exhibit near exponential convergence.](image1)

![FIG. 2. (Color online) The total instantaneous energy of a system of twenty non-interacting neutrons evolving from an initial 3D harmonic oscillator potential to a final symmetrized Woods-Saxon potential. The curves correspond to quasi-adiabatic evolution with friction \((1 - s_l)H_0 + s_l H_1 + U_l \) for various switching periods \( T \) (two-thirds of the simulation time) and just friction \( H_1 + U_l \) for the remaining third of the simulation. That the energy is constant during this time demonstrates that the ground state has been reached. Note: there are three curves for the longest \( T \) corresponding to different simulations with \( \{24^3, 32^3, 40^3\} \) lattices of 1 fm spacing: this demonstrates the infrared (IR) convergence.](image2)
state in an elongated three-dimensional trap $V_1(x, y, z) = m\omega_1^2 (x^2 + y^2)/2 + m\omega_2^2 z^2/2$ with a 1:4 aspect ratio in a box with $16 \times 16 \times 64$ spatial lattice points. The single-particle Hamiltonian here is a $32\,768 \times 32\,768$ matrix, and $15\,322$ coupled nonlinear partial differential equations (PDEs) in 3D and time are solved. The solution — using twenty four GPUs on the UW Hyak cluster — takes about one hour to converge to the ground state.

The final configuration of Titan (NCCS) [23] will have 18680 GPUs, and we expect to be able to solve several million PDEs on spatial lattices of $\sim 100^3$ points.

A natural extension to including local quantum friction is to include a fluctuating potential to create a quantum equivalent of the Langevin equation. By adjusting the nature and amplitudes of the fluctuating and dissipating terms, one can generate different ensembles. Note that this is similar to the stochastic projected GPE (SPGPE), see [25] and references therein. Efficient real-time evolution of this modified Schrödinger equation can then be used as a tool to study non-equilibrium quantum systems at finite temperatures. Local quantum friction might provide a more efficient approach to study quantum dissipation than the Markovian Kossakowski-Lindblad master equation, and provide an ideal tool for simulating non-equilibrium dynamics where interactions with the environment are modeled by the time-dependent local quantum friction potential $U_t$ and a stochastic driving term. This interaction is essentially classical, lacking entanglement between the quantum system and the environment. As such, the implementation is a simple extension of the time-dependent Schrödinger equation for wavefunctions and one does not have to evolve a reduced density matrix as in traditional approaches to quantum dissipative evolution [1–5].

We have shown how quantum friction can be introduced through a local potential that may be efficiently computed using standard techniques. The resulting evolution is manifestly unitary, preserving the orthonormality of states. This allows one to leverage efficient algorithms for simulating real-time dynamics with time-dependent density functional theories (TDDFTs), and we have demonstrated the efficacy of combining quasi-adiabatic state preparation with local quantum friction to prepare initial states. This algorithm greatly extends the reach of quantum many-body simulations since solving the time-dependent Schrödinger equation becomes easier than solving its static counterpart.

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