Quantum systems coupled to a structured reservoir with multiple excitations

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We present a method for dealing with quantum systems coupled to a structured reservoir with any density of modes and with more than one excitation. We apply the method to a two-level atom coupled to the edge of a photonic band gap and a defect mode. Results pertaining to this system provide the solution to the problem of two photons in the reservoir, and a possible generalization is discussed. [S1050-2947(99)10512-2]

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The problem of the interaction of small systems with structured reservoirs is of central importance to a number of areas including nanostructures in semiconductors, atom lasers [1], aspects of molecular dynamics [2] and atoms embedded in photonic band-gap materials. A fundamental difficulty in the theoretical formulation of such problems stems from the invalidation of the Born-Markov approximations, essential in obtaining a master equation, which is the standard vehicle in the presence of smooth reservoirs. Models approximating some of the features of such reservoirs such as superpositions of Lorentzians can be useful, as the introduction of ''pseudomodes'' can lead to a Markovian master equation for a system slightly enlarged through the introduction of the pseudomodes [3–6]. Alternatively, one may introduce decorrelation approximations in the Heisenberg equations of motion for the operators of interest. But in any case, one cannot be confident of the validity and degree of accuracy of the approximations. For a general density of states that cannot be modeled by a superposition of Lorentzians, the dynamics can only be obtained if there is at most one photon in the structured reservoir [7]. At this point, there is no generally established approach that can provide a description of the dynamics for a general density of states and multiple excitations in the structured continuum.

It is the purpose of this paper to present such an approach with illustrative applications. The basic idea relies on the discretization of the continuum, which is thus replaced in the formulation by a finite (but large) number of discrete modes. Their couplings and frequencies are chosen so as to model the effect of the structured continuum to the desired accuracy. The judicious choice of this parametrization is of critical importance to the success of this idea. Given the discretization, the system ''atom plus discretized continuum'' can be handled through differential equations governing the evolution of the amplitudes entering the Schrödinger equation. These differential equations are then solved numerically. The discretization of continua in other contexts [8] is an established but always dangerous approach requiring much care, as it can lead to unphysical artifacts.

To introduce and demonstrate the method, we consider a two-level atom coupled near-resonantly to the edge of a photonic band gap (PBG) [9–14]. The photonic band-gap material has a strongly modified dispersion relation, and, employing the isotropic dispersion relation introduced by John and Wang [11], the corresponding density of states reads

$$\rho(\omega)=\frac{k}{\sqrt{\omega-\omega_e}}\Theta(\omega-\omega_e), \tag{1}$$

where k is a material specific constant, ω_e is the band-edge frequency, and $\Theta(x)$ is the Heaviside step function. Clearly, the density of modes diverges at the edge frequency, which invalidates the standard Born-Markov approximations normally employed when dealing with a smooth reservoir. As a consequence the reservoir cannot be eliminated.

The idea is to replace the density of modes in Eq. (1) near the atomic transition (which for our purposes will be in the vicinity of the edge frequency) by a collection of discrete harmonic oscillators, while the rest of the mode density can be treated perturbatively since it is far from resonance. The frequencies and the couplings of the discrete modes are chosen such that the discrete oscillators best model the structured continuum near the edge frequency. To this end, we write Eq. (1) in a differential form,

$$\Delta N=\rho(\omega)\Delta\omega. \tag{2}$$

For $\Delta N=1$, and introducing a discrete index, we find $\Delta\omega_i=1/\rho(\omega_i)$, and thus

$$\omega_{i+1}=\omega_i+\Delta\omega_i=\omega_i+1/\rho(\omega_i) \tag{3}$$

and $\omega_1=\omega_e+\delta$, where δ is chosen sufficiently small ($\delta\approx 10^{-2}C^{2/3}$). The coupling g_r to the discrete modes is found by integration of Eq. (2),

$$\sum g_r^2\Delta N\approx\int_{\omega_e}^{\omega_u}d\omega|\kappa_\omega|^2\rho(\omega), \tag{4}$$

where ω_u is the upper limit of the discretized part of the density of states, κ_ω is the coupling between the continuum mode with frequency ω and the atom and, $|\kappa_\omega|^2\rho(\omega)=(C/\pi)[1/\sqrt{(\omega-\omega_e)}]$, where C is the effective coupling of the atom to the PBG structure. We thus find

$$g_r\approx\sqrt{\frac{2C}{N\pi}\sqrt{\omega_u-\omega_e}}, \tag{5}$$

where N is the number of discrete modes. An alternative form of Eq. (3) is

$$\omega_{i+1}=\omega_{i-1}+\Delta\omega_i=\omega_{i-1}+2/\rho(\omega_i), \tag{6}$$

which is actually the form that we have used in our implementation.

We consider a two-level atom with ground ($|g\rangle$) and excited ($|e\rangle$) states whose energy difference is $\hbar\omega_o$. The atom is coupled to the structured reservoir and a defect mode centered at the frequency ω_d inside the gap. The Hamiltonian for this system in an interaction picture rotating at the band-edge frequency ω_e ($\hbar=1$), and in the rotating-wave approximation reads

$$H=\Delta_0\sigma_{ee}+\Delta_d a_d^\dagger a_d+\sum_\lambda \Delta_\lambda a_\lambda^\dagger a_\lambda+g_d(a_d\sigma^+ + a_d^\dagger\sigma^-)$$

$$+\sum_\lambda g_\lambda(a_\lambda\sigma^+ + a_\lambda^\dagger\sigma^-), \tag{7}$$

where $\Delta_o=\omega_o-\omega_e$, and $\Delta_d=\omega_d-\omega_e$, and $\Delta_\lambda=\omega_\lambda-\omega_e$; $\sigma^+=|e\rangle\langle g|$ and $\sigma^-=|g\rangle\langle e|$ are the atomic raising and lowering operators, and $\sigma_{ee}=\sigma^+\sigma^-$. The field operators $(a_d,a_d^\dagger)$ and $(a_\lambda,a_\lambda^\dagger)$ correspond to the defect mode and PBG reservoir, respectively, which are coupled to the atom via the respective coupling constants g_d and g_λ.

In order to demonstrate the validity of this method, we first present the results for spontaneous decay, i.e., the atom is initially excited, and we neglect the defect mode, i.e., $g_d=0$. Replacing the density of modes of Eq. (1) for $\omega<\omega_u$, by a collection of discrete modes, the wave function for the full system reads

$$|\psi\rangle=a_0|e,0\rangle+\sum_j b_j|g,1_j\rangle+\sum_\lambda b_\lambda|g,1_\lambda\rangle, \tag{8}$$

where the amplitudes b_j correspond to the discrete modes, while b_λ correspond to the modes with frequency $\omega_\lambda>\omega_u$, which are treated pertubatively, i.e., they are eliminated adiabatically.

The time evolution of the amplitudes is governed by the Schrödinger equation, from which we obtain

$$\dot a_0=\frac{1}{i}\Delta_0 a_0+\frac{1}{i}\sum_{j=1}^{N} g_j b_j+\frac{1}{i}\sum_\lambda g_\lambda b_\lambda, \tag{9}$$

$$\dot b_j=\frac{1}{i}\Delta_j b_j+\frac{1}{i}g_j a_0, \tag{10}$$

$$\dot b_\lambda=\frac{1}{i}\Delta_\lambda b_\lambda+\frac{1}{i}g_\lambda a_0. \tag{11}$$

Formal integration of Eq. (11) gives

$$b_\lambda(t)-b_\lambda(t_0)e^{\Delta_\lambda(t-t_0)/i}=\frac{g_\lambda}{i}\int_{t_0}^{t}dt' a_0(t')e^{\Delta_\lambda(t-t')/i}. \tag{12}$$

Since these modes are strongly off-resonant, i.e., $\Delta_\lambda\gg g_\lambda$, and for short times $a_0(t')$ remains almost constant, $a_0(t')$ can be replaced by $a_0(t)$. The remaining integral over the exponential is easily performed, with the result

$$b_\lambda(t)\simeq\frac{g_\lambda}{i^2\Delta_\lambda}a_0(t). \tag{13}$$

Substituting Eq. (13) into Eq. (9), we have

$$\dot a_0=\frac{1}{i}\Delta_o a_0+\frac{1}{i}\sum_{j=1}^{N} g_j b_j-\sum_\lambda\frac{g_\lambda^2}{i\Delta_\lambda}a_0, \tag{14}$$

$$\dot b_j=\frac{1}{i}\Delta_j b_j+\frac{1}{i}g_j a_0. \tag{15}$$

Converting the mode sum over λ into an integral from $\omega=\omega_u$ to infinity and using Eq. (1), we obtain

$$\dot a_0=\frac{1}{i}\left(\Delta_0-\frac{g_j^2 N}{\omega_u-\omega_e}\right)a_0+\frac{1}{i}\sum_{j=1}^{N} g_j b_j, \tag{16}$$

$$\dot b_j=\frac{1}{i}\Delta_j b_j+\frac{1}{i}g_j a_0, \tag{17}$$

where for all discretized modes $g_j=g_r$, as given in Eq. (5). The effect of the smoothly varying part of the density of modes is thus to add a vacuum shift term to the equation of motion for the upper-state amplitude which effectively shifts the level down in energy and thus toward the band gap, where it is protected from decay. This approximation leads to a significantly reduced number of differential equations, and the remaining amplitudes are distributed over a much narrower frequency interval. Beyond that, the approximation also provides a surprising insight into the physical process, as discussed above.

To ensure satisfactory numerical agreement with the known exact solution [12,14] for this test problem, we find that we need at least 150 modes. In Fig. 1, we present the results obtained by propagation of Eqs. (16) and (17). The dotted line is for a calculation with 50 discrete modes, the long-dashed line is for 150 discrete modes, and the dash-dotted line is for 500 modes. For comparison, we also plot the exact known solution [12–14] (solid line), which shows very good agreement with the calculation involving 150 modes (estimated error 2%). The curve corresponding to 500 modes is practically indistinguishable from the exact solution. The calculation involving 50 modes exhibits revivals for longer times. These are a consequence of the discretization, one of the dangerous artifacts that one must be cognizant of. Increasing the number of discrete modes, the revivals appear at later and later times. The number of modes in our calculations thus determines the time scale on which the propagation is free of artificial oscillations, while ω_u determines the proximity of the envelope to the correct result. This implies considerable flexibility in the method; in the sense that the size of the calculation can be tailored to the time scale, over which the behavior of the system is sought, and the desired accuracy.

Having demonstrated the validity of the method, we now address an open problem. Adding to the system described above a defect mode near resonant with the atom, this defect

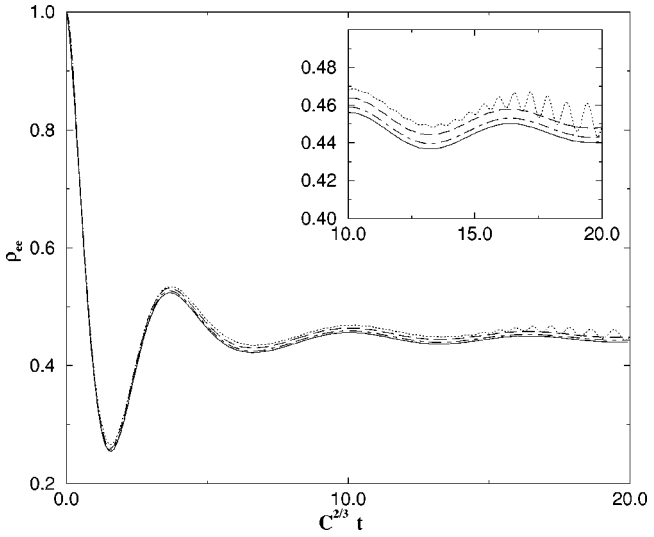

FIG. 1. The population in the excited state as function of time (dimensionless). The solid line is the exact solution. The dotted line is for $N=50$. The long-dashed line is for $N=150$, and the dot-dashed line is for $N=500$. The inset shows a close-up of the long-time behavior. Parameters: $\Delta_0=0$ and $g_d=0$.

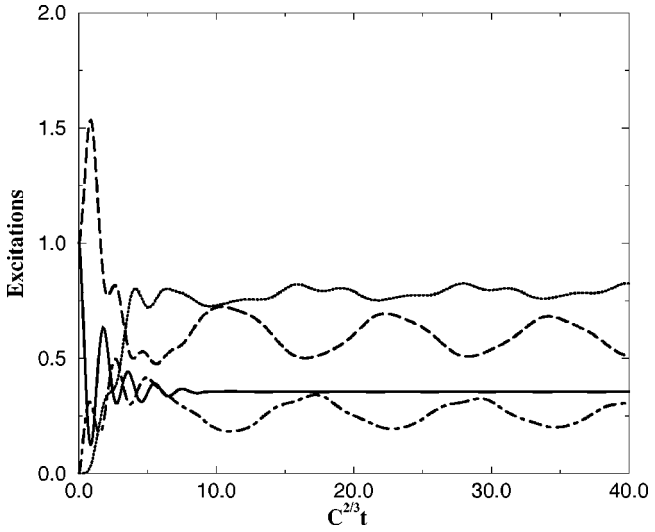

FIG. 2. The evolution of the system is plotted as function of time (dimensionless). The solid line is the population in the upper atomic state. The long-dashed line is the mean photon number in the defect mode, the dot-dashed line is the population in the one-photon sector of the reservoir Hilbert space, and the dotted curve is the population in the two-photon sector of the reservoir Hilbert space. Parameters: $N=150$, $g_d=C^{2/3}$, and $\Delta_0=\Delta_d=-0.1C^{2/3}$.

mode acts as a photon source that can pump the atom. With one photon in the defect mode and the atom excited at $t=0$, we have the possibility of two photons in the reservoir, a problem not amenable to techniques employed so far. The wave function for the system can be written

$$|\Psi(t)\rangle=a_0|e,1_d,0\rangle+b_0|g,2_d,0\rangle+\sum_j b_j|g,1_d,1_j\rangle+\sum_j a_j|e,0,1_j\rangle+\sum_{j,k} b_{jk}|g,0,1_j,1_k\rangle, \tag{18}$$

where the states involved are product states and, for instance, $|g,1_d,1_j\rangle=|g\rangle|1_d\rangle|1_j\rangle$ where $|1_d\rangle$ is the one-photon state of the defect mode and $|1_j\rangle$ is a one-photon state of the reservoir. The amplitudes obey the Schrödinger equation, and through the perturbative elimination of off-resonant modes as described above, we find

$$\dot{a}_0=\frac{1}{i}\left(\Delta_0+\Delta_d-\frac{g_j^2N}{\omega_u-\omega_e}\right)a_0+\frac{1}{i}\sqrt{2}g_db_0+\frac{1}{i}\sum_{j=1}^{N} g_jb_j, \tag{19}$$

$$\dot{b}_0=\frac{2}{i}\Delta_db_0+\frac{1}{i}\sqrt{2}g_da_0, \tag{20}$$

$$\dot{a}_j=\frac{1}{i}\left(\Delta_0+\Delta_j-\frac{g_k^2N}{\omega_u-\omega_e}\right)a_j+\frac{1}{i}g_db_j+\frac{1}{i}\sum_{\substack{k=1\\(k\neq j)}}^{N} g_kb_{jk}+\frac{1}{i}\sqrt{2}g_jb_{jj}, \tag{21}$$

$$\dot{b}_j=\frac{1}{i}(\Delta_j+\Delta_d)b_j+\frac{1}{i}g_ja_0+\frac{1}{i}g_da_j, \tag{22}$$

$$\dot{b}_{jk}=\frac{1}{i}(\Delta_k+\Delta_j)b_{jk}+\frac{1}{i}g_ka_j+\frac{1}{i}g_ja_k, \tag{23}$$

$$\dot{b}_{jj}=\frac{2}{i}\Delta_jb_{jj}+\frac{1}{i}\sqrt{2}g_ja_j, \tag{24}$$

where j and k are mode indices, and for all discretized modes $g_j=g_k=g_r$. For the purposes of this example, the frequency ω_d of the defect mode is inside the gap as determined by the value of Δ_d and the atomic transition on resonance with ω_d, i.e., $\Delta_0=\Delta_d$.

This set of equations is solved numerically with the results presented in Fig. 2. We plot the atomic inversion (solid line), the mean photon number in the defect mode (long-dashed line) and the populations in the one-photon sector (dot-dashed line) and two-photon sector (dotted line) of the reservoir Hilbert space, respectively, as functions of time. From the figure, we find that there is an exchange of energy (oscillation) between the defect mode and the one-photon sector of the reservoir. This oscillation must involve the atom, since the defect mode is not directly coupled to the reservoir, but is not reflected in the atomic inversion. As is evident in Fig. 2, although photons are exchanged between the defect mode and the reservoir through the atom, after some initial time, the atomic population remains practically constant: a rather surprising effect. The results presented in Fig. 2, have of course been tested for convergence in terms of number of modes, ω_u, etc.

As the defect mode is pushed further into the gap, we find that the oscillations of the atomic population begin to extend to increasingly longer times. Conversely, a change in the magnitude of g_d in relation to $C^{2/3}$ does not seem to affect the atomic oscillations for longer times, but it does affect the relative oscillations of the excitations in the defect mode and the reservoir, as we will discuss in detail elsewhere.

In conclusion, we have developed an approach that is capable of providing solutions to a class of problems which can only be treated approximately through other techniques. It is applicable to small systems coupled to a density of modes of any form, and has allowed us to solve problems involving multiple excitations in the continuum. In addition to the implementation outlined here, we have explored various other forms of discretizations, as well as other densities of modes, with good agreement with other exact results in those cases that are available. This demonstrates the generality and versatility of the approach, which could be readily employed in other contexts such as, for example, waveguides where the density of modes is also singular. [15,16]

We demonstrated, in addition, that off-resonant continuum modes can be eliminated perturbatively. The effect of this approximation is to reduce the number of differential equations to be propagated, thus leading to a drastic enhancement of the computation speed, essentially without compromise in accuracy. The number of equations to propagate scales roughly as N^p, where N is the number of discrete modes and p the number of excitations. The ultimate limitation of the method is determined by computer memory as demanded by each problem. In particular, the study of multiple excitations will probably for the time being be limited to 4 or 5. For the purpose of presenting the method, we limited our discussion here to two photons. Results from work for more photons will be presented elsewhere, but we do mention here that we have also obtained fully converged results for three photons in the reservoir.

Providing solutions for the dynamics of the system is one aspect of this approach. Perhaps an equally important aspect is the insight gained by the possibility to combine the perturbative treatment with the nonperturbative treatment of the rest. As discussed above, this sheds light on the physical effect of the modes around the band edge as compared to the smooth distant part of the density of modes. In addition, the possibility to monitor the dynamics of additional photons in the structured reservoir may prove very valuable when considering the validity of approximations necessary in other schemes.

It should be mentioned in closing that a recently proposed formal approach to similar non-Markovian problems, based on the quantum state diffusion formalism, was presented by Diosi, Strunz, and Gisin [17]. At this point we are aware of the application of the method to a relatively tractable problem involving a standard cavity reservoir. Its potential, however, does not seem at first sight to be limited, and it will be interesting to see and explore its applications to problems involving more complicated densities of modes.

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