Many-body quantum Monte Carlo wave-function approach to the dissipative atom-field interaction

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We develop a many-body quantum Monte Carlo wave-function approach to analyze the dissipative interaction of ultracold free atoms with the radiation field reservoir. A Markovian master equation for the identical atoms that neglects the dipole-dipole interaction is derived within the framework of quantum field theory. The effective Hamiltonian obtained by a decomposition of the master equation explicitly depends on the quantum statistics.

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Laser cooling below the photon recoil limit has been recently demonstrated [1] and one-dimensional effective temperatures as low as 100 nK have been measured [2]. At these ultracold temperatures, the thermal de Broglie wavelength of the atoms are on the order of the wavelength of the optical fields or larger, and the wave nature of the atoms become important. Atomic interferometers that utilize the wave nature of single atoms have been successfully demonstrated [3–5]. One of the objectives of this new field of atom optics, however, is the observation of the effect of quantum statistics on the dynamics, and particularly, the Bose-Einstein condensation of bosonic atoms. The proper theoretical description of an ensemble of ultracold atoms requires a quantum field-theoretical approach, and such a theory has been developed by Svistunov and Shlyapnikov [6], Politzer [7], and Lewenstein and You [8]. Zhang and Walls [9] used a similar description in the context of coherent laser-atom interactions.

In this article, we develop a quantum Monte Carlo wave-function (MCWF) approach [10–12] to the analysis of an ensemble of ultracold identical atoms, interacting with the radiation field reservoir. Following Zhang and Walls [9], we describe the atoms using quantum density fields, by extending the Schrödinger wave functions to quantum field operators. These field operators satisfy either the canonical commutation or anticommutation relations, depending on the quantum statistical nature of atoms being bosonic or fermionic. Using the second quantized interaction Hamiltonian, we derive a Markovian master equation describing the atomic dynamics. We then decompose this master equation to obtain a set of (angle-dependent) collapse operators (similar to the case of single atom laser cooling theory [11]), and an effective Hamiltonian that explicitly depends on the quantum statistics. The predictions of the theory include (1) for bosonic atoms, an effective spontaneous emission rate that is proportional to the product of the occupancy of the final atomic state and the single-atom decay rate; and (2) for fermionic atoms, inhibition of spontaneous emission into final atomic states that are already occupied. The effective Hamiltonian that we obtain exhibits features such as virtual transverse photon exchange between different atomic modes.

The recent interest in the stochastic wave function approach to dissipative processes in quantum optics is principally due to the simplification of the computational procedure for systems with many degrees of freedom [11,12]. Another feature is the physical insight provided by the wave-function description of a single (open) quantum system [10]. This work, together with the recent MCWF analysis of electron-phonon interaction in semiconductors [13], extends the previous stochastic wave-function methods to the analysis of dissipative many-body systems.

The stochastic wave-function theory for dissipative many-atom systems that we develop neglects the dipole-dipole interaction between the atoms and is based on the Born-Markov approximation. The free-atom formalism that we present below is otherwise general, and can be easily extended to include interactions with a coherent laser field and a trap potential confining the atoms in real space. Here, we consider the low temperature (the thermal de Broglie wavelength λ_T is much longer than the resonant photon wavelength λ_L), low atomic density ($\mathcal{N}$) case where $\mathcal{N}\lambda_T^3 \geq 1 \gg \mathcal{N}\lambda_L^3$. In this limit, the interactions arising from the composite nature of the atoms (i.e., dipole-dipole coupling) can be neglected, even though the many-body features remain pertinent.

We consider an ensemble of identical two-level atoms where the excited-state $|e\rangle$ couples to radiation field modes and decays spontaneously to the ground state $|g\rangle$. The starting point of our analysis is the interaction Hamiltonian of the radiation and atomic (quantum) fields in the Schrödinger picture [9],

$$\hat{H}_{\rm int} = i\hbar \sum_{\mathbf{k}}{}' g_{\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger \int d\mathbf{r}\, \hat{\psi}_g^\dagger(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} \hat{\psi}_e(\mathbf{r}) + \text{H.c.}\,, \quad (1)$$

where $\hat{a}_{\mathbf{k}}$ denotes the annihilation operator of the radiation field mode $\mathbf{k}$ and $\hat{\psi}_\nu(\mathbf{r})$ denotes the field operator that annihilates an atom with internal state $|\nu\rangle$ at position $\mathbf{r}$ ($\nu = g, e$). $g_{\mathbf{k}}$ is the coupling constant of the atoms to the radiation field mode $\mathbf{k}$. In contrast to Zhang and Walls [9], we expand the atomic field operators in terms of free propagation modes,

$$\hat{\psi}_g(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{p}} \hat{g}_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}},$$
$$\hat{\psi}_e(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{p}} \hat{e}_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}}. \tag{2}$$

Here, $\hat{g}_{\mathbf{p}}$ ($\hat{e}_{\mathbf{p}'}$) denotes the annihilation operator of a ground (excited) state atom in mode $\mathbf{p}$ ($\mathbf{p}'$) and V is the quantization volume. Substituting Eq. (2) in Eq. (1), we obtain the atom-field interaction Hamiltonian in the second quantized form,

$$\hat{H}_{\rm int} = i\hbar \sum_{\mathbf{k},\mathbf{p}} g_{\mathbf{k}} (\hat{a}^\dagger_{\mathbf{k}} \hat{g}^\dagger_{\mathbf{p}-\mathbf{k}} \hat{e}_{\mathbf{p}} - \hat{e}^\dagger_{\mathbf{p}} \hat{g}_{\mathbf{p}-\mathbf{k}} \hat{a}_{\mathbf{k}}). \tag{3}$$

The Hamiltonian of Eq. (3) can be used in the Liouville–von Neumann equation to evaluate the time evolution of the density operator of the atom-field system. Following the derivation of Ref. [14], we will first go to the interaction picture ($\hat{a}_{\mathbf{k}} \to \hat{a}_{\mathbf{k}} e^{-i\omega_k t}; \hat{g}_{\mathbf{p}} \to \hat{g}_{\mathbf{p}} e^{-i(\epsilon_p+\omega_g)t}; \hat{e}_{\mathbf{p}} \to \hat{e}_{\mathbf{p}} e^{-i(\epsilon_p+\omega_e)t}$). We assume that the initial radiation field density operator commutes with the free Hamiltonian, and that the reservoir is not affected by the presence of the atoms. These assumptions imply $\hat{\sigma}_R(t) = {\rm Tr}_A[\hat{\rho}(t)] = \hat{\sigma}_R(0)$, where $\hat{\sigma}_R(t)$ and $\hat{\rho}(t)$ denote the density operator for the reservoir and the atom-reservoir system, respectively. We make the Born approximation and obtain the equation of motion of the reduced atomic density operator in the interaction picture,

$$\frac{d\hat{\sigma}(t)}{dt} = \left(\frac{1}{i\hbar}\right)^2 \int_0^t dt' \times {\rm Tr}_R\Big([\hat{H}_{\rm int}(t), [\hat{H}_{\rm int}(t'), \hat{\sigma}(t') \otimes \hat{\sigma}_R(0)]]\Big). \tag{4}$$

The first order term ${\rm Tr}_R[\hat{H}_{\rm int}(t), \hat{\rho}(0)]$ that comes from the formal integration of the equation of motion for the density operator is identically zero, since ${\rm Tr}_R[\hat{\sigma}_R(0)\hat{H}_{\rm int}(t)]$ vanishes for the interaction Hamiltonian of Eq. (3).

Due to the dense ensemble of levels in the radiation field reservoir, the reservoir operators have a characteristic correlation time $\tau_{\rm corr}$, which is in general shorter than the reciprocal atomic transition frequency $\omega_{eg} = \omega_e - \omega_g$. Provided that the atomic phase-space density is low enough (to be specified), we can make the Markov approximation and replace $\hat{\sigma}(t')$ by $\hat{\sigma}(t)$ in Eq. (4). For simplicity, we are also going to set the radiation field temperature to zero.

We now evaluate the time integral in Eq. (4). The principal value terms could result in nontrivial energy shifts and many-body coherences. Since our main goal is to analyze dissipation, we discard these terms with the assumption that they could in principle be included in the (Hermitian) free atomic Hamiltonian (see below). We then obtain

$$\frac{d\hat{\sigma}(t)}{dt} = -\sum_{\mathbf{p}_1,\mathbf{p}_2} \sum_{\mathbf{k}} \Bigg(\pi |g_{\mathbf{k}}|^2 \delta(\epsilon_{\mathbf{p}_2-\mathbf{k}} - \epsilon_{\mathbf{p}} - \omega_{eg} + \omega_{\mathbf{k}}) e^{-i(\epsilon_{\mathbf{p}_1-\mathbf{k}} - \epsilon_{\mathbf{p}_1} - \epsilon_{\mathbf{p}_2-\mathbf{k}} + \epsilon_{\mathbf{p}_2})t} \times \Big[\hat{e}^\dagger_{\mathbf{p}_1} \hat{g}_{\mathbf{p}_1-\mathbf{k}} \hat{g}^\dagger_{\mathbf{p}_2-\mathbf{k}} \hat{e}_{\mathbf{p}_2} \hat{\sigma}(t) - \hat{g}^\dagger_{\mathbf{p}_2-\mathbf{k}} \hat{e}_{\mathbf{p}_2} \hat{\sigma}(t)\, \hat{e}^\dagger_{\mathbf{p}_1} \hat{g}_{\mathbf{p}_1-\mathbf{k}} \Big] + {\rm H.c.} \Bigg). \tag{5}$$

We can use the δ function in Eq. (5) to evaluate the photon-energy ($|\mathbf{k}| = k$) integral, which determines the magnitude of the emitted photon momentum $\bar{k}(\mathbf{p}_2)$. For the atom-radiation field interaction (especially at low temperatures) the atomic momentum dependence of the photon momentum is negligible and we can simply take $\bar{k}(\mathbf{p}_2) = \bar{k}$. We then identify the spontaneous photon-emission rate along a given direction (Ω) as $\Gamma(\Omega) = \sum_k 2\pi |g_{k,\Omega}|^2 \delta(\epsilon_{\mathbf{p}_2-\mathbf{k}} - \epsilon_{\mathbf{p}} - \omega_{eg} + \omega_{\mathbf{k}})$. We neglect the weak dependence of the spontaneous emission rate on the atomic momentum that actually is an artifact of the approximate interaction Hamiltonian that we use [15]. Switching back to the Schrödinger picture, we obtain the many-body atomic master equation in the Born-Markov approximation

$$\frac{d\hat{\sigma}_s(t)}{dt} = \frac{1}{i\hbar}[\hat{H}_0, \hat{\sigma}_s(t)] + \tfrac{1}{2} \sum_{\Omega} \Gamma(\Omega) \sum_{\mathbf{p}_1,\mathbf{p}_2} \Big(2\hat{g}^\dagger_{\mathbf{p}_2-\bar{\mathbf{k}}} \hat{e}_{\mathbf{p}_2} \hat{\sigma}_s(t) \hat{e}^\dagger_{\mathbf{p}_1} \hat{g}_{\mathbf{p}_1-\bar{\mathbf{k}}} - \hat{e}^\dagger_{\mathbf{p}_1} \hat{g}_{\mathbf{p}_1-\bar{\mathbf{k}}} \hat{g}^\dagger_{\mathbf{p}_2-\bar{\mathbf{k}}} \hat{e}_{\mathbf{p}_2} \hat{\sigma}_s(t) - \hat{\sigma}_s(t) \hat{e}^\dagger_{\mathbf{p}_2} \hat{g}_{\mathbf{p}_2-\bar{\mathbf{k}}} \hat{g}^\dagger_{\mathbf{p}_1-\bar{\mathbf{k}}} \hat{e}_{\mathbf{p}_1} \Big). \tag{6}$$

Here, $\hat{\sigma}_s(t)$ and $\hat{H}_0$ denote the Schrödinger picture reduced density operator and the (free) atomic Hamiltonian, respectively. $\bar{\mathbf{k}}$ is the photon wave vector emitted along direction Ω. $\hat{H}_0$ may in general contain the principal value terms arising from the reservoir interactions as well as interactions with other sources, such as weak coherent electromagnetic fields.

Equation (6) gives the master equation that describes an ensemble of many-body quantum systems that undergo dissipation due to their interaction with the radiation field reservoir and is the starting point for a quantum MCWF description. Following Refs. [10,16], we *decompose* the master equation to obtain a set of collapse operators that depend on the emitted (detected) photon direction,

$$\hat{C}_\Omega = \sum_{\mathbf{p}} \sqrt{\Gamma(\Omega)} \hat{g}^\dagger_{\mathbf{p}-\bar{\mathbf{k}}} \hat{e}_{\mathbf{p}}, \tag{7}$$

and an effective Hamiltonian

$$\begin{aligned}\hat{H}_{\text{eff}} &= \hat{H}_0 - \frac{i\hbar}{2} \sum_\Omega \hat{C}^\dagger_\Omega \hat{C}_\Omega \\ &= \hat{H}_0 - \frac{i\hbar}{2} \sum_\Omega \Gamma(\Omega) \sum_{\mathbf{p},\mathbf{p}'} \hat{e}^\dagger_{\mathbf{p}'} \hat{g}_{\mathbf{p}'-\bar{\mathbf{k}}} \hat{g}^\dagger_{\mathbf{p}-\bar{\mathbf{k}}} \hat{e}_{\mathbf{p}} \\ &= \hat{H}_0 - \frac{i\hbar}{2} \sum_\Omega \Gamma(\Omega) \sum_{\mathbf{p},\mathbf{p}'} \hat{e}^\dagger_{\mathbf{p}'} \hat{e}_{\mathbf{p}} (\delta_{\mathbf{p},\mathbf{p}'} + q \hat{g}^\dagger_{\mathbf{p}-\bar{\mathbf{k}}} \hat{g}_{\mathbf{p}'-\bar{\mathbf{k}}}).\end{aligned} \tag{8}$$

Here, q is defined by the commutation relations that the atoms satisfy $[\hat{g}_{\mathbf{p}'}, \hat{g}^\dagger_{\mathbf{p}}]_q = \hat{g}_{\mathbf{p}'} \hat{g}^\dagger_{\mathbf{p}} - q\, \hat{g}^\dagger_{\mathbf{p}} \hat{g}_{\mathbf{p}'}$, i.e., $q = +1$ for bosons and -1 for fermions.

The effective Hamiltonian given by Eq. (8) along with the collapse operators of Eq. (7) constitute the principle result of this paper: They show that the dissipative dynamics of a many-atom system interacting with the radiation field reservoir explicitly depends on the quantum statistics that the atoms obey. More specifically, the (imaginary) diagonal terms of the $\hat{H}_{\text{eff}}$ that correspond to the total decay rates are (1) enhanced by a factor proportional to $[1 + \langle \hat{g}^\dagger_{\mathbf{p}-\bar{k}} \hat{g}_{\mathbf{p}-\bar{k}} \rangle]$ for bosons, and (2) reduced by $[1 - \langle \hat{g}^\dagger_{\mathbf{p}-\bar{k}} \hat{g}_{\mathbf{p}-\bar{k}} \rangle]$ for fermions. The off-diagonal terms of Eq. (8) correspond to non-Hermitian virtual-photon exchange between the atoms, and are also subject to enhancement (bosons) and reduction (fermions) due to the final-state occupancies. This coupling term is similar to the nonsecular terms arising in Fano-type systems, and may lead to interference effects in Raman or Rayleigh scattering experiments [17].

The fact that the radiative decay of bosons is stimulated [7] by both the initial (superfluorescence effect) and final state occupancies (quantum statistical effect) limits the applicability of the Markov approximation to relatively low phase-space densities. An approximate validity condition may be obtained by requiring that the net decay rate be much smaller than the transition frequency: $\Gamma(\Omega)[1 + \langle \hat{g}^\dagger_{\mathbf{p}-\bar{k}} \hat{g}_{\mathbf{p}-\bar{k}} \rangle] \langle \hat{e}^\dagger_{\mathbf{p}} \hat{e}_{\mathbf{p}} \rangle \ll \omega_{eg}$. For typical atomic transitions, the upper limit in the phase-space densities introduced by this requirement is about 1×10^6, under weak-excitation conditions $(\langle \hat{e}^\dagger_{\mathbf{p}} \hat{e}_{\mathbf{p}} \rangle \ll \langle \hat{g}^\dagger_{\mathbf{p}-\bar{k}} \hat{g}_{\mathbf{p}-\bar{k}} \rangle)$.

As indicated before, the Hermitian part of the effective Hamiltonian $\hat{H}_0$ may in general include coherent-optical interactions. From a practical point of view, any measurement on the atomic ensemble would be done by probing the system using a (weak) laser beam. Provided that the Rabi frequency of the laser-atom coupling is much smaller than the transition frequency, the Born-Markov approximation and hence the master equation of Eq. (6) remain valid. If we neglect the principal value terms and the dipole-dipole interactions, the form of $\hat{H}_0$ is

$$\begin{aligned}\hat{H}_0 = \hbar \sum_{\mathbf{p}} &[\epsilon_{\mathbf{p}} \hat{g}^\dagger_{\mathbf{p}} \hat{g}_{\mathbf{p}} + (\epsilon_{\mathbf{p}} + \omega_{eg}) \hat{e}^\dagger_{\mathbf{p}} \hat{e}_{\mathbf{p}}] \\ &+ i\hbar \sum_{\mathbf{p}} g_L (\hat{a}^\dagger_L \hat{g}^\dagger_{\mathbf{p}-\mathbf{k}_L} \hat{e}_{\mathbf{p}} - \hat{e}^\dagger_{\mathbf{p}} \hat{g}_{\mathbf{p}-\mathbf{k}_L} \hat{a}_L) .\end{aligned} \tag{9}$$

In Eq. (9), $\hat{a}_L$ $(\hat{a}^\dagger_L)$ denotes the annihilation (creation) operator of the laser mode $\mathbf{k}_L$, and g_L denotes the atom-laser coupling constant. We reemphasize that only in the low atomic density and weak laser excitation limit we can neglect the dipole-dipole interactions.

The many-body stochastic wave-function approach that we introduce here should simplify the numerical simulations considerably. In a typical simulation, we expand the many-body wave function using multimode atomic-number states, where the maximum occupancy of each mode is limited to the total number of atoms N_a: For M discretized momentum states, the eigenstates of the noninteracting Hamiltonian that we use are of the form $|n_{g,p_1}, n_{e,p_1}, n_{g,p_2}, n_{e,p_2}, \ldots, n_{e,p_M}\rangle$, where $n_{g,p_1} + n_{e,p_1} + \cdots + n_{e,p_M} = N_a$. The interesting many-body effects can only be seen in systems with a large state space, which for bosonic systems would have

$$\frac{(sM + N_a - 1)!}{N_a!\,(sM - 1)!}$$

coupled quantum states ($s = 2$ is the number of internal atomic states). Due to our limited computational facilities, we shall consider a hypothetical case where a few atoms ($N_a \le 10$) are interacting with the tailored radiation field reservoir of a one-dimensional photonic bandgap structure [18], which only permits spontaneous photon emission along two directions ($\pm\hat{\mathbf{z}}$). A resonant coherent laser field propagating along $\hat{\mathbf{z}}$ weakly couples the two atomic states. We assume in addition that the initial momentum distribution of the atoms are such that their momentum standard deviation Δp satisfies $\Delta p \ll \bar{k}$.

In general, one would expect that the bosons would have a stronger forward scattering rate [19] due to the stimulation by the final state occupancy. For fermions however, the opposite is true: The fact that the final states for forward scattering are mostly full makes backscattering more likely. In the simple one-dimensional case that we are considering, the situation is somewhat different: The dynamics of fermionic atoms are almost identical to independent atoms since the final state of the forward scattering is necessarily empty and the forward and backward scattering are therefore equally likely.

Figure 1 shows the results of our simulations for bosonic atoms under weak resonant laser excitation where $g_L\sqrt{\bar{n}_L} = 0.025\Gamma$. Here, $\bar{n}_L$ denotes the mean occupancy of the laser mode, $\Gamma = \Gamma_+ + \Gamma_-$ denotes the total (single-atom) spontaneous emission rate, and Γ_+ and Γ_- are the decay rates along $+\hat{\mathbf{z}}$ and $-\hat{\mathbf{z}}$ directions, respectively ($\Gamma_+ = \Gamma_-$). We see that as the atomic number N_a is increased, the forward scattering becomes more favored to the extent that for $N_a \ge 5$, practically all the scattered photons are emitted along $+\hat{\mathbf{z}}$. For the assumed exactly resonant laser case, however, an increase in the

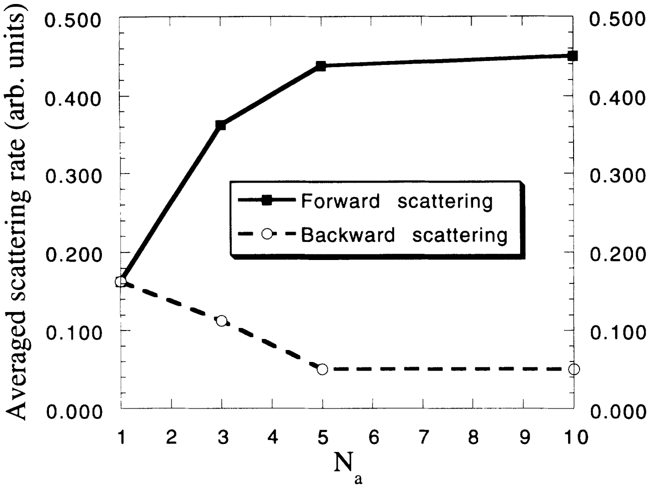

FIG. 1. The forward and backward scattering rates for bosonic atoms as a function of the total number of atoms under weak resonant laser excitation. Atoms are assumed to occupy the lowest allowed energy state before the coherent laser is turned on.

atomic number does not result in a considerable increase in the total scattering rate, due to the increase in the linewidth associated with the cooperative decay. The total many-atom (weak-field) scattering rate is about twice as high as the single-atom rate, as would be predicted by a perturbative approach based on the effective Hamiltonian. In these simulations, all the atoms are initially in the lowest *discrete* momentum state and it is assumed that only four momentum states are coupled by the interactions.

The extension of the many-body MCWF method to finite radiation field temperatures is straightforward. For bosonic atoms interacting with a thermal field with average occupancy $\bar{n}_T$ at frequency ω_{eg}, we obtain in steady state (absorption equals emission),

$$\frac{\langle \hat{e}^\dagger_{\mathbf{p}} \hat{e}_{\mathbf{p}} \rangle}{1 + \langle \hat{e}^\dagger_{\mathbf{p}} \hat{e}_{\mathbf{p}} \rangle} = \frac{\bar{n}_T}{1 + \bar{n}_T} \quad , \tag{10}$$

provided that $\langle \hat{g}^\dagger_{\mathbf{p}-\bar{k}} \hat{g}_{\mathbf{p}-\bar{k}} \rangle \gg 1$. Therefore, once large phase-space densities are reached, the excited-state population is fixed by the radiation field temperature and is independent of the total number of atoms. The resulting population distribution in internal atomic states is nonthermal.

Many-body atomic physics with all the interesting prospects for linear and nonlinear atom optics [20] is fast becoming an active subfield of atomic and optical physics. The ultralarge state space necessarily associated with the interesting many-body effects make a wave-function approach indispensable. We believe that the simple many-body quantum MCWF approach developed in this letter will be very useful, especially if it is extended to include dipole-dipole interactions.

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