Annals of Physics 371 (2016) 368–378

Contents lists available at ScienceDirect

Annals of Physics

journal homepage: www.elsevier.com/locate/aop

Quantum dynamics at finite temperature: Time-dependent quantum Monte Carlo study

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ARTICLE INFO

Article history:
Received 24 March 2016
Accepted 20 May 2016
Available online 2 June 2016

Keywords:
Quantum Monte Carlo
Finite temperature
Density matrix

ABSTRACT

In this work we investigate the ground state and the dissipative quantum dynamics of interacting charged particles in an external potential at finite temperature. The recently devised time-dependent quantum Monte Carlo (TDQMC) method allows a self-consistent treatment of the system of particles together with bath oscillators first for imaginary-time propagation of Schrödinger type of equations where both the system and the bath converge to their finite temperature ground state, and next for real time calculation where the dissipative dynamics is demonstrated. In that context the application of TDQMC appears as promising alternative to the path-integral related techniques where the real time propagation can be a challenge.

1. Introduction

The area of non-equilibrium quantum statistical physics is still an object of rapid expansion in view of the new challenges posed by the recent developments in quantum transport in nano-materials, strongly correlated systems, dynamics of Bose–Einstein condensates at finite temperature, etc. The many-body open quantum systems have been treated perturbatively using the Green function formalism [1] and numerically by different Monte Carlo techniques [2,3]. Unlike in classical mechanics the incorporation of finite temperature effects is not trivial in quantum physics. The extension of the theoretical models at nonzero temperature involves environmental effects in the dynamics of the system by introducing nonlinearity into the Schrödinger equation itself [4] as well as using stochastic system-bath approaches where the quantum system which consists of relatively few degrees of

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http://dx.doi.org/10.1016/j.aop.2016.05.013
0003-4916/

freedom is coupled to a much larger bath through a system-bath coupling thus introducing quantum decoherence and dissipation [5]. The advantage of the latter is that it reduces in the classical limit to the familiar description based on generalized Langevin equation. However, most of the existing methods at finite temperature are focused on finding the ground state of the quantum system under consideration. Rare examples of real-time simulation techniques at finite temperature include multi configuration time-dependent self-consistent field [6] and real-time path integral [7]. Although time-polynomial the efficiency of the former method is hampered by the calculation of large number of Coulomb and exchange integrals while the latter may suffer from the rapid oscillations of the quantum propagator [8]. Therefore further development of non-perturbative time-dependent methods at finite temperature is indispensable to meet the challenges triggered by the experimental progress. A recent method with linear-to-low order polynomial scaling, the time-dependent quantum Monte-Carlo (TDQMC), combines self-consistently the non-stationary statistics of waves and particles (walkers) which evolve in physical space–time [9–11]. While the walker's distribution in space corresponds to the electron density, the quantum waves which guide those particles evolve according to a set of coupled nonlinear time-dependent Schrödinger equations. During the preparation stage of imaginary-time propagation TDQMC has a variational structure with the only variational parameter being the nonlocal quantum correlation length. Besides its conceptual simplicity TDQMC is unitary and numerically stable against rapid oscillations in the phase of the quantum state.

In this paper, the TDQMC method is applied to study finite-temperature effects in model quantum systems based on system-bath approach where a small system is coupled to a large bath of quantum oscillators at fixed temperature.

2. Preliminaries

For a non-relativistic system consisting of N particles of different kinds (quantum species) the Schrödinger equation reads:

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{R},t)=H\Psi(\mathbf{R},t), \tag{1}$$

where:

$$H=-\sum_{i}^{N}\frac{\hbar^2}{2M_i}\nabla_i^2+V(\mathbf{R},t), \tag{2}$$

is the many-body quantum Hamiltonian, and $\mathbf{R}=\{\mathbf{r}_1,\ldots,\mathbf{r}_N\}$ are the degrees of freedom. The potential in Eq. (2) may include electron–nuclear, nuclear–electron, electron–electron, nuclear–nuclear, and external potentials and M_i is the mass of ith species. Since, in general, the Hamiltonian in Eq. (2) is not separable in coordinates the numerical solution of Eq. (1) scales exponentially with the number of particles involved. Then, a factorization of the wave function of the type:

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N,t)=\prod_{i=1}^{N}\varphi_i(\mathbf{r}_i,t) \tag{3}$$

reduces Eqs. (1), (2) to the well-known set of self-consistent mean field (Hartree–Fock) equations (e.g. [12]) where the effect of the motion of each quantum particle on the rest of the particles is accounted for in an averaged manner such that the detailed quantum correlations are ignored. One way to recover those is to introduce an additional degree of freedom such that besides the wave function each quantum particle is described also by a set of classical particles (walkers) which are guided by separate guiding wave functions in the spirit of de Broglie–Bohm wave mechanics. Then, if the ith quantum particle is described by M walkers, we have for the walker's motion:

$$\mathbf{v}(\mathbf{r}_i^k)=\frac{\hbar}{M_i}\mathrm{Im}\left[\frac{1}{\varphi_i^k(\mathbf{r}_i,t)}\nabla_i\varphi_i^k(\mathbf{r}_i,t)\right]_{\mathbf{r}_i=\mathbf{r}_i^k(t)}, \tag{4}$$