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Fully coupled model versus rotating-wave approximation in the asymptotic time evolution of spin systems

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Abstract. In the frame of the generalized master equation (GME) approach, an analysis of the asymptotic spin relaxation is made for different j values. The fully coupled (FC) model and the rotating-wave approximation (RWA) for the system-reservoir coupling are considered and it is seen that they give rise to structurally different GMEs. In particular, we examine the evolution of the diagonal and off-diagonal matrix elements of the density operator, the mean values of the relevant observables and the equilibrium solution for both coupling models and display their significant differences. Particularly the spin $j = 1$ case is examined.

1. Introduction

The GME approach [1] for describing the irreversible dynamics of a quantum macroscopic system that interacts with a heat reservoir has proven to be an essential tool for understanding not only the equilibration process but also the nature of the equilibrium state encountered. In particular, the possibility of reaching non-Gibbsian equilibria [2], a feature that appears to be related to the breakup of the weak-coupling approximation, has been investigated. The most widespread 'toy problems' subjected to this analysis are the harmonic oscillator [3] and the single spin [4] in the Markovian limit. In this case, the asymptotic GME is of the gain-minus-loss form, which corresponds to a situation where only population probabilities of the spectrum of the evolving system are involved.

The validity of the Markovian limit is already an important issue to keep in mind before attempting to employ the GME approach. It is frequently preferred in the literature due to its simplicity, and indeed it has been shown resorting to the time-convolutionless projection operator method [5] that in the non-Markovian situation, i.e. when memory effects in the reservoir cannot be disregarded within the time-scale of the motion, the GME can be cast into the same form as its Markovian version, with time-dependent transition rates. These ideas have been applied to investigate the possibility of non-exponential relaxation and the role of the long-lived reservoir correlations in the dynamics of a two-level system [6]. More recently, the Markovian evolution in the presence of different kinds of coupling mechanisms and heat baths have been studied within essentially the same theoretical frame [7].

However, several questions remain to be investigated and among them, an important one is the assertion that in the vicinity of the equilibrium situation the density matrix of the system is purely diagonal [8]. Another question concerns the validity of the RWA as an approximation to the FC model. In this paper, we show through a specific example, consisting of a single spin system immersed into a heat bath, that such a statement may be not true and discuss the conditions under which this actually occurs.

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This paper is organized in the following way. In section 2 the spin relaxation model is investigated; the corresponding GME is obtained and the evolution equation for the diagonal and off-diagonal density matrix elements are given. In particular, the $j = \frac{1}{2}$ case is solved analytically in section 3. Section 4 contains an analysis of the equilibrium and dynamical properties of a system with spin $j = 1$. Finally, in section 5 we present our conclusions.

2. The generalized quantum master equation for a spin system

In this section we introduce and discuss a particular model in atomic physics, where one spin—or several non-interacting ones—subjected to a magnetic field, relax due to the coupling to a normal reservoir. This model applies as well to vibrational and optical spectroscopy [6] and to atomic two-level systems interacting with a radiation field, as described by the quasi-spin formalism [9]. The interaction with the reservoir will induce transitions between the $2j + 1$ angular momentum eigenstates $|jm\rangle$ of the unperturbed Hamiltonian

$$H_S = -BJ_z \tag{2.1}$$

which correspond to the different orientations of the spin j with respect to the magnetic field.

In what follows we consider the system-plus-reservoir Hamiltonian

$$H = H_S + H_R + H_{SR} \tag{2.2}$$

where H_R is the isolated reservoir Hamiltonian. The interaction term is assumed to be of the generalized FC form [4, 10]

$$H_{SR} = \alpha(J_- + J_+)(R + R^\dagger) \tag{2.3}$$

where α is a parameter that measures the average strength of the interaction, $\hat{J} = (J_z, J_+, J_-)$ is the set of generators of an $SU(2)$ algebra, and the operators R and $R^\dagger$ belong to the operator space of the reservoir and contain infinite summations over all degrees of freedom in the environment.

The dynamical behavior of the spin system can be computed from the knowledge of the reduced density, $\sigma(t) = \mathrm{Tr}_R\rho(t)$, where $\rho(t)$ is the full spin-plus-reservoir density operator that satisfies the Liouville equation

$$\frac{\partial}{\partial t}\rho(t) = -\frac{i}{\hbar}[H, \rho(t)] \tag{2.4}$$

and Tr_R indicates tracing in the Hilbert space with respect to the quantum numbers of the reservoir R.

Using standard projection operator techniques, assuming the Born approximation (valid in a weak coupling scheme) and taking the Markovian limit, the corresponding GME can be obtained. This equation is the same as equation (9) in [3], which for the particular model of equations (2.1) to (2.3), and after some algebra, leads to the following law of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\sigma = -\frac{\mathrm{i}}{\hbar}[H_S^r, \sigma] + (\Lambda + \varepsilon\Lambda')\sigma \tag{2.5}$$

where

$$H_S^r = H_S + \hbar\Delta^+ J_- J_+ + \hbar\Delta^- J_+ J_- \tag{2.6}$$

is the renormalized Hamiltonian that appears when we couple the system to the reservoir, and Λ and Λ' represent the collision kernels acting upon σ. These kernels can be written as

$$\Lambda\sigma = -\tfrac{1}{2}W^{+}(J_{-}J_{+}\sigma - 2J_{+}\sigma J_{-} + \sigma J_{-}J_{+}) - \tfrac{1}{2}W^{-}(J_{+}J_{-}\sigma - 2J_{-}\sigma J_{+} + \sigma J_{+}J_{-}) \tag{2.7}$$

and

$$\begin{aligned}\Lambda'\sigma = &-\left(\tfrac{1}{2}W^{+} + \mathrm{i}\Delta^{+}\right)[J_{+}, J_{+}\sigma] + \left(\tfrac{1}{2}W^{+} - \mathrm{i}\Delta^{+}\right)[J_{-}, \sigma J_{-}] \\ &-\left(\tfrac{1}{2}W^{-} + \mathrm{i}\Delta^{-}\right)[J_{-}, J_{-}\sigma] + \left(\tfrac{1}{2}W^{-} - \mathrm{i}\Delta^{-}\right)[J_{+}, \sigma J_{+}].\end{aligned} \tag{2.8}$$

For the FC model ε is just unity. In the RWA we exclude from the GME the 'anti-resonating' terms that correspond to the simultaneous creation or annihilation of system and bath excitations, discarding those terms that contain two J_+ or J_- operators. Therefore, as one can see from (2.7) and (2.8), ε vanished in this case. We mention here that there exists another way to carry out the RWA [10], namely consider $H_{\mathrm{SR}} = \alpha(J_{+}R^{\dagger} + J_{-}R)$ instead of (2.3). In this case, the corresponding GME is (2.5) with $\varepsilon = 0$ and with slightly different expressions for $\Delta^{\pm}$ [7].

The real quantities $W^{\pm}$, $\Delta^{\pm}$ are respectively the downwards and upwards transition rates and the conservative corrections to the free-flow rate, defined as

$$\tfrac{1}{2}W^{\pm} + \Delta^{\pm} = \frac{\alpha^2}{\hbar^2}\int_0^{\infty} \mathrm{d}\tau\, \mathrm{e}^{\pm \mathrm{i}B\tau}\left(\Phi_{R^{\dagger}R}(t) + \Phi_{RR^{\dagger}}(t)\right) \tag{2.9}$$

where $\Phi_{R^{\dagger}R}(t) = \langle R^{\dagger}(\tau)R\rangle$ and $\Phi_{RR^{\dagger}}(t) = \langle R(\tau)R^{\dagger}\rangle$ are the correlation functions of the heat bath operators. Here $R^{\dagger}(\tau)$ and $R(\tau)$ are computed in the non-interacting scheme for the bath. Taking into account that the Fourier transform of the reservoir correlation function

$$\Phi_{R^{\dagger}R}[\omega] = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}t\mathrm{e}^{-\mathrm{i}\omega t}\Phi_{R^{\dagger}R}(t) \tag{2.10}$$

satisfies the parity relationship [11]

$$\Phi_{R^{\dagger}R}[-\omega] = \mathrm{e}^{\beta\hbar\omega}\Phi_{RR^{\dagger}}[\omega] \tag{2.11}$$

with $\beta = 1/T$ the inverse equilibrium temperature, one can demonstrate that the coefficients (2.9) can be written as

$$W^{\pm} = \frac{2\pi}{\hbar^2}\alpha^2\Phi_{R^{\dagger}R}[B] \times \begin{cases} e^{\beta\hbar B} \\ 1 \end{cases} \tag{2.12}$$

and

$$\Delta^{\pm} = \frac{\alpha^2}{\hbar^2}P\int_0^{\infty} \mathrm{d}\omega\,\Phi_{R^{\dagger}R}[\omega]\left(\frac{1}{\omega \pm B} - \frac{\mathrm{e}^{\beta\hbar\omega}}{\omega \mp B}\right) \tag{2.13}$$

where P denotes Cauchy's principal value of the integral. In the above analysis, the only assumption regarding the reservoir is that the thermal averages $\langle R^{\dagger}R^{\dagger}\rangle$ and $\langle RR\rangle$ vanish, a condition satisfied for the most usual models.

We mention here that this problem can be invesigated as well beyond the weak-coupling approximation, since one can show that the coefficients can be written as expansions in the coupling parameter, whose first terms are the ones displayed above. In the non-Markovian case the evolution equation is identical to (2.5) with time-dependent coefficients; however, for times greater than the characteristic decaying time τ_{R} of the autocorrelation function of the isolated reservoir—which may be strongly dependent on the temperature—the Markovian approximation is suitable. Hereafter, the evolution for times $t \gg \tau_{\mathrm{R}}$ will be referred to as the asymptotic regime.

In what follows, we will discuss the characteristics of the motion of both the diagonal and off-diagonal matrix elements $\sigma_{m,n}$. The occupation probabilities σ_m of the angular momentum eigenstates $|jm\rangle$ evolve according to

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\sigma_m = \hbar^2 W^+(C_m^2\sigma_{m-1} - C_{m+1}\sigma_m) + \hbar^2 W^-(C_{m+1}^2\sigma_{m+1} - C_m^2\sigma_m) \\ +\hbar^2\varepsilon\left\{C_m C_{m+1}\left[(W^+ + W^-)R_{m+1,m-1} + 2(\Delta^+ - \Delta^-)I_{m+1,m-1}\right]\right. \\ -C_{m+1}C_{m+2}\left[W^- R_{m,m+2} + 2\Delta^- I_{m,m+2}\right] \\ \left. -C_m C_{m-1}\left[W^+ R_{m,m-2} + 2\Delta^+ I_{m,m-2}\right]\right\}\end{aligned} \tag{2.14}$$

where

$$R_{m,n} = \mathrm{Re}\{\sigma_{m,n}\} = \frac{1}{2}(\sigma_{m,n} + \sigma_{n,m}) \tag{2.15a}$$

$$I_{m,n} = \mathrm{Im}\{\sigma_{m,n}\} = \frac{1}{2\mathrm{i}}(\sigma_{m,n} - \sigma_{n,m}) \tag{2.15b}$$

the real and imaginary part of the reduced density, and

$$C_m = \hbar\sqrt{j(j+1) - m(m-1)}\,. \tag{2.16}$$

The explicit expressions for the evolution equations of the matrix elements $\sigma_{m,n} = \langle jm|\sigma|jn\rangle$ are given in the appendix.

We can appreciate that, while the RWA (i.e. $\varepsilon = 0$) yields a master equation with the typical gain-minus-loss appearance, such a feature is no longer valid in the FC frame in view of the coupling between occupation numbers and off-diagonal transition amplitudes. After some algebraic steps, the latter can be seen to fulfill the set of equations

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}R_{m,n} = -\left\{\left[B + \hbar^2(\Delta^+ - \Delta^-)\right](m-n) + \hbar^2(\Delta^+ + \Delta^-)(m^2 - n^2)\right\} I_{m,n} \\ +\hbar^2 W^+[C_m C_n R_{m-1,n-1} - \tfrac{1}{2}(C_{m+1}^2 + C_{n+1}^2)R_{m,n}] \\ +\hbar^2 W^-[C_{m+1}C_{n+1}R_{m+1,n+1} - \tfrac{1}{2}(C_m^2 + C_n^2)R_{m,n}] \\ +\tfrac{1}{2}\hbar^2\varepsilon\left\{C_m C_{n+1}\left[(W^+ + W^-)R_{m-1,n+1} - 2(\Delta^+ - \Delta^-)I_{m-1,n+1}\right]\right. \\ +C_{m+1}C_n\left[(W^+ + W^-)R_{m+1,n-1} + 2(\Delta^+ - \Delta^-)I_{m+1,n-1}\right] \\ -C_m C_{m-1}\left[W^+ R_{m-2,n} - 2\Delta^+ I_{m-2,n}\right] \\ -C_{m+1}C_{m+2}\left[W^- R_{m+2,n} - 2\Delta^- I_{m+2,n}\right] \\ -C_n C_{n-1}\left[W^+ R_{m,n-2} + 2\Delta^+ I_{m,n-2}\right] \\ \left. -C_{n+1}C_{n+2}\left[W^- R_{m,n+2} + 2\Delta^- I_{m,n+2}\right]\right\}\end{aligned} \tag{2.17}$$

and

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}I_{m,n} = \left\{\left[B + \hbar^2(\Delta^+ - \Delta^-)\right](m-n) + \hbar^2(\Delta^+ + \Delta^-)(m^2 - n^2)\right\} R_{m,n} \\ +\hbar^2 W^+\left[C_m C_n I_{m-1,n-1} - \tfrac{1}{2}\left(C_{m+1}^2 + C_{n+1}^2\right)I_{m,n}\right] \\ +\hbar^2 W^-\left[C_{m+1}C_{n+1}I_{m+1,n+1} - \tfrac{1}{2}\left(C_m^2 + C_n^2\right)I_{m,n}\right] \\ +\tfrac{1}{2}\hbar^2\varepsilon\left\{C_m C_{n+1}\left[(W^+ + W^-)I_{m-1,n+1} + 2(\Delta^+ - \Delta^-)R_{m-1,n+1}\right]\right. \\ +C_{m+1}C_n\left[(W^+ + W^-)I_{m+1,n-1} - 2(\Delta^+ - \Delta^-)R_{m+1,n-1}\right] \\ -C_m C_{m-1}\left[W^+ I_{m-2,n} + 2\Delta^+ R_{m-2,n}\right] \\ -C_{m+1}C_{m+2}\left[W^- I_{m+2,n} + 2\Delta^- R_{m+2,n}\right] \\ -C_n C_{n-1}\left[W^+ I_{m,n-2} - 2\Delta^+ R_{m,n-2}\right] \\ \left. -C_{n+1}C_{n+2}\left[W^- I_{m,n+2} - 2\Delta^- R_{m,n+2}\right]\right\}\,.\end{aligned} \tag{2.18}$$

The spin $j = \frac{1}{2}$ has been investigated by several authors (see, for example, [6] for updated references) and explicit expressions can be written in the Markovian limit. The major results can be summarized as follows. With the renaming $\sigma_+ = \sigma_{\frac{1}{2},\frac{1}{2}}$, $\sigma_- = \sigma_{-\frac{1}{2},-\frac{1}{2}}$, $R = R_{\frac{1}{2},-\frac{1}{2}}$, $I = I_{\frac{1}{2},-\frac{1}{2}}$, the GME makes room to two uncoupled differential systems, namely

$$\frac{\mathrm{d}}{\mathrm{d}t}\sigma_+ = \hbar^2\left(W^+\sigma_- - W^-\sigma_+\right) \tag{2.19a}$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\sigma_- = \hbar^2\left(-W^+\sigma_- + W^-\sigma_+\right) \tag{2.19b}$$

and

$$\frac{\mathrm{d}}{\mathrm{d}t}R = -\tfrac{1}{2}\nu(1-\varepsilon)R - [B + \delta(1-\varepsilon)]\, I \tag{2.20a}$$
$$\frac{\mathrm{d}}{\mathrm{d}t}I = -\tfrac{1}{2}\nu(1+\varepsilon)I + [B + \delta(1+\varepsilon)]\, R \tag{2.20b}$$

where $\nu = \hbar^2(W^+ + W^-)$ and $\delta = \hbar^2(\Delta^+ - \Delta^-)$. Hence, the evolution of the diagonal part is independent of the coupling model, which is no longer true for higher j values as one can verify from (2.14).

One easily sees that the matrix in the linear system (2.19) possesses eigenvalues 0 and ν, the solution for the probabilities being

$$\sigma_\pm(t) = \left(\sigma_\pm(0) - \frac{1}{1+\alpha^{\pm 1}}\right)\mathrm{e}^{-\nu t} + \frac{1}{1+\alpha^{\pm 1}} \tag{2.21}$$

where we use the normalization condition $\sigma_+ + \sigma_- = 1$ and α denotes the quotient $\alpha = W^+/W^-$. One can realize that the Markovian decay is of the exponential type regardless the coupling strenght. This is no longer true in the non-Markovian case [6].

The equilibrium solution of (2.21) is

$$\sigma_\pm(\infty) = \frac{1}{1+\alpha^{\pm 1}} \tag{2.22}$$

which in the weak coupling limit is precisely the canonical distribution

$$\sigma_\pm^{\mathrm{can}} = \frac{\mathrm{e}^{\pm\beta\hbar B}}{\mathrm{e}^{\beta\hbar B} + \mathrm{e}^{-\beta\hbar B}} \tag{2.23}$$

in view of the detailed balance relationship $\alpha = \mathrm{e}^{-\beta\hbar B}$.

On the other hand, the system (2.20) possesses the eigenvalues,

$$\lambda^\pm = -\tfrac{1}{2}\nu \pm \mathrm{i}\sqrt{(B+\delta)^2 - \varepsilon\left(\tfrac{1}{4}\nu^2 + \delta^2\right)} \tag{2.24}$$

which means

$$\lambda^\pm_{(\mathrm{FC})} = -\tfrac{1}{2}\nu \pm \mathrm{i}\sqrt{B(B+2\delta) - \tfrac{1}{4}\nu^2} \tag{2.25a}$$
$$\lambda^\pm_{(\mathrm{RWA})} = -\tfrac{1}{2}\nu \pm \mathrm{i}(B+\delta)\,. \tag{2.25b}$$

We then recover the well known fact that the off-diagonal elements of the density matrix $\sigma_{\frac{1}{2},-\frac{1}{2}}, \sigma_{-\frac{1}{2},\frac{1}{2}}$ undergo damped oscillations with a characteristic time twice as large as the damping for the occupation numbers, consequently we are facing a specific example where the usual statement [3, 12] concerning the asymptotic diagonal form of the density matrix is not valid. Such an assertion holds under the FC and the RWA (except in the case of vanishing initial off-diagonal elements), a fact that imposes a limit on the use of the gain-minus-loss master equation (2.19) to describe the damping process to full extent. Furthermore, in the strictly weak coupling limit where both ν and δ are much more smaller than B, one has $\lambda^{\pm}_{\mathrm{RWA}} \approx \lambda^{\pm}_{\mathrm{FC}}$.

We end this chapter with some comments concerning the evolution of the spin $\bar{J}$. Noticing that in the $j=\frac{1}{2}$ case, one has $\langle J_z\rangle = \frac{1}{2}\hbar(\sigma_{+}-\sigma_{-})$, $\langle J_{+}\rangle = \hbar\sigma_{-\frac{1}{2},\frac{1}{2}}$, $\langle J_{-}\rangle = \hbar\sigma_{\frac{1}{2},-\frac{1}{2}}$, we realize that $\langle J_x\rangle = \hbar R$ and $\langle J_y\rangle = -\hbar I$. The motion of $\langle J_z\rangle$ is thus independent of the motion of the polar components and given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle J_z\rangle = -\nu\left[\langle J_z\rangle - \frac{\hbar}{2}\left(\frac{1-\alpha}{1+\alpha}\right)\right] \tag{2.26}$$

which in the weak coupling limit displays the canonical equilibrium value $\langle J_z(\infty)\rangle = \frac{1}{2}\hbar\tanh(\frac{1}{2}\beta\hbar B)$.

The evolution of the averages $\langle J_x\rangle$ and $\langle J_y\rangle$ is given by the coupled equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle J_x\rangle = -\tfrac{1}{2}\nu(1-\varepsilon)\langle J_x\rangle + [B+\delta(1-\varepsilon)]\langle J_y\rangle \tag{2.27a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle J_y\rangle = -[B+\delta(1+\varepsilon)]\langle J_x\rangle - \tfrac{1}{2}\nu(1+\varepsilon)\langle J_y\rangle \tag{2.27b}$$

which together with (2.26) constitute the vector Bloch equation and are similar to those obtained for a harmonic oscillator with frequency ω_0 and mass m linearly coupled to a reservoir [3] if one makes the replacement: $(J_x, BJ_y) \to (mQ, P)$, $\nu \to (W^+ - W^-)$, $\delta \to (\Delta^+ + \Delta^-)$ and $B \to \omega_0$. This analogy and the linearity of (2.26) and (2.27) are only valid for a $j=\frac{1}{2}$ spin system, while for higher spin values the corresponding equations are nonlinear ones (see equations (3.8) below).

3. Application to $j = 1$ spin systems

In this section we consider explicitly a spin $j=1$ and discuss the results of a numerical study of the GME. First, we select for the Hermitian matrix ρ, the occupation probabilities σ_{-1}, σ_0, σ_1 and the real and imaginary parts of the off-diagonal elements $\sigma_{1,0}$, $\sigma_{0,-1}$, $\sigma_{1,-1}$. The GME (2.5) gives rise to two uncoupled differential sets, as follows

$$\frac{\mathrm{d}}{\mathrm{d}t}\sigma_1 = -2\hbar^2\left[W^-\sigma_1 - W^+\sigma_0 + \varepsilon(W^+R_{1,-1} + 2\Delta^+ I_{1,-1})\right] \tag{3.1a}$$

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\sigma_0 = {}& 2\hbar^2\left[W^-\sigma_1 - (W^+ + W^-)\sigma_0 + W^+\sigma_{-1}\right]\\ &+2\hbar^2\varepsilon\left[(W^+ + W^-)R_{1,-1} + 2(\Delta^+ - \Delta^-)I_{1,-1}\right]\end{aligned} \tag{3.1b}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\sigma_{-1} = 2\hbar^2\left[W^-\sigma_0 - W^+\sigma_{-1} - \varepsilon(W^-R_{1,-1} - 2\Delta^- I_{1,-1})\right] \tag{3.1c}$$

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}R_{1,-1} = {}& -\hbar^2\left\{(W^+ + W^-)R_{1,-1} + 2\left[\frac{B}{\hbar^2} + (\Delta^+ - \Delta^-)\right]I_{1,-1}\right\}\\ &-\hbar^2\varepsilon\left\{W^-\sigma_1 - (W^+ + W^-)\sigma_0 + W^+\sigma_{-1}\right\}\end{aligned} \tag{3.1d}$$

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}I_{1,-1} = {}& \hbar^2\left\{2\left[\frac{B}{\hbar^2} + (\Delta^+ - \Delta^-)\right]R_{1,-1} - (W^+ + W^-)I_{1,-1}\right\}\\ &+2\hbar^2\varepsilon\left\{\Delta^-\sigma_1 + (\Delta^+ - \Delta^-)\sigma_0 - \Delta^+\sigma_{-1}\right\}\end{aligned} \tag{3.1e}$$

and

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}R_{1,0} = {}& -\hbar^2\left[(W^+ + 2W^-)R_{1,0} + \left(\frac{B}{\hbar^2} + 2\Delta^+\right)I_{1,0} + 2W^+R_{0,-1}\right]\\ &-\hbar^2\varepsilon\left[(W^+ + W^-)R_{1,0} - 2(\Delta^+ - \Delta^-)I_{1,0} + W^+R_{0,-1} + 2\Delta^+ I_{0,-1}\right]\end{aligned} \tag{3.2a}$$

$$\frac{d}{dt}I_{1,0} = \hbar^2\left[\left(\frac{B}{\hbar^2}+2\Delta^+\right)R_{1,0}-(W^+ + 2W^-)I_{1,0}+2W^+I_{0,-1}\right]$$
$$+\hbar^2\varepsilon\left[2(\Delta^+-\Delta^-)R_{1,0}-(W^+ + W^-)I_{1,0}-2\Delta^+R_{0,-1}+W^+I_{0,-1}\right] \tag{3.2b}$$

$$\frac{d}{dt}R_{0,-1} = \hbar^2\left[2W^-R_{1,0}-(2W^+ + W^-)R_{0,-1}-\left(\frac{B}{\hbar^2}-2\Delta^-\right)I_{0,-1}\right]$$
$$+\hbar^2\varepsilon\left[-W^-R_{1,0}+2\Delta^-I_{1,0}+(W^+ + W^-)R_{0,-1}+2(\Delta^+-\Delta^-)I_{0,-1}\right] \tag{3.2c}$$

$$\frac{d}{dt}I_{0,-1} = \hbar^2\left[2W^-I_{1,0}+\left(\frac{B}{\hbar^2}-2\Delta^-\right)R_{0,-1}-(2W^+ + W^-)I_{0,-1}\right]$$
$$+\hbar^2\varepsilon\left[2\Delta^-R_{1,0}+W^-I_{1,0}+2(\Delta^+-\Delta^-)R_{0,-1}-(W^+ + W^-)I_{0,-1}\right]. \tag{3.2d}$$

A look at (3.1) and (3.2) shows the general feature of the diagonal and off-diagonal matrix elements that evolve independently in the RWA. In such a case, one may compute the three eigenvalues of the evolution matrix for the occupation numbers in (3.1), being

$$\lambda_1 = 0 \tag{3.3a}$$
$$\lambda_{2,3} = -2\nu \pm 2\hbar W^+ e^{-\beta\hbar B/2} \tag{3.3b}$$

which coincide with those obtained in [4]. The eigenvalues for the transition amplitudes between levels $m = 1$ and -1 are obtained from (3.1*d*) and (3.1*e*) and reads

$$\lambda'_\pm = -\nu \pm i2(B+\delta). \tag{3.4}$$

In the FC case one cannot analytically compute the eigenvalues of (3.1). However, up to second order in the coupling constant λ the characteristic polynomials of these equations have the eigenvalues (3.3) and (3.4). In the same approximation, one can compute the four eigenvalues of (3.2), which are

$$\lambda_{1,2} = \pm iB \tag{3.5a}$$
$$\lambda_{3,4} = -3\nu \pm i\sqrt{B(B-4\delta)-9\nu^2} \tag{3.5b}$$

for the FC and RWA. Consequently, while the off-diagonal elements $\sigma_{1,-1}$ and $\sigma_{-1,1}$ exhibit a characteristic time twice as large as the diagonal ones, the adjacent elements $\sigma_{1,0}$, $\sigma_{0,1}$, $\sigma_{-1,0}$ and $\sigma_{0,-1}$ approximately relax with the fastest rate 3ν.

In the previous section we have seen that the equilibrium solution for the $j = \frac{1}{2}$ system is the canonical one either in the FC or in the RWA frames, but this is not true in the present case. From equations (3.1) it is easy to check that in the RWA the stationary diagonal elements obey the distribution

$$\sigma_0^{\mathrm{RWA}} = 1/(1+\alpha+\alpha^{-1}) \tag{3.6a}$$
$$\sigma_{\pm1}^{\mathrm{RWA}} = \alpha^{\mp1}/(1+\alpha+\alpha^{-1}) \tag{3.6b}$$

while the off-diagonal elements $\sigma_{1,-1}$, $\sigma_{-1,1}$ vanish. Note that in the weak coupling limit the distribution (3.6) correspond to the canonical one. Nevertheless, in the FC case the situation is different. A straightforward calculation leads from (3.1) to the following stationary solution:

$$\sigma_{\pm1}^{\mathrm{FC}} = \sigma_{\pm1}^{\mathrm{RWA}}(1-R_{1,-1}^{\mathrm{FC}}) \tag{3.7a}$$
$$\sigma_0^{\mathrm{FC}} = \sigma_0^{\mathrm{RWA}}(1-R_{1,-1}^{\mathrm{FC}})+R_{1,-1}^{\mathrm{FC}} \tag{3.7b}$$

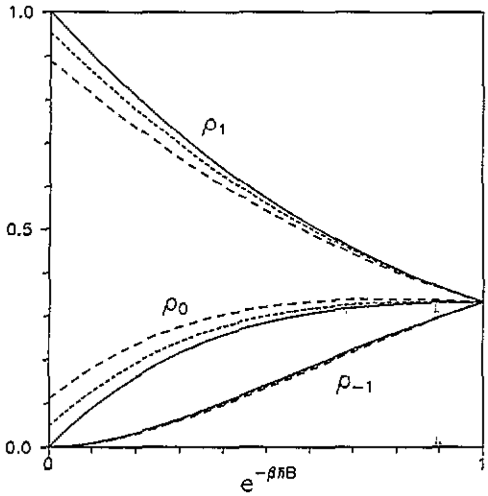

Figure 1. Equilibrium distribution for the RWA (full curve) and FC model (broken curve) as a function of the parameter $\exp(-\beta\hbar B)$. The latter is displayed for $\chi = B/\gamma = 10^{-4}$ and $\mu = 2\times10^{-5}$ (short broken curve) and $\mu = 5\times10^{-5}$ (long broken curve).

$$R^{FC}_{1,-1} = \frac{\hbar^2[\Delta^+(\sigma^{RWA}_{-1} - \sigma^{RWA}_0) - \Delta^-(\sigma^{RWA}_1 - \sigma^{RWA}_0)]}{B + \hbar^2[\Delta^+(2\sigma^{RWA}_1 + \sigma^{RWA}_0 + 3\sigma^{RWA}_{-1}) - \Delta^-(3\sigma^{RWA}_1 + \sigma^{RWA}_0 + 2\sigma^{RWA}_{-1})]} \tag{3.7c}$$

$$I^{FC}_{1,-1} = 0 \tag{3.7d}$$

where the deviation from the RWA distribution is proportional to $R^{eq}_{1,-1}$ which at least is of second order in the coupling strength contained in $\Delta^{\pm}$. Note that in the high temperature regime ($\beta\hbar B \ll 1$), $R^{eq}_{1,-1} \to 0$ and one recovers the RWA distribution.

On the other hand, the determinant of the matrix (3.2) is non-vanishing for both models. Then, the remaining off-diagonal elements vanish at equilibrium.

For the weak coupling limit case, in figure 1 the RWA (canonical) and FC equilibrium distributions are shown as functions of $\exp(-\beta\hbar B)$. For the latter, the corresponding $\Delta^{\pm}$ coefficients appearing in (3.7) were calculated for a harmonic oscillatory reservoir model with ohmic dissipation using a Lorentz–Drude cut-off [13].

We have depicted the FC equilibrium distribution for two values of the parameter $\mu = \lambda^2\kappa\hbar^2$ while $\chi = B/\gamma = 10^{-4}$. The departure from the canonical distribution increases as the parameter μ/χ grows and the temperature decreases. In particular, we verify that for $\mu/\chi < 0.01$ both distributions coincide.

Since, in general, (3.1) and (3.2) are not analytically solvable, we have performed numerical integrations, considering different values of the system-plus-reservoir parameters in the case of the same reservoir utilized for compute the equilibrium solution. A diagonal initial condition $\sigma_{i,j}(0) = \delta_{i,j}\delta_{i,1}$ has been enforced in every case. Typical results display the following features: first, for high temperatures ($\beta\hbar B \ll 1$), oscillations are present in the FC calculations as opposed to the purely exponential relaxation predicted in the RWA. This can be appreciated in figure 2 where we show, for $\mu = 2\times10^{-5}$ and $\chi = \beta\hbar B = 10^{-4}$, (i) the time evolution of the occupation numbers $\sigma_{\pm}$, σ_0 and (ii) the off-diagonal components $R_{1,-1}$ and $I_{1,-1}$. Notice that the remaining density matrix elements identically vanish at all times. The appearance of some smooth oscillations in the diagonal elements can be attributed to the fact that the current regime does not comply with the 'weak coupling' demands leading to exponential decay; indeed, for the selected parameters one obtains a ratio $\nu/B \sim 0.4$. As the temperature is lowered—i.e. $\beta\hbar B$ increases—the above oscillations in the occupation number disappear. In figures 3(*a*) and (*b*), with $\beta\hbar B = 1$, we may observe, on the one hand the slight departure of the FC equilibrium distribution with respect to the RWA canonical one, and

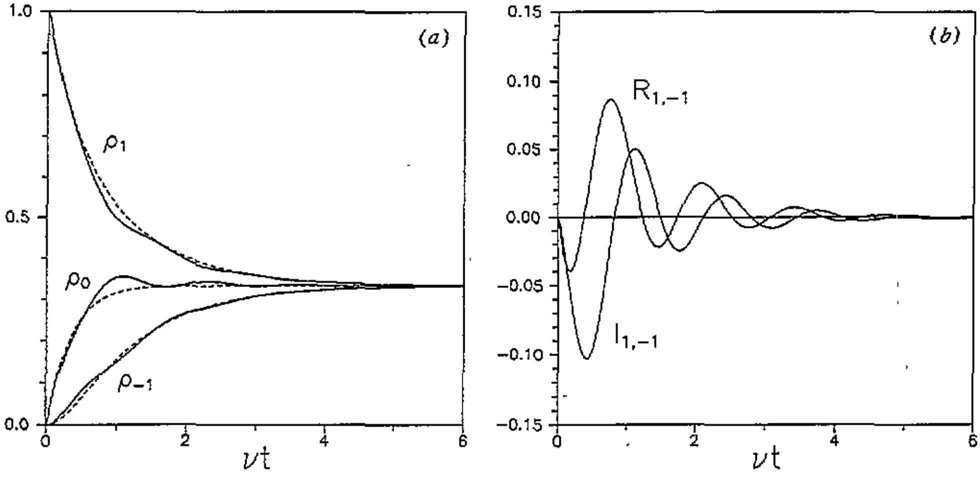

Figure 2. The time evolution of (a) the occupation numbers $\rho_{\pm}$, ρ_0 and (b) the off-diagonals components $R_{1,-1}$ and $I_{1,-1}$ for the FC (full curve) and RWA (broken curve) cases displayed for $\mu = 2 \times 10^{-5}$ and $\chi = \beta\hbar B = 10^{-4}$.

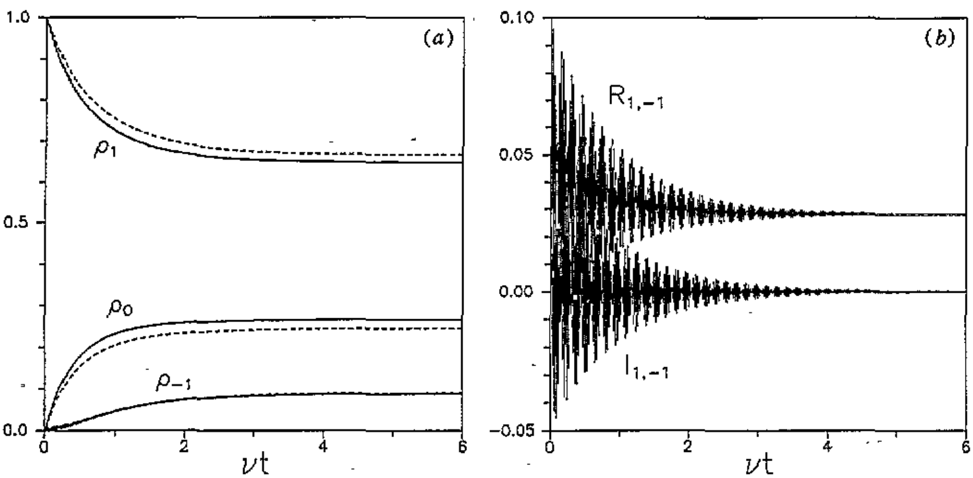

Figure 3. As for figure 2 for $\beta\hbar B = 1$.

on the other, the occurrence of a non-vanishing equilibrium value of $R_{1,-1}$, which is reached through a high-frequency motion provoked by the large imaginary part of the rate in (3.4).

Secondly, we have verified that as the parameter χ increases, the FC and RWA evolutions resemble each other more closely. For $\mu/\chi < 10^{-2}$ the diagonal matrix elements are identical within the current drawing scale, while the amplitude of the off-diagonal components $R_{1,-1}$ and $I_{1,-1}$ are significantly lowered with respect to the cases illustrated in figures 2 and 3.

In the $j = 1$ case one can easily verify that

$$\langle J_z \rangle = \hbar(\sigma_1 - \sigma_{-1}) \tag{3.8a}$$

$$\langle J_z^2 \rangle = \hbar^2(\sigma_1 + \sigma_{-1}) \tag{3.8b}$$

$$\langle J_x \rangle = \hbar\sqrt{2}(R_{1,0} + R_{0,-1}) \tag{3.8c}$$

$$\langle J_x^2\rangle = \tfrac{1}{2}\hbar^2(1+\sigma_0+2R_{1,-1}) \tag{3.8d}$$

$$\langle J_y\rangle = -\hbar\sqrt{2}(I_{1,0}+I_{0,-1}) \tag{3.8e}$$

$$\langle J_y^2\rangle = \tfrac{1}{2}\hbar^2(1+\sigma_0-2R_{1,-1}) \tag{3.8f}$$

from which we realize that the motion of $\langle J_x\rangle$ and $\langle J_y\rangle$ is independent of the remaining quantities as a consequence of the fact that (3.1) and (3.2) are uncoupled. Specially, if the off-diagonal elements $\sigma_{1,0}$, $\sigma_{0,-1}$ initially vanished, $\langle J_x\rangle$ and $\langle J_y\rangle$ remain identical to zero along the evolution.

In figures 4 and 5 we show, under labels (*a*)–(*d*), respectively, the quantities $\langle J_z\rangle$, $\langle J_z^2\rangle$, $\langle J_x^2\rangle$ and $\langle J_y^2\rangle$. In turn, these pictures correspond to the same parameter values as figures 2 and 3. Their major features are (i) the FC oscillations in $\langle J_z^2\rangle$ are smoothed away as $\beta\hbar B$ is increased; (ii) the FC frequency of $\langle J_x^2\rangle$ and $\langle J_y^2\rangle$ becomes much higher, the lowest the temperature; (iii) for the highest temperatures, the asymptotic values of all the quantities are the same in the FC and RWA cases and (iv) significant differences in the equilibrium situation show up at low temperatures. In particular, in the latter condition one encounters

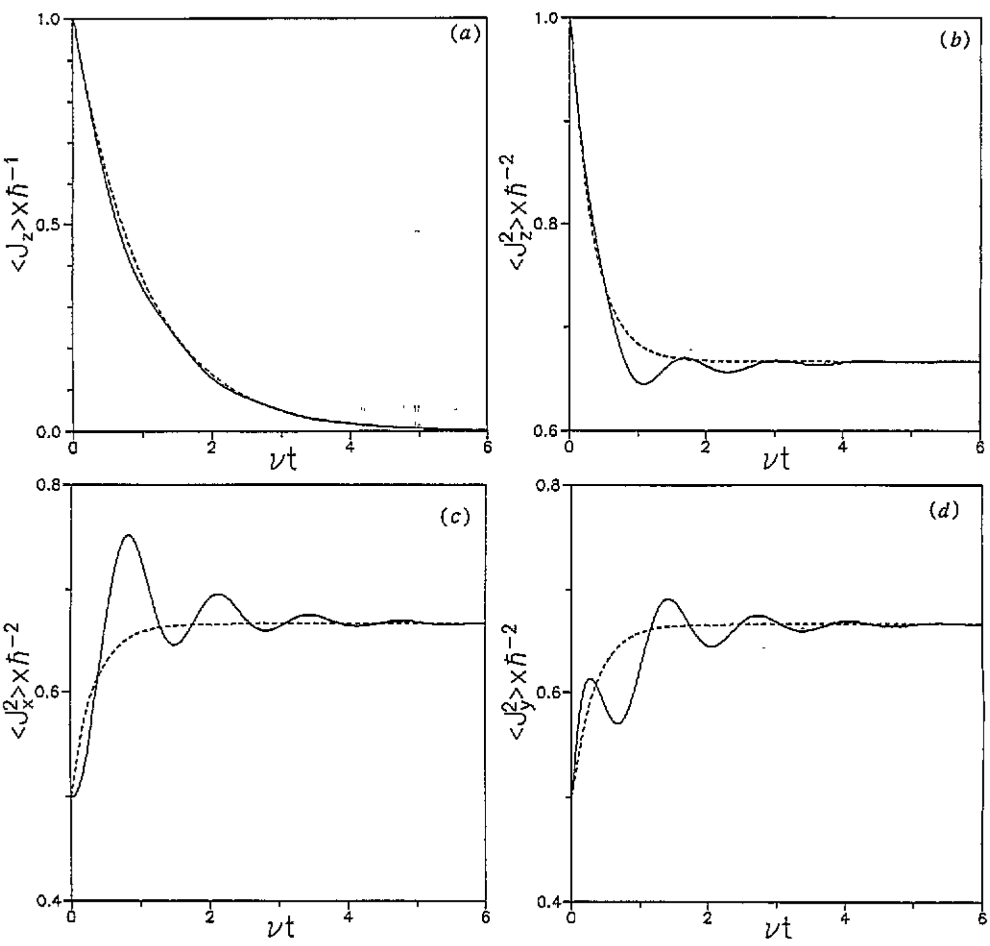

Figure 4. Time evolution of (*a*) $\langle J_z\rangle$, (*b*) $\langle J_z^2\rangle$, (*c*) $\langle J_x^2\rangle$ and (*d*) $\langle J_y^2\rangle$ for the the FC (full curve), RWA (broken curve) and the same parameters values of figure 2.

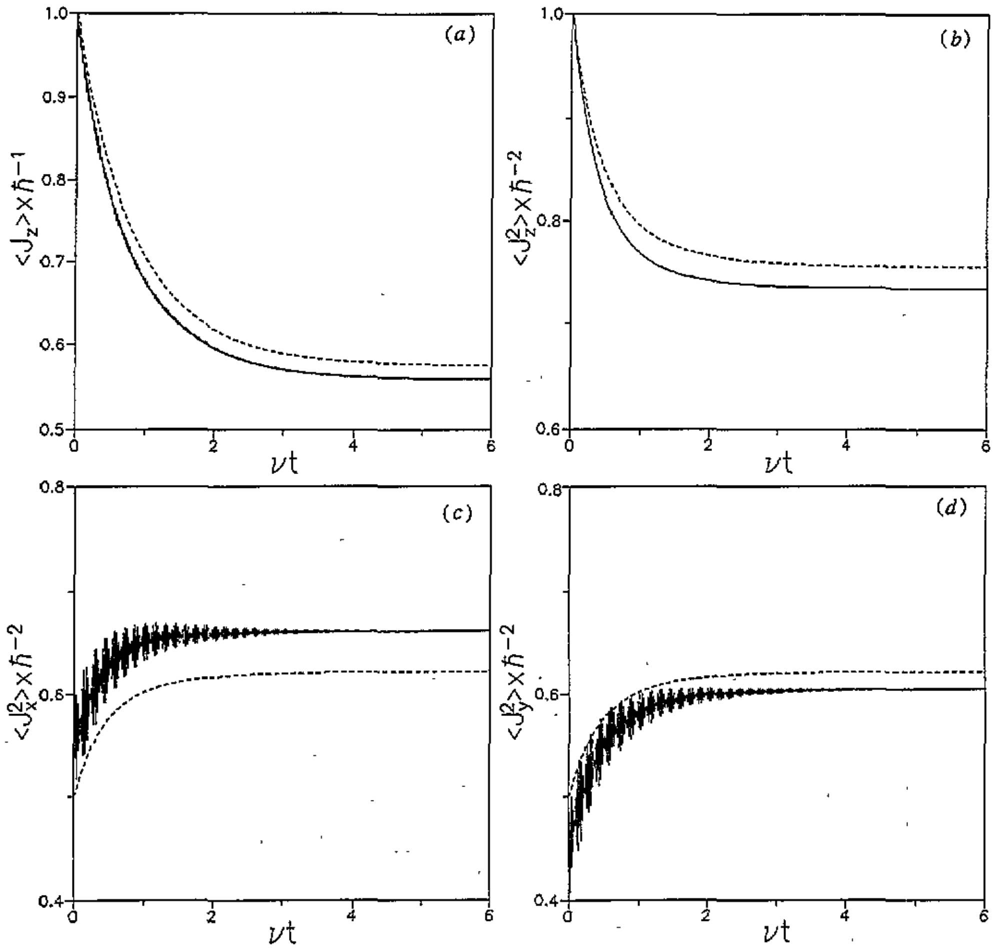

Figure 5. As for figure 4 for the same parameters values of figure 3.

that $\langle J_x^2 \rangle_{\rm FC} \geqslant \langle J_x^2 \rangle_{\rm RWA}$ and $\langle J_y^2 \rangle_{\rm FC} \leqslant \langle J_y^2 \rangle_{\rm RWA}$. However, these differences are washed out as the ratio μ/χ becomes smaller.

4. Conclusions

In this work we have examined the approach to equilibrium of a spin-j system irreversibly coupled to a heat reservoir, in the frame of the Markovian GME. The very different relaxation dynamics that may show up as one selects either the FC model or the RWA, has been examined in two definite cases. While the spin-$\frac{1}{2}$ system can be solved analytically, the spin-1 case demands a numerical approach as carried down in this paper. This procedure allowed us to demonstrate, on the one hand, that non-Gibbsian or non-canonical equilibrium distributions may appear, and on the other, that off-diagonal elements of the density matrix of the relaxing system may persist over very long times.

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Appendix.

The evolution of the matrix elements $\sigma_{m,n}$ corresponding to a spin system can be evaluated projecting the corresponding GME in the $|jm\rangle$ basis and using that

$$J_z|j,m\rangle = \hbar m|j,m\rangle \tag{A.1a}$$

$$J_\pm|j,m\rangle = \hbar\sqrt{j(j+1)-m(m\pm 1)}\,|j,m\rangle\,. \tag{A.1b}$$

With this in mind, from (2.5)–(2.8) one can easily obtain that

$$\begin{aligned}\dot{\sigma}_{m,n} = \mathrm{i}\left\{\left[B+\hbar^2(\Delta^+-\Delta^-)\right](m-n)+\hbar^2(\Delta^++\Delta^-)(m^2-n^2)\right\}\sigma_{m,n}\\ +\hbar^2W^+[C_mC_n\sigma_{m-1,n-1}-\tfrac{1}{2}(C_{m+1}^2+C_{n+1}^2)\sigma_{m,n}]\\ +\hbar^2W^-[C_{m+1}C_{n+1}\sigma_{m+1,n+1}-\tfrac{1}{2}(C_m^2+C_n^2)\sigma_{m,n}]+\langle jm|\Lambda'\sigma|jn\rangle\end{aligned} \tag{A.2}$$

where the last term is a contribution only for the FC case and reads

$$\begin{aligned}\langle jm|\Lambda'\sigma|jn\rangle = \tfrac{1}{2}\hbar^2\varepsilon\,\{\,C_{m+1}C_n\left[(W^++W^-)-\mathrm{i}2(\Delta^+-\Delta^-)\right]\sigma_{m+1,n-1}\\ +C_mC_{n+1}\left[(W^++W^-)+\mathrm{i}2(\Delta^+-\Delta^-)\right]\sigma_{m-1,n+1}\\ -C_mC_{m-1}\left(W^++\mathrm{i}2\Delta^+\right)\sigma_{m-2,n}-C_{m+1}C_{m+2}\left(W^-+\mathrm{i}2\Delta^-\right)\sigma_{m+2,n}\\ -C_nC_{n-1}\left(W^+-\mathrm{i}2\Delta^+\right)\sigma_{m,n-2}-C_{n+1}C_{n+2}\left(W^--\mathrm{i}2\Delta^-\right)\sigma_{m,n+2}\right\}\,.\end{aligned} \tag{A.3}$$

Finally, from (A.1b), (A.3) and (2.15) one can compute the expressions (2.17) and (2.18) for the real and imaginary part of the non diagonal matrix elements $\sigma_{m,n}$.

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