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Degenerate spin-boson system

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The temporal evolution of a degenerate two-level system (spin) coupled to a dissipative bath (bosons) is studied in this Rapid Communication. Closed-form expressions for the occupancy probabilities and correlation functions are found by functional methods. The non-Markovian characteristics such as explicit dependence on the initial condition and a possible long-time tail behavior are shown to be present. We also suggest a reasonable procedure for the construction of the Green's function of the nondegenerate system.

The interaction of a two-level system with a dissipative bath serves to model a large class of phenomena occurring in condensed-matter physics: for example, the x-ray-absorption and emission spectra of simple metals,[1] the Kondo-Anderson effect,[2] and macroscopic quantum tunneling,[3] etc. These have been studied both intensively and extensively for a long time. In a more recent investigation, a related model—the Jaynnes-Cummings model—has been studied by the method of dynamical superalgebra.[4] An interesting response of the two-level system was found when the external perturbation has quasiperiodic time dependence.[5] In a rigorous study, phase transition was shown to exist in the limit of infinitely many spins, where the system (spins plus bosons) exhibits a high-temperature phase in which the spins and bosons decouple.[6]

The approximation solution to this problem was first given by Pauli,[7] where he wrote down a master or rate equation describing the time development of the transition probability P_n (n labels the states of the discrete system) on physical grounds:

$$\partial_t P_n = -\sum_k (W_{nk}P_k - W_{kn}P_k)\,, \tag{1}$$

where W_{nk} is the amplitude of transition from state n to state k. The rate equation was shown to be valid by Weisskopf and Wigner[8] and by Van Hove[9] under certain conditions. The essential point in these approximations is that one assumes the relaxation process of the discrete system is Markovian and hence neglects the effect of memory. These considerations were discussed in great detail by Fain,[10] where he also pointed out the qualitatively different behavior resulting from lifting the Markovian approximation. A representative of this class of problems is simply that of a two-level system coupled to a continuum boson field supporting fluctuation of all frequencies. The coupling between the two is what causes the spin flip. We shall study the problem in the case where the two-level system is degenerate in energy without the Markovian approximation. The exact expression for $P_n(t)$ was found by Fain.[11] Expressions for the line-shape and scattering operators were found[12] under the rotating-wave approximations of Hepp and Lieb.[13] Instead we shall adopt functional methods which include the finite-temperature effect.[14,15] The exact probability[11] is reproduced and we are able to obtain exact spin-spin correlations. The system is modeled by the Hamiltonian:

$$H = \psi^\dagger \omega_0 \sigma_3 \psi + \sum_k \omega_k \phi_k^\dagger \phi_k - \sum_k (B_k/2)(\phi_k^\dagger + \phi_k)\psi^\dagger \sigma_1 \psi\,, \tag{2}$$

where ψ_α, $\psi_\alpha^\dagger$ ($\alpha=1,2$), ϕ_k, and $\phi_k^\dagger$ are the usual Fermi and Bose creation and annihilation operators and σ_a ($a=1,2,3$) are the Pauli matrices. The units are $\hbar = k_B = 1$. We shall study the time evolution of the probability amplitude from a given initial state $\psi_1 = 1$, $\psi_2 = 0$, and unprescribed boson distribution at $t=0$. The finite-temperature action with $\omega_0 = 0$ is

$$S = \int_0^\beta d\tau \psi^\dagger (\partial_\tau)\psi + \int_0^\beta d\tau \sum_k \phi_k^\dagger(\partial_\tau + \omega_k)\phi_k - \int_0^\beta d\tau \sum_k \frac{B_k}{2}(\phi_k^\dagger + \phi_k)\psi^\dagger \sigma_1 \psi\,. \tag{3}$$

S can be made diagonal in spin space by a rotation of ψ:

$$S = \int_0^\beta d\tau \sum_k \phi_k^\dagger(\partial_\tau + \omega_k)\phi_k + \int_0^\beta d\tau \xi^\dagger \left[\partial_\tau - \sum_k \frac{B_k}{2}(\phi_k^\dagger + \phi_k)\sigma_3\right]\xi\,, \tag{4}$$

where

$$\Lambda = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}, \quad \Lambda^\dagger \sigma_1 \Lambda = \sigma_3$$

and $\psi = \Lambda \xi$. From Eq. (4) the Matsubara Green's function of the discrete system under the influence of the boson field is easily found because the fermionic part of the action is quadratic. Therefore,

$$\{\partial_\tau - \sigma_3 V(\tau;[\phi^\dagger,\phi])\}\mathcal{G}(\tau,\tau';[V]) = -\delta(\tau-\tau')\,, \tag{5}$$

where

$$V(\tau;[\phi^\dagger,\phi])=\sum_k \frac{B_k}{2}(\phi_k^\dagger+\phi_k)\,,$$

$$\mathcal{G}_{\alpha\beta}(\tau,\tau';[\phi^\dagger,\phi]):=-\langle\xi_\alpha(\tau)\xi_\beta^\dagger(\tau')\rangle_F:=\frac{\int\mathcal{D}\xi^\dagger\mathcal{D}\xi\exp(-S_F[\xi^\dagger,\xi;\phi^\dagger,\phi])\xi_\alpha(\tau)\xi_\beta^\dagger(\tau)}{\int\mathcal{D}\xi^\dagger\mathcal{D}\xi e^{-S_F}}\,, \tag{5a}$$

$$S_F:=\int_0^\beta d\tau\xi^\dagger\left[\partial_\tau-\sum_k\frac{B_k}{2}(\phi_k^\dagger+\phi_k)\sigma_3\right]\xi\,.$$

Since the phonon distribution is unprescribed, the transition probability is

$$P_{++}(\tau):=\left\langle\sum_\alpha\mathcal{G}_{\alpha\alpha}(\tau,0;[\phi^\dagger,\phi])\sum_\beta\mathcal{G}_{\beta\beta}(0,\tau;[\phi^\dagger,\phi])\right\rangle_B\,, \tag{6}$$

where

$$\langle\cdots\rangle_B:=\frac{\int\prod_k\mathcal{D}\phi_k^\dagger\mathcal{D}\phi_k e^{-S_B[\phi^\dagger,\phi]}\cdots}{\int\prod_k\mathcal{D}\phi_k^\dagger\mathcal{D}\phi_k e^{-S_B}}$$

The Matsubara Green's function can be found via the Schwinger Ansatz:[16]

$$\mathcal{G}(\tau,\tau';[V])=\mathcal{G}_0(\tau,\tau')e^{I(\tau)-I(\tau')}\,,$$

where $I(\tau)$ is an unknown functional of V to be determined and $\mathcal{G}_0$ satisfies Eq. (5) with $V=0$. Using the ansatz, we find $\partial_\tau I(\tau)=\sigma_3 V(\tau)$. Because $\mathcal{G}(\tau,\tau')$ describes propagation of fermionic excitation in the imaginary time, it must be periodic in τ and τ' with period β, while V being a functional of the boson field is periodic in τ with period β. Therefore, $I(\tau)$ must be periodic in τ with period β and can be developed into a Fourier series,

$$I(\tau)=-(\sigma_3/\beta)\sum_{n=-\infty}^{+\infty}e^{i\omega_n\tau}V(i\omega_n)/i\omega_n\,,$$

where $\omega_n=2n\pi/\beta:=2n\pi T$ is the boson Matsubara frequency and $V(i\omega_n)$ are the Fourier coefficients of $V(\tau)$. The ansatz fails when ω_0 is nonzero. Physically, the boson bath experiences a perturbation over a finite "time" duration ($|\tau-\tau'|$) and we are studying the response of the bath, whereas in the x-ray problem, the response of the conduction electrons is being examined. Therefore, we may expect a long-time tail behavior to develop in the present problem. This will be borne out in later calculations. The final form of $\mathcal{G}(\tau,\tau')$ now reads

$$\mathcal{G}=\mathcal{G}_0(\tau,\tau')\exp\left[\frac{-\sigma_3}{\beta}\sum_n\frac{V(i\omega_n)}{i\omega_n}(e^{i\omega_n\tau}-e^{i\omega_n\tau'})\right]\,, \tag{7}$$

from which

$$\langle\mathrm{tr}\mathcal{G}(\tau,0)\mathrm{tr}\mathcal{G}(0,\tau)\rangle_B=\mathcal{G}_0(\tau)\mathcal{G}_0(-\tau)(2+2\langle e^F\rangle_B)\,, \tag{8}$$

where $\mathrm{tr}\mathcal{G}=\sum_\alpha\mathcal{G}_{\alpha\alpha}$, with $F(\tau,\tau')$ defined according to Eqs. (7) and (8) and $\langle e^F\rangle_B=\langle e^{-F}\rangle_B$. The boson average in Eq. (8) can be calculated by the following formulas:

$$\frac{\int\mathcal{D}\phi^\dagger\mathcal{D}\phi\exp\left[-\int_x\int_y\phi_x^\dagger K_{xy}\phi_y+\int_x(J_x^\dagger\phi_x+\phi_x^\dagger J_x)\right]}{\int\mathcal{D}\phi^\dagger\mathcal{D}\phi\exp\left[-\int_x\int_y\phi_x^\dagger K_{xy}\phi_y\right]}=\exp\left[\int_x\int_y J_x^\dagger K_{xy}^{-1}J_y\right]\,,$$

with

$$\int_y K_{xy}^{-1}K_{yx'}=\delta_{xx'}\,.$$

This gives:

$$\langle e^F\rangle_B=\exp\left[-(2/\beta)\sum_n\sum_k\frac{B_k^2[1-\cos\omega_n(\tau-\tau')]}{\omega_n^2(i\omega_n-\omega_k)}\right]\,.$$

Performing the frequency sum and upon continuation to real time, the above becomes:

$$\langle e^F\rangle_B=\exp\left[\sum_k\frac{B_k^2[1-\cos\omega_k(t-t')]}{\omega_k^2(1-e^{-\beta\omega_k})}\right]\,, \tag{9}$$

where $t=i\tau$. Note that at zero temperature, the Bose factor in Eq. (9) becomes unity and

$$G_0(t-t')=-\tfrac{1}{2}\,\mathrm{sgn}(t-t')\,.$$

Using these on the definition of P_{++}, we recover the results of Fain,[11]

$$P_{++}(t)=\tfrac{1}{2}(1+e^{-\Sigma(t,T=0)})\,, \tag{10}$$

where

$$\Sigma(t,T=0):=2\sum_k\frac{B_k^2}{\omega_k^2}[1-\cos\omega_k(t-t')]\,.$$

Note also that at $t=0$, the correct normalization is found. The probability of spin down is thus, $P_{--}=1-P_{++}$, and is zero at $t=0$, thus showing the dependence on the initial condition. To study more precisely the long-time relaxation, let us take the case where the pseudospin is coupled to a two-dimensional boson bath with dispersion relation $\omega_k=ck$ and consider contact interaction $B_k=Be^{(-a/2)|k|}$ (a a small positive number to limit the large momentum processes). Converting the sum into an integral over k, we find

$$\Sigma(t,T=0)=\left(\frac{B}{c}\right)^2\int_0^\infty \frac{dk}{2k\pi}(1-\cos ckt)e^{-ka}=\frac{1}{2\pi}\left(\frac{B}{c}\right)^2\ln\left(\frac{(ct)^2+a^2}{a^2}\right)\sim(B^2/c^2\pi)\ln\left(\frac{ct}{a}\right), \tag{11}$$

in the limit of $ct \gg a$, exhibiting the long-time tail, a very slow relaxation process highly non-Markovian in character. At low temperature, the tail is enveloped by stretched exponentials:

$$\Sigma(t,T)-\Sigma(t,T=0)=(1/2\pi)(B/c)^2\sum_{n=1}^{\infty}\ln[1+(t/n\beta)^2]=(B^2/2\pi^2c)\int_0^{\pi(t/\beta)}dx(\coth x-1/x)=\ln[\sinh\pi(t/\beta)/\pi(t/\beta)] \tag{12}$$

$$\sim\frac{1}{2\pi}\left(\frac{B}{c}\right)^2\sum_{n=1}^{\infty}(-1)^{n+1}\left(\frac{t}{\beta}\right)^{2n}\frac{\zeta(2n)}{n}, \tag{13}$$

where Eq. (12) is found by using

$$\ln(1+x)=\int_0^1 d\lambda\frac{x}{1+\lambda x}$$

and

$$\sum_{n=1}^{\infty}1/(n^2+a^2)=(\pi/2a)[\coth\pi a-(1/\pi a)].$$

Equation (13) follows by a series expansion in t/β, valid in the low-temperature region and $\zeta(x)$ is the Riemann ζ function. The simplicity of this method is reflected in the calculation of correlation functions. Consider, for example,

$$\chi^{ab}(\tau,0):=\langle S^a(\tau)S^b(0)\rangle-\langle S^a(\tau)\rangle\langle S^b(0)\rangle, \tag{14}$$

where

$$S^a(\tau):=(\psi^\dagger\sigma^a\psi)(\tau),$$

$$\langle\cdots\rangle:=\frac{\int\mathcal{D}\phi^\dagger\mathcal{D}\phi\mathcal{D}\psi^\dagger\mathcal{D}\psi e^{-S}\cdots}{\int\mathcal{D}\phi^\dagger\mathcal{D}\phi\mathcal{D}\psi^\dagger\mathcal{D}\psi e^{-S}},$$

$a=0,1,2,3$ and $\sigma^0=\underline{I}$. From a straightforward calculation, Eq. (14) becomes

$$\chi^{ab}(\tau)=\sum_{\alpha_1\alpha_2}\bar{\sigma}^a_{\alpha_1\alpha_2}\bar{\sigma}^b_{\alpha_2\alpha_1}\langle\mathcal{G}_{\alpha_1\alpha_2}(0,\tau)\mathcal{G}_{\alpha_2\alpha_1}(\tau,0)\rangle_B, \tag{15}$$

where $\bar{\sigma}^a:=\Lambda^\dagger\sigma^a\Lambda$ and $\mathcal{G}$ is defined by Eq. (7).

Using the results given above, the susceptibility at imaginary time is given by

$$\chi^{ab}(\tau)=\mathcal{G}_0(\tau)\mathcal{G}_0(-\tau)[\bar{\sigma}^a_{11}\bar{\sigma}^b_{11}+\bar{\sigma}^a_{22}\bar{\sigma}^b_{22}+(\bar{\sigma}^a_{12}\bar{\sigma}^b_{21}+\bar{\sigma}^a_{21}\bar{\sigma}^b_{12})e^{-\Sigma(\tau,T)}]. \tag{16}$$

Written explicitly,

$$(\chi^{ab})=\begin{pmatrix}A_1 & 0\\ 0 & A_2\end{pmatrix}, \tag{17}$$

where

$$(A_1):=\begin{pmatrix}\chi_0^{00} & \chi_0^{01}\\ \chi_0^{01} & \chi_0^{11}\end{pmatrix},\quad (A_2):=\begin{pmatrix}f & 0\\ 0 & f\end{pmatrix},$$

$$f:=2\mathcal{G}_0(\tau)\mathcal{G}_0(-\tau)e^{-\Sigma(\tau,T)},$$

and the subscript 0 denotes the situation where the spin is decoupled from the bath, i.e., $\Sigma=0$.

Having done these calculations we shall now address the issue of the existence of the discrete nondissipative (i.e., sharp) levels in the spectrum of the couple system. It was pointed out by Fain,[11] that the non-Markovian relaxation is due to the "sharpness" of the discrete levels, where a value $\sum_k B_k^2/\omega_k$ was assigned to them. In order to determine the existence of these levels, we must calculate the density of states (DOS) of the spin subsystem. If the DOS has δ-function peaks, then we conclude that the levels are sharp, otherwise the nondissipative structures do not exist. As will be shown in the following calculations, one does not find any δ-function peaks but rather more exotic behavior in the DOS. The DOS at $T=0$ is defined as

$$D(\omega)=-2\,\mathrm{Im}\int_0^\infty dt\cos(\omega t)\mathrm{tr}G_R(t), \tag{18}$$

where

$$G_R(t):=i\theta(t)[G(t)-G(-t)]$$

is the retarded real-time Green's function of the spin system, $G(t)$ is the Green's function obtained from the analytic continuation of the Matsubara Green's function at $T=0$ and is

$$G(t)=-\tfrac{1}{2}\,\mathrm{sgn}(t)e^{-\Sigma(t)}\underline{I}. \tag{19}$$

Taking the coupling which produces the long-time tail and putting Eq. (19) into Eq. (18), we find

$$D(\omega)=(2/\omega_c)\int_0^\infty dx(1+x^2)^{-\mu}\cos(\omega x/\omega_c)=(2\pi^{1/2}/\omega_c)(2\omega_c/\omega)^{1/2-\mu}K_{\mu-1/2}(\omega/\omega_c)/\Gamma(\mu), \tag{20}$$

where $\omega_c:=a/c$ is the cutoff frequency, $\mu:=B^2/2c^2\pi>0$, $K_\nu(x)$ is the Macdonald's function, and Eq. (20) can be found from Ref. 17. The low-frequency asymptote ($\omega\ll\omega_c$) of $D(\omega)$ depends on the dimensionless parameter μ in a nontrivial manner. For $0<\mu<\frac{1}{2}$,

$$D(\omega)\sim(2^{1-2\mu}\pi^{1/2}/\omega_c)[\Gamma(\tfrac{1}{2}-\mu)/\Gamma(\mu)](\omega/\omega_c)^{-(1-2\mu)},$$

exhibiting a weak algebraic divergence. Upon reaching $\mu=\frac{1}{2}$, $D(\omega)\sim(2/\omega_c)\ln(2\omega_c/\omega)$, and for $\mu>\frac{1}{2}$, the DOS becomes independent of ω,

$$D(\omega)=(\pi^{1/2}/\omega_c)[\Gamma(\mu-\tfrac{1}{2})/\Gamma(\mu)].$$

At high frequency ($\omega\gg\omega_c$), one expects the DOS to be exponentially damped. For $0<\mu<1$,

$$D(\omega)\sim[2^{1-\mu}\pi/\omega_c\Gamma(\mu)](\omega/\omega_c)^{-(1-\mu)e^{-(\omega/\omega_c)}}$$

At $\mu=1$, one finds pure exponential decay, $D(\omega)\sim(\pi/\omega_c)e^{-(\omega/\omega_c)}$. The ultraviolet shift in energy $(\sum_k B_k^2/\omega_k)$ cancel each other from the numerator and denominator in the functional averages.[18] Furthermore, this problem can be seen to correspond to the x-ray limit of the Kondo problem[19] and μ is the same as the parameter α used in Ref. 3. The "vacuum" polarization,

$$\det(\partial_\tau-\sigma_3 V)/\det(\partial_\tau)=\exp\left[\mathrm{tr}\sigma_3\int_0^1 d\lambda\int_0^\beta d\tau V(\tau)\mathcal{G}(\tau,\tau+0;\lambda[V])\right],$$

where the above is derived from the identity,

$$\ln[\det(A+B)/\det(A)]=\mathrm{tr}B\int_0^1 d\lambda(A+\lambda B)^{-1},$$

and $\mathcal{G}$ satisfies Eq. (5), is unity. In other words, upon tracing out the spin degrees of freedom, the bath is unaffected and the total energy of the system is given by that of the bath alone. If we have instead inserted an extra term, $\varepsilon\psi^\dagger\psi$, in the Hamiltonian of the spin system, the total energy decomposed into the sum of the bath energy and ε. The energy of the spin system remains unshifted. However, the DOS has no δ-function peaks. The no-recoil approximation has been used by Edwards and Peierls[20] in studies of quantum field theory resulting in a nontrivial asymptote of the electron Green's and vertex functions.[21] In summary, we have given closed-form expressions for the occupancy probability and the generalized susceptibility of the degenerate spin-boson system. This, in our opinion, is better than using the many-body wave function of the system, whose explicit form is difficult to determine. The non-Markovian relaxation of the discrete system is related to the fact that its behavior is nonergodic. As to the experimental observation of the long-time tail, we would like to refer the reader to a standard treatise in the field.[22] Similarity to the x-ray problem[1] can be made more pronounced, if one considers the Schotte-Schotte[23] oscillator representation of the conduction electrons, due originally to Tomonaga.[24] In this representation, the conduction electrons near the Fermi energy are bosonized in terms of fictitious sound wave and since the deep hole in the x-ray problem is structureless, the conduction electrons experience a transient perturbation. Thus the present problem is equivalent to the x-ray problem. When $\omega_0>0$, spin-flipping processes can no longer be "rotated" away, thus the present problem becomes the Kondo problem, which was discussed in great detail in Ref. 3. In the extreme where $\omega_0\gg\omega_c\sim c/a$, we may disregard the coupling to the bath in the first approximation and an (trivial) exact solution can be found. The correction to this may be constructed by the Wentzel-Kramers-Brillouin (WKB) method, in which one regards the "bath variables" as slowly varying. The partition function of the system can be expressed in terms of the off-diagonal elements of $\mathcal{G}$, which in turn satisfy a "time"-independent Schrödinger equation with the imaginary time playing the role of the spatial coordinates of the quantum-mechanical particle and ω_0^2 playing the role of the energy. Coupling to the bath introduces a random potential in the Schrödinger equation. The solution of this remains an outstanding problem. This can also be viewed as interaction between two types of "particles," one of which—the bath-variables—is massless. The WKB approximation corresponds to the heavy-mass limit[15] of the quantum-mechanical particle. The above is deferred to a later publication.

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