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NON-MARKOVIAN RELAXATION OF A QUANTUM SYSTEM

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A non-Markovian treatment of the relaxation of a spin j is developed. The corresponding reduced collision operator admits a discrete spectral representation whose eigenvalues are extracted in a high temperature limit. Then, assuming a phonon reservoir with a Debye-like density of phonon states, the time evolution of the collision operator is explicitly given, showing that the corresponding time decay arises from the branch points of its Laplace transform. The extraction of the analytic continuation of the transform allows the memory effects on the relaxation frequencies (resolvent poles) to be analyzed and the validity of the rotating-wave approximation to be tested.

1. Introduction

One of the central problems that generally make the non-Markovian treatment of irreversible dynamics difficult is that of the calculation of analytic continuations for the collision and the resolvent operators. This matter has been treated mainly by the Brussels school in connection with the theory of subdynamics [1, 2] and several methods of analytic continuation suitable for operators having a continuous spectrum in the thermodynamic limit were proposed [3–5]. On the other hand, the case of discrete spectrum operators was formally treated in ref. [6] and in the present paper we will focus upon a physical situation within a similar formalism. We are interested in studying the memory effects on the dynamics of a "small quantum system" with a discrete energy spectrum that is coupled to a "large reservoir" with a continuous energy spectrum (the so-called quantal Brownian motion problem[#1]). Then the collision operator of the whole system should possess a continuous spectrum but, since we are interested in the motion of the small subsystem, we should focus upon a reduced collision operator which indeed would possess a discrete spectrum.

[#1] There exists an extensive literature on quantum Brownian motion, see for instance refs. [7, 8].

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We will consider the simplest case of a system having a discrete and, furthermore, a finite energy spectrum, namely a spin of arbitrary angular momentum in an externally imposed magnetic field. Thus the starting point is a Hamiltonian for the whole system given by

$$H = H_S + H_R + H_{SR} , \tag{1.1}$$

with H_R and H_{SR} representing the Hamiltonians of the reservoir and the interaction respectively and

$$H_S = -BJ_z \tag{1.2}$$

representing the Hamiltonian of the spin, B being a nonnegative parameter related to the field and J_z the operator for the z component of the spin angular momentum $\boldsymbol{J}$. Therefore the unperturbed Hamiltonian H_S has $2j+1$ eigenvalues corresponding to the different orientations of the spin j with respect to the magnetic field. The interaction H_{SR} can induce transitions between the above eigenstates of H_S that could eventually (see below) lead the spin to a final steady state.

Starting from the Liouville–von Neumann equation of motion, using standard projection operator techniques, and under rather general assumptions regarding the interaction and the reservoir, a generalized master equation for the diagonal component of the density operator of the spin, $\rho(t)$, can be extracted [9–12],

$$\dot{\rho}(t) = -\int_0^t d\tau\, \phi(\tau)\, \rho(t-\tau) , \tag{1.3}$$

where $\phi(\tau)$ symbolizes a reduced collision operator which is obtained from the whole one [1, 2] by averaging it over the reservoir degrees of freedom. Assuming the first Born approximation, which is valid in a weak-coupling scheme [9, 11, 13], the following explicit form correct to second order in H_{SR} arises:

$$\phi(\tau) \cong \phi_0(\tau) = \mathrm{Tr}_R(L_{SR}\, e^{-i(L_S+L_R)\tau} L_{SR}\rho_R) , \tag{1.4}$$

where Tr_R denotes tracing over the reservoir variables, $L = \hbar^{-1}[H,\ \ ]$ are Liouville operators and ρ_R represents the density operator of the (steady) reservoir. If, in addition, we consider an interaction Hamiltonian linear in $\boldsymbol{J}$, the action of the weak-coupling collision operator (1.4) can be written as

$$\phi_0(\tau)\,\rho = \frac{1}{2\hbar^2}\, W_-(\tau)\,(J_+J_-\rho + \rho J_+J_- - 2J_-\rho J_+)$$
$$+ \frac{1}{2\hbar^2}\, W_+(\tau)\,(J_-J_+\rho + \rho J_-J_+ - 2J_+\rho J_-)\,, \tag{1.5}$$

where J_+ (J_-) is the usual raising (lowering) operator of the spin. The explicit form of the time functions $W_\pm(\tau)$, which we shall call instantaneous transition rates (ITRs), can be obtained after the reservoir and the interaction are specified.

We must also recall the usual assumption in the derivation of eq. (1.3), namely that the initial correlations between the spin and the heat bath are negligible. In other words, one is making the hypothesis that the initial density operator of the total system can be factorized as a product of a spin operator and a reservoir operator. In addition, the latter operator should correspond to a canonical distribution at a temperature T and the former to a diagonal density matrix in the basis of eigenstates of J_z. Such conditions are suitable for studying the relaxation of a spin with an initially well defined component of the angular momentum.

The Laplace transformation theory yields immediately a formal solution for the generalized master equation (1.3),

$$\rho(t) = \frac{1}{2\pi \mathrm{i}} \int_{k-\mathrm{i}\infty}^{k+\mathrm{i}\infty} \mathrm{d}s\, \mathrm{e}^{st}[\tilde{\phi}(s) + s]^{-1}\rho(0)\,, \qquad k > 0\,, \tag{1.6}$$

where

$$\tilde{\phi}(s) = \int_0^\infty \mathrm{e}^{-s\tau}\phi(\tau)\,\mathrm{d}\tau \tag{1.7}$$

is the Laplace transform of the collision operator.

According to the Brussels school [1, 2], we may distinguish a number of general properties regarding the solution (1.6):

1) The behaviour of the collision operator $\tilde{\phi}(s)$ in the limit $s \to 0^+$ is crucial in the determination of the existence of an irreversible subdynamics. Briefly speaking, the systems exhibiting the normal thermodynamic irreversibility are characterized by the existence of an operator $\tilde{\phi}(0^+)$ which does not vanish identically [1, 2]. In fact, the existence of $\tilde{\phi}(0^+)$ is closely related to the finite lifetime of the collision operator $\phi(\tau)$, as can be seen from eq. (1.7), and this decaying behavior ensures the finite lifetime of correlations, which is the source of irreversibility. Particularly, a usually assumed limiting case arises if the above lifetime is microscopical compared to the relaxation time. Then the

Markovian approximation for the generalized master equation (1.3) leads to the well-known differential master equation

$$\dot{\rho}(t) = -\int_0^\infty \mathrm{d}\tau\, \phi(\tau)\, \rho(t) = -\tilde{\phi}(0^+)\, \rho(t)\,, \tag{1.3'}$$

where we can identify $\tilde{\phi}(0^+)$ as the generator of the dynamics in the Markovian limit.

2) The collision operator $\tilde{\phi}(s)$, defined through eq. (1.7) for $\mathrm{Re}(s) > 0$, is assumed to admit analytic continuation in the left half plane. Then the poles of the resolvent $[\tilde{\phi}(s) + s]^{-1}$ (eq. (1.6)) which must be located on $\mathrm{Re}(s) \leq 0$ give the asymptotic irreversible evolution of $\rho(t)$ [5, 6].

3) Finally, it is well known (and was remarked almost in the beginning of the formulation of quantum theory [14, 15]) that a necessary condition for an irreversible microscopic evolution is the occurrence of a continuous energy spectrum, which in our case must correspond to the reservoir.

Having summarized the general features of the formal solution (1.6), from now on we shall focus upon the collisional kernel (1.5). Firstly, from eqs. (1.5) and (1.7) we realize that the s-dependence of the collision operator $\tilde{\phi}_0(s)$ must come through the Laplace transforms of the ITRs,

$$\tilde{W}_\pm(s) = \int_0^\infty \mathrm{e}^{-s\tau} W_\pm(\tau)\, \mathrm{d}\tau\,. \tag{1.8}$$

Then a sufficient condition for the *existence* of a *non vanishing* $\tilde{\phi}(0^+)$ is [#2]

$$0 < |\tilde{W}_+(0^+)| + |\tilde{W}_-(0^+)| < \infty \tag{1.9}$$

and the analytic continuation of $\tilde{\phi}(s)$ can be explored through the analytic continuations of the functions (1.8). The Markovian limit will be valid if the ITRs $W_\pm(\tau)$ have sufficiently short lifetimes and in such a case the equation of motion will be (1.3′). The main features of the Markovian relaxation of a spin are well known, specially for the simplest case of a spin $\frac{1}{2}$ [9, 10, 16, 17] and it is not the aim of the present paper to focus upon this regime. However, as we shall see in section 3, the study of the non-Markovian dynamics requires the knowledge of the spectrum of Markovian eigenfrequencies. In addition, there exist some questions on the Markovian regime of a spin j that remain unexplored (e.g., the explicit general solution). This is the case for the linked

[#2] Eq. (1.9) expresses the necessary and sufficient condition for the existence of a nonvanishing weak-coupling collision operator $\tilde{\phi}_0(0^+)$.

hierarchy of moment equations [17]. Therefore we devote section 2 to displaying those results of the Markovian dynamics. In section 3 we study the spectral representation of the collision and resolvent operators. The non-Markovian dynamics is focused upon in section 4 assuming a phonon reservoir and a general linear interaction in a thermodynamic limit given by a Debye-like density of phonon states. Finally, in section 5 we study in a high temperature regime the time evolution of the collision operator and the analytic continuation of its Laplace transform, which permits us to investigate various features of the relaxation frequencies.

2. Markovian regime

From eqs. (1.3′) and (1.5) it is easy to extract the following Markovian master equation:

$$\begin{aligned} \dot{\rho}_m = {} & \tilde{W}_-\{[(j+1)j-(m+1)m]\rho_{m+1}-[(j+1)j-(m-1)m]\rho_m\} \\ & +\tilde{W}_+\{[(j+1)j-(m-1)m]\rho_{m-1}-[(j+1)j-(m+1)m]\rho_m\} \\ & (-j \leqslant m \leqslant j)\,, \end{aligned} \tag{2.1}$$

where we have denoted $\tilde{W}_\pm \equiv \tilde{W}_\pm(0^+)$ (eq. (1.8)) while the ρ_m's represent the diagonal elements of the spin density matrix, i.e.,

$$\rho = \sum_{m=-j}^{j} \rho_m |jm\rangle\langle jm|\,. \tag{2.2}$$

From eqs. (2.1), (2.2) and (1.3′) it is clear that the operator $\tilde{\phi}(0^+)$ is represented by a $(2j+1)\times(2j+1)$ non-Hermitian matrix. The "upwards" transition rate $\tilde{W}_+$ is responsible for the spin transitions toward the alignment with the magnetic field whereas $\tilde{W}_-$ is related to the opposite motion ("downwards" transition rate). It is easy to verify that the canonical distribution

$$\rho_m^0 = \frac{1}{Z}\left(\frac{\tilde{W}_+}{\tilde{W}_-}\right)^m, \tag{2.3}$$

with $Z=\Sigma_{m=-j}^{j}(\tilde{W}_+/\tilde{W}_-)^m$, is a fixed point of eq. (2.1). The parameter $\tilde{W}_+/\tilde{W}_-$ will usually coincide with the Boltzmann factor (see section 4):

$$\tilde{W}_+/\tilde{W}_- = \exp(\hbar B/k_B T)\,, \tag{2.4}$$

where k_B is the Boltzmann constant, T is the temperature of the heat bath and B is proportional to the magnetic field (eq. (1.2)). The general solution of eq. (2.1) arises from the diagonalization of the matrix $\tilde{\phi}_0(0^+)$ and its adjoint [18], and this task seems to be rather involved. However, we shall see that it is easy to extract the set of eigenfrequencies in the high temperature limit. Before displaying these results, we want to focus upon the equations for the moments,

$$M_p = \langle J_z^p \rangle / \hbar^p = \sum_{m=-j}^{j} m^p \rho_m \,. \tag{2.5}$$

A straightforward calculation leads from eq. (2.1) to the following linked hierarchy in which the equation for each moment of order p involves the moment of order $p+1$ (cf. ref. [17]):

$$\begin{aligned}\dot{M}_p = \tilde{W}_- \Big\{ & (-1)^p j(j+1) M_0 + \sum_{k=1}^{p-1} (-1)^{p-k} M_k \Big[j(j+1)\binom{p}{k} - \binom{p+1}{k-1} \Big] \\ & - \frac{p}{2}(p+1) M_p + p M_{p+1} \Big\} \\ + \tilde{W}_+ \Big\{ & j(j+1) M_0 + \sum_{k=1}^{p-1} M_k \Big[j(j+1)\binom{p}{k} - \binom{p+1}{k-1} \Big] \\ & - \frac{p}{2}(p+1) M_p - p M_{p+1} \Big\} \,. \end{aligned} \tag{2.6}$$

In particular, the first two equations read

$$\dot{M}_0 = 0 \qquad (M_0 = 1) \,, \tag{2.6a}$$

$$\begin{aligned}\dot{M}_1 &= j(j+1)(\tilde{W}_+ - \tilde{W}_-) - (\tilde{W}_+ + \tilde{W}_-) M_1 + (\tilde{W}_- - \tilde{W}_+) M_2 \\ &= (\tilde{W}_+ - \tilde{W}_-) \Big[\langle J^2 \rangle - M_2 - \coth\Big(\frac{\hbar B}{2 k_B T}\Big) M_1 \Big] \,. \end{aligned} \tag{2.6b}$$

Eq. (2.6a) obviously reflects the trace conservation of the density matrix. Eq. (2.6b) was first reported in ref. [17] in a classical limit ($k_B T \gg \hbar B$). In addition, it was also shown that a suitable truncation of the hierarchy at eq. (2.6b) leads to the well-known [19] linear Bloch equation.

It is interesting to make the comparison between hierarchy (2.6) and that of the moments of the phonon distribution of a harmonic oscillator in Brownian motion [8], which turns out to be unlinked, i.e., the equation for the p-moment does not involve the moment of order $p+1$. This property is verified by our hierarchy (2.6) in the high-temperature limit $\tilde{W}_- \cong \tilde{W}_+ \equiv \tilde{W}$ (eq. (2.4)) when (2.6) becomes

$$\dot{M}_p = \tilde{W}\Big\{[1+(-1)^p]j(j+1)M_0 + \sum_{k=1}^{[(p-1)/2]} 2M_{p-2k}\left[j(j+1)\binom{p}{p-2k} - \binom{p+1}{p-2k-1}\right] - p(p+1)M_p\Big\} . \tag{2.7}$$

This system of differential equations is of the form

$$\dot{\boldsymbol{M}} = \tilde{\mathbf{W}}\boldsymbol{M} , \tag{2.8}$$

where $\boldsymbol{M}$ represents a vector of components M_p and $\tilde{\mathbf{W}}$ symbolizes an infinite triangular matrix which, as is well known, displays its eigenvalues in the diagonal; hence, the spectrum of eigenfrequencies of the general hierarchy (2.7) must be

$$-p(p+1)\tilde{W} , \qquad p = 0, 1, 2, \ldots \tag{2.9}$$

This spectrum corresponds to all possible values of j and therefore the eigenfrequencies of a given spin j must be included in the set (2.9). In order to determine the latter spectrum, it suffices to diagonalize the matrices of the collision operator for the first values of j (see the appendix); thus we can find the general rule: The Markovian eigenfrequencies of a spin j in the high temperature limit are

$$-p(p+1)\tilde{W} , \qquad p = 0, 1, \ldots , 2j . \tag{2.10}$$

The vanishing frequency ($p = 0$) corresponds to the equilibrium distribution (2.3) which turns out to be scalar, i.e., the high-temperature–weak-field limit $k_B T \gg \hbar B$ leads to isotropy as expected.

It is interesting to notice that in the classical limit $j \gg 1$, the spectrum (2.10) is isomorphic to the spectrum of eigenfrequencies of a rigid rotor performing Brownian motion in the high-friction limit, since the time evolution of its coordinate distribution function is governed by the spherical diffusion equation [20, 21]. A similar analogy between the quantum Markovian regime and the classical high-friction limit has also been observed for a harmonic oscillator [22].

3. Spectral representation of the collision and resolvent operators

The full diagonalization of the non-self-adjoint operator $\tilde{\phi}_0(0^+)$ for arbitrary values of the transition rates $\tilde{W}_\pm(0^+)$ provides a useful spectral representation for the collision operator $\tilde{\phi}_0(s)$. In fact, as we have discussed in section 1, $\tilde{\phi}_0(s)$ is simply related to $\tilde{\phi}_0(0^+)$ by means of the replacement $\tilde{W}_\pm(0^+) \to \tilde{W}_\pm(s)$. Then, the diagonalization of $\tilde{\phi}_0(0^+)$ leads to the following spectral decomposition[#3] (cf. ref. [6]):

$$\tilde{\phi}_0(s) = \sum_r \mu_r(s) |U_r(s)\rangle \langle V_r(s)| , \tag{3.1}$$

in terms of a complete biorthogonal set of right $\{|U_r(s)\rangle\}$ and left $\{\langle V_r(s)|\}$ eigenvectors with eigenvalues $\mu_r(s)$, i.e.,

$$\begin{aligned} &\tilde{\phi}_0(s)|U_r(s)\rangle = \mu_r(s)|U_r(s)\rangle , \\ &\langle V_r(s)|\tilde{\phi}_0(s) = \langle V_r(s)|\mu_r(s) , \end{aligned} \tag{3.2}$$

and

$$\begin{aligned} &\langle V_r(s)|U_q(s)\rangle = \delta_{rq} , \\ &\sum_r |U_r(s)\rangle\langle V_r(s)| = \mathbb{1} . \end{aligned} \tag{3.3}$$

The expansion (3.1) is simply found (see the appendix) for $j = 1/2$ and $j = 1$; however, in a general case it is not easily available since the extraction of the eigenvalues cannot be analytically performed. There is an exception to this rule that we have discussed in section 2: if $\tilde{W}_+(s) = \tilde{W}_-(s) = \tilde{W}(s)$ then

$$\{\mu_r(s)\} \to p(p+1)\tilde{W}(s) , \qquad p = 0, 1, \dots, 2j . \tag{3.4}$$

Expression (3.1) immediately yields the spectral representation of the resolvent $[\tilde{\phi}_0(s) + s]^{-1}$ of eq. (1.6),

$$[\tilde{\phi}_0(s) + s]^{-1} = \sum_r [\mu_r(s) + s]^{-1} |U_r(s)\rangle\langle V_r(s)| . \tag{3.5}$$

Then the set of relaxation frequencies of the non-Markovian dynamics arise from the solutions of the "dispersion relations" [6]

[#3] This kind of spectral representation was fully extracted for a Brownian harmonic oscillator in ref. [8].

$$s = -\mu_r(s)\,; \tag{3.6}$$

in particular, there must be a solution in $s = 0$ which, of course, corresponds to the equilibrium distribution.

The Markovian limit corresponds to a weak dependence of $\mu_r(s)$ on s, i.e., $\mu_r(s) \cong \mu_r(0^+)$ and thus (cf. section 2)

$$s_{\mathrm{M}} = -\mu_r(0^+)\,. \tag{3.7}$$

Notice that the nonvanishing solutions of (3.6) are expected to belong to the region of analytic continuation of $\tilde{\phi}_0(s)$, $\mathrm{Re}(s) < 0$. Let us finally mention that the above solutions need not be the only singularities of the resolvent $[\tilde{\phi}_0(s) + s]^{-1}$ (see section 5).

4. Explicit expressions for the instantaneous transition rates

Hitherto we have not specified the form of the ITRs $W_\pm(\tau)$ (eq. (1.5)); in order to analyze their properties we shall consider a particular model for the heat bath and the interaction. Then let us suppose a usual phonon heat bath, i.e. (obvious notation),

$$H_{\mathrm{R}} = \sum_\alpha \hbar\omega_\alpha a_\alpha^\dagger a_\alpha \tag{4.1}$$

which is coupled to the spin through the Hamiltonian

$$H_{\mathrm{SR}} = \sum_\alpha [(\lambda_\alpha^+ a_\alpha^\dagger + \lambda_\alpha^- a_\alpha)J_+ + (\lambda_\alpha^{+*} a_\alpha + \lambda_\alpha^{-*} a_\alpha^\dagger)J_-]\,. \tag{4.2}$$

The selected interaction is most general since it includes as particular cases:

a) a rotating-wave approximation for $\lambda_\alpha^- = 0$ (cf. refs. [7, 23, 24]);

b) the proper full coupling for $\lambda_\alpha^- = \lambda_\alpha^+$ (refs. [7, 12]).

Then inserting in eq. (1.4) the Hamiltonians (4.1), (4.2) and (1.2) as well as the canonical distribution, $\rho_{\mathrm{R}} = \exp(-H_{\mathrm{R}}/k_{\mathrm{B}}T)/\mathrm{Tr}[\exp(-H_{\mathrm{R}}/k_{\mathrm{B}}T)]$, a straightforward although lengthy calculation leads to the form (1.5) with

$$W_\pm(\tau) = 2\sum_\alpha \{\underbrace{|\lambda_\alpha^\mp|^2 \bar{n}_\alpha \cos[(B \pm \omega_\alpha)\tau]}_{a_\alpha J_\pm} + \underbrace{|\lambda_\alpha^\pm|^2(\bar{n}_\alpha + 1)\cos[(B \mp \omega_\alpha)\tau]\}}_{a_\alpha^\dagger J_\pm}\,, \tag{4.3}$$

where

$$\bar{n}_\alpha = [\exp(\hbar\omega_\alpha / k_B T) - 1]^{-1} \tag{4.4}$$

is the Bose distribution for the number of phonons in mode α.

Each term of the upwards $W_+(\tau)$ and the downwards $W_-(\tau)$ ITRs may be identified with a corresponding collision vertex of the interaction Hamiltonian, as we indicate below expression (4.3). Note also that the field inversion $B \to -B$ should cause the inversion of the ITRs, i.e., $W_\pm \to W_\mp$ and this is only achieved for the full coupling $\lambda_\alpha^- = \lambda_\alpha^+$.

The Laplace transform of (4.3) is easily obtained yielding

$$\tilde{W}_\pm(s) = 2 \sum_\alpha \left(|\lambda_\alpha^\mp|^2 \bar{n}_\alpha \frac{s}{s^2 + (B \pm \omega_\alpha)^2} + |\lambda_\alpha^\pm|^2 (\bar{n}_\alpha + 1) \frac{s}{s^2 + (B \mp \omega_\alpha)^2} \right). \tag{4.5}$$

Observing eq. (4.3), we easily realize that in its present form the ITRs are quasiperiodic time functions that will not show any decay for $\tau \to \infty$. This behavior is reflecting an infinite lifetime of correlations which excludes an irreversible time evolution. Such a conclusion arises as well from the irreversibility criterion (1.9). In fact, in the limit $s \to 0^+$, eq. (4.5) becomes

$$\tilde{W}_\pm(0^+) = 2\pi \sum_\alpha |\lambda_\alpha^+|^2 \left(\bar{n}_\alpha + \begin{Bmatrix} 1 \\ 0 \end{Bmatrix} \right) \delta(B - \omega_\alpha) , \tag{4.6}$$

where we have considered $B > 0$ and $\omega_\alpha > 0$. Then, the existence of resonant modes $\omega_\alpha = B$ or their nonexistence both lead to the same conclusion: condition (1.9) is not fulfilled. In section 1 we have remarked that a necessary condition for irreversibility is the existence of a continuous energy spectrum for the reservoir. In fact, let us suppose a thermodynamic limit in which

$$\sum_\alpha |\lambda_\alpha^\pm|^2 \to D\lambda_\pm^2 \int_0^{\omega_D} \omega^{\gamma+2} \, d\omega . \tag{4.7}$$

Such a limit could arise from a Debye-like density of phonon states,

$$\sum_\alpha \to D \int_0^{\omega_D} \omega^2 \, d\omega , \tag{4.8}$$

and from an interaction of the form

$$|\lambda_\alpha^\pm|^2 \to \lambda_\pm^2 \omega^\gamma . \tag{4.9}$$

Then inserting (4.7) in (4.6), we find

$$\tilde{W}_{\pm}(0^+) = 2\pi D\lambda_{\mp}^2 \int_0^{\omega_D} \mathrm{d}\omega\, \omega^{\gamma+2}\left(\bar{n}(\omega) + \begin{Bmatrix}1\\0\end{Bmatrix}\right) \delta(B-\omega)\,, \tag{4.10}$$

where

$$\bar{n}(\omega) = [\exp(\hbar\omega/k_B T) - 1]^{-1}\,. \tag{4.11}$$

First of all we realize that eq. (4.10) vanishes if $B > \omega_D$; thus the parameter B ($\propto$ magnetic field) must be lower than the "Debye frequency" ω_D in order to fulfill the dissipativity condition (1.9). In addition, if we admit that a vanishing magnetic field cannot affect the dissipativity, the parameter γ must be -1. In fact, assuming $\hbar B \ll k_B T$, eq. (4.10) becomes

$$\tilde{W}_{\pm}(0^+) \cong \frac{2\pi}{\hbar B} D\lambda_{+}^2 B^{\gamma+2} k_B T = \frac{2\pi}{\hbar} D\lambda_{+}^2 k_B T B^{\gamma+1}\,. \tag{4.12}$$

Therefore it must be $\gamma = -1$ in order to preserve (1.9) even if the field is turned off. From eq. (4.12) we can also see that in a high-temperature–weak-field limit, we have $\tilde{W}_{+}(0^+) \cong \tilde{W}_{-}(0^+)$. The general case arises from eq. (4.10) taking $\gamma = -1$,

$$\tilde{W}_{\pm}(0^+) = 2\pi D\lambda_{+}^2 B \exp\left(\begin{Bmatrix}\hbar B/k_B T\\0\end{Bmatrix}\right) \Big/ [\exp(\hbar B/k_B T) - 1]\,, \tag{4.13}$$

and the above expression leads to the usual Boltzmann factor (2.4) for the equilibrium distribution (2.3).

It is interesting to remark that only resonant phonons with $\omega = B$ contribute to the functions $\tilde{W}_{\pm}(s)$ of the $s = 0^+$ steady state [eq. (4.10)]. This fact can be regarded as a consequence of the time–energy uncertainty principle. That is, in a steady state ($\Delta t \to \infty$) only processes which conserve energy ($\Delta E = 0$) are possible. The same is valid in the Markovian regime (section 2) whose asymptotic dynamics is "seen as a steady state" by the correlation dynamics.

Now let us write the ITRs (4.3) in the thermodynamic limit (4.7) taking $\gamma = -1$,

$$\begin{aligned} W_{\pm}(\tau) = {} & 2D\lambda_{\mp}^2 \int_0^{\omega_D} \mathrm{d}\omega\, \omega\bar{n}(\omega) \cos[(B \pm \omega)\tau] \\ & + 2D\lambda_{\pm}^2 \int_0^{\omega_D} \mathrm{d}\omega\, \omega[\bar{n}(\omega) + 1] \cos[(B \mp \omega)\tau]\,. \end{aligned} \tag{4.14}$$

In the following section we shall study the above functions in a high temperature limit.

5. High temperature regime ($\hbar\omega_D \ll k_B T$)

In this limit we can replace in eq. (4.14) the phonon number $\bar{n}(\omega)$ by $k_B T/\hbar\omega \gg 1$; thus

$$
\begin{aligned}
W_{\pm}(\tau) &= \frac{2D}{\hbar}\,\lambda_-^2 k_B T \int_0^{\omega_D} \mathrm{d}\omega\,\cos[(B+\omega)\tau] \\
&\quad + \frac{2D}{\hbar}\,\lambda_+^2 k_B T \int_0^{\omega_D} \mathrm{d}\omega\,\cos[(B-\omega)\tau] \\
&= 2D\lambda_-^2 k_B T\,\frac{1}{\hbar\tau}\,\{\sin[(\omega_D+B)\tau] - \sin(B\tau)\} \\
&\quad + 2D\lambda_+^2 k_B T\,\frac{1}{\hbar\tau}\,\{\sin[(\omega_D-B)\tau] + \sin(B\tau)\}\,,
\end{aligned}
\tag{5.1}
$$

and therefore the corresponding Laplace transform reads

$$
\begin{aligned}
\tilde{W}(s) \equiv \tilde{W}_{\pm}(s) &= \frac{2D}{\hbar}\,\lambda_-^2 k_B T\{\mathrm{tg}^{-1}[(\omega_D+B)/s] - \mathrm{tg}^{-1}(B/s)\} \\
&\quad + \frac{2D}{\hbar}\,\lambda_+^2 k_B T\{\mathrm{tg}^{-1}[(\omega_D-B)/s] + \mathrm{tg}^{-1}(B/s)\}\,.
\end{aligned}
\tag{5.2}
$$

Firstly notice that

$$0 < B < \omega_D \Rightarrow \tilde{W}(0^+) = \frac{2\pi D}{\hbar}\,\lambda_+^2 k_B T\,, \tag{5.3a}$$

$$B = 0 \Rightarrow \tilde{W}(0^+) = \frac{\pi D}{\hbar}\,k_B T(\lambda_+^2 + \lambda_-^2)\,. \tag{5.3b}$$

The above expressions show once more that the proper interaction must be the full coupling (FC) $\lambda_+^2 = \lambda_-^2$ (for which (5.3) equals (4.12)) and also that the approximations $\lambda_+^2 \neq \lambda_-^2$ are expected to fail for low magnetic fields [12]. Later in this section we shall analyze the validity of the usually assumed rotating-wave approximation (RWA) $\lambda_-^2 = 0$ (cf. refs. [7, 23, 24]).

Then the proper ITRs are

$$W_{\pm}(\tau) = \frac{2D}{\hbar\tau}\,\lambda_+^2 k_B T\{\sin[(\omega_D+B)\tau] + \sin[(\omega_D-B)\tau]\} \tag{5.1'}$$

and the Laplace transform reads

$$\tilde{W}(s) = \frac{2D}{\hbar}\,\lambda_+^2 k_B T\{\mathrm{tg}^{-1}[(\omega_D + B)/s] + \mathrm{tg}^{-1}[(\omega_D - B)/s]\}\,. \tag{5.2'}$$

From expression (5.1′) we can appreciate that the ITRs have lost indeed their quasiperiodicity in the continuum limit, and they became decaying time functions with characteristic decay times given by $(\omega_D \pm B)^{-1}$. If these times are microscopic compared to the relaxation times, the Markovian approximation is valid. In other words, the usual Markovian approximation $W_\pm(\tau) \propto \delta(\tau)$ is formally obtained by considering

$$\lim_{\omega_D \pm B \to +\infty} \frac{1}{\tau}\sin[(\omega_D \pm B)\tau] = \frac{\pi}{2}\,\delta(\tau) \tag{5.4}$$

and thus

$$W_\pm(\tau) = \frac{2\pi D}{\hbar}\,\lambda_+^2 k_B T\delta(\tau)\,. \tag{5.5}$$

Observe that the Laplace transform of (5.5) is a constant, i.e., $\tilde{W}(s) = \tilde{W}(0^+)$ (cf. discussion regarding eq. (3.7)).

Comparing eqs. (5.1) and (5.1′) we see that a non-FC interaction introduces the spurious decay time B^{-1}. Thus, an approximated coupling (e.g., RWA) combined with the Markov assumption and a low magnetic field will yield poor results since now the formal Markovian limit (cf. eq. (5.4)) arises for $\omega_D \pm B \to +\infty$ and $B \to +\infty$ (cf. refs. [12, 24]).

The time evolution of the ITRs constitutes an interesting feature of the dynamics since it displays the corresponding evolution of the weak-coupling collision operator $\phi_0(\tau)$. Recall that such a motion is thoroughly hidden in the Markovian approximation since $\phi(\tau) \propto \delta(\tau)$. In fig. 1 we have depicted the time evolution of the ITRs $W_\pm(\tau)$ for three values of the relation B/ω_D. The comparison between the FC ($\lambda_-^2 = \lambda_+^2$) and the RWA ($\lambda_-^2 = 0$) ITRs shows that the latter follow as an envelope the more rapid oscillations of the former. The frequency of such oscillations appears to be an increasing function of the parameter B/ω_D, i.e., of the magnetic field.

Now we shall focus upon the Laplace transformed ITRs (5.2′). Firstly, taking into account that $\mathrm{tg}^{-1}(z) = (2\mathrm{i})^{-1}\log[(\mathrm{i} - z)/(\mathrm{i} + z)]$, we realize that (5.2′) possesses four branch points on the imaginary axis, namely

$$\pm\mathrm{i}(\omega_D + B)\,, \qquad \pm\mathrm{i}(\omega_D - B)\,. \tag{5.6}$$

That is, we find that the time decay of the collision operator $\phi_0(\tau)$ arises from

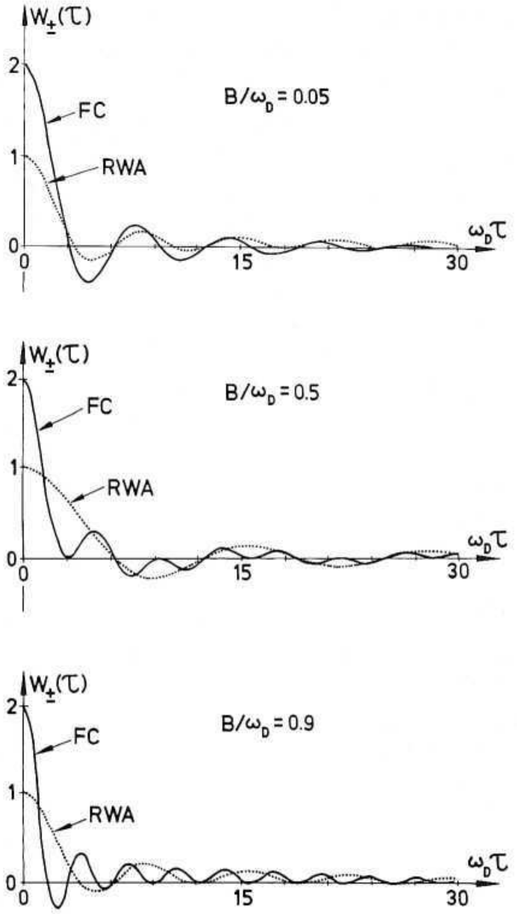

Fig. 1. The time evolution of the ITRs $W_{\pm}(\tau)$ (in units of $2D\lambda_+^2 k_B T\omega_D/\hbar$) is displayed for three values of B/ω_D (see text for further explanation).

the singularities of its Laplace transform but such singularities are branch points rather than poles. The question of the analytic continuation of $\tilde{\phi}_0(s)$ then reduces to the selection of the orientation of each cut issuing from the corresponding branch point. In analyzing this matter, we shall firstly focus upon the simplest case of a vanishing magnetic field $B = 0$. In such a case, (5.2′) reduces to

$$\tilde{W}(s) = \frac{4D}{\hbar}\,\lambda_+^2 k_B T\,\mathrm{tg}^{-1}(\omega_D/s)\,. \tag{5.7}$$

The analytic continuation of $\mathrm{tg}^{-1}(\omega_D/s)$ for $\mathrm{Re}(s)<0$ must be explored taking into account the values of this function on the frontier $\mathrm{Re}(s)=0^+$. Firstly, from

$$\mathrm{tg}^{-1}(\omega_D/s)=\frac{1}{2\mathrm{i}}\log\left|\frac{\mathrm{i}-\omega_D/s}{\mathrm{i}+\omega_D/s}\right|+\frac{1}{2}\arg\left(\frac{\mathrm{i}-\omega_D/s}{\mathrm{i}+\omega_D/s}\right) \tag{5.8}$$

we realize that the multivaluedness comes through the real part. In fig. 2 we have drawn a "map" of $\mathrm{Re}[\mathrm{tg}^{-1}(\omega_D/s)]$; along the real positive axis it reduces to the well-known real function tg^{-1}, i.e.,

$$0<s<+\infty \Rightarrow \pi/2>\mathrm{tg}^{-1}(\omega_D/s)>0 \tag{5.9}$$

and the values on the imaginary axis follows easily from (5.8). It is then obvious that there are two straightforward procedures of analytic continuation toward the left half-plane:

1) Drawing a cut between $-\mathrm{i}\omega_D$ and $+\mathrm{i}\omega_D$ which implies that the values adjacent to $+\pi/2$ in fig. 2 shall be $-\pi/2$.

2) Drawing two cuts i.e., from $\pm\mathrm{i}\omega_D$ to $\pm\mathrm{i}\infty$ implying continuity for the values $+\pi/2$ in fig. 2 across the imaginary axis between $-\mathrm{i}\omega_D$ and $+\mathrm{i}\omega_D$.

In discussing the selection of the proper cut, it is convenient to analyze the singularities of the collision operator $\tilde{\phi}_0(s)$ in the limiting process leading to the thermodynamic limit. In fact, from eq. (4.5) we can see that if the reservoir has a discrete spectrum, the singularities of $\tilde{\phi}_0(s)$ are imaginary first order poles given by the phonon frequencies $+\mathrm{i}\omega_\alpha$ (for $B=0$). In passing to the continuum limit, such a dense sequence of poles formally becomes a cut. We thus realize

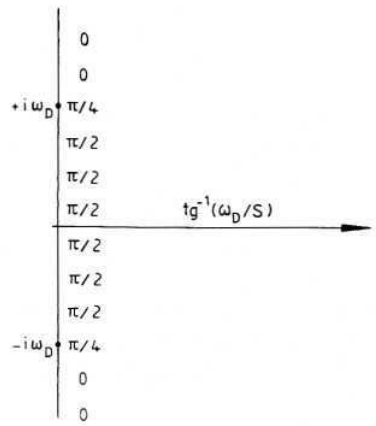

Fig. 2. The function $\mathrm{Re}[\mathrm{tg}^{-1}(\omega_D/s)]$ in the half plane $\mathrm{Re}(s)>0$ is displayed through its values on the real and imaginary axis.

that the existence of the branch points $\pm i\omega_D$ is a direct consequence of the assumed sharp cutoff of the Debye-like density (4.8) and hence, if we were considering a soft cutoff with a phonon density vanishing smoothly as $\omega \to \infty$, the whole imaginary axis would become a cut through which the analytic continuation should be performed. This analysis shows in general that the proper analytic continuation must include the origin. In our case, this fact arises as well, noticing that

$$\mathrm{Re}(s) > 0 \Rightarrow 0 < \mathrm{Re}[\mathrm{tg}^{-1}(\omega_D/s)] < \pi/2\,, \tag{5.10a}$$

$$\mathrm{Re}(s) < 0 \Rightarrow \begin{cases} (1) \quad -\pi/2 < \mathrm{Re}[\mathrm{tg}^{-1}(\omega_D/s)] < 0\,, & (5.10\mathrm{b}) \\ \text{or} & \\ (2) \quad \pi/2 < \mathrm{Re}[\mathrm{tg}^{-1}(\omega_D/s)] < \pi\,, & (5.10\mathrm{c}) \end{cases}$$

and hence the dispersion relations (cf. eqs. (3.4) and (3.6))

$$s = -p(p+1)\tilde{W}(s)\,, \qquad p = 0, 1, \ldots, 2j\,, \tag{5.11}$$

can only give solutions for (5.10c). In other words, the procedure 2) of analytic continuation is the correct one that should yield the relaxation frequencies through (5.11)[#4].

The above analysis applies immediately to the general case of a nonvanishing magnetic field. In fact, the cuts then must be drawn issuing from each branch point and directed to $\pm i\infty$, but without affecting the origin $s = 0$. Then from eq. (5.2′) it is easy to see that the analytic continuation along the real axis follows from an odd-parity rule:

$$\tilde{W}(-s) = 2\tilde{W}(0^+) - \tilde{W}(s)\,, \qquad s \geqslant 0\,. \tag{5.12}$$

This formula deserves several remarks: first of all, it expresses the corresponding analytic continuation for the weak-coupling collision operator $\tilde{\phi}_0(s)$. In this respect, it can be shown that the same odd-parity rule is valid as well for a very different configuration of quantal Brownian motion, namely, the relaxation process of a harmonic oscillator linearly coupled to a highly degenerate Fermi gas (this conclusion arises easily from eq. (3.10) of ref. [26]). Secondly, we stress that our calculation of analytic continuations was made possible by means of a knowledge of the corresponding analytic expressions in the right half plane; however, it is easy to see that such kind of expressions are not readily available in a general case of arbitrary temperature. Nevertheless, we remark that such a general case will be treated in a separate paper [27] since it can be shown that the theory of Cauchy integrals [28] provides a mathematical background suitable for studying expressions like (4.5) in a continuum limit.

[#4] However we must remark that the existence of branch points should give rise to a nonexponential decay for $t \to \infty$ (cf. eq. (5.1)).

The relaxation frequencies can be obtained as the roots of (5.11) with $\tilde{W}(s)$ given by (5.2′). Then the general conditions for the existence of Markovian solutions are (cf. the discussion regarding eq. (5.5))

$$s_M = -p(p+1)\tilde{W}(s_M) \cong -p(p+1)\tilde{W}(0^+)\,, \tag{5.13a}$$

$$|s_M| \cong p(p+1)\tilde{W}(0^+) = p(p+1)\,\frac{2\pi D}{\hbar}\,k_B T\lambda_+^2 \ll \omega_D \pm B\,. \tag{5.13b}$$

Roughly speaking, the condition is a sufficiently weak coupling compared to the Debye frequency. However, such a weak coupling condition is much more restrictive than the one required by the Born approximation [11, 13, 25]. This can be easily understood by calculating the unperturbed and the interaction mean square energies. In fact, for $\hbar\omega_D \ll k_B T$ the former reads

$$\langle H_R^2\rangle \propto D^2(k_B T)^2\omega_D^6 \gg \langle H_S^2\rangle \propto \hbar^2 B^2 j^2\,, \tag{5.14}$$

while the latter reads

$$\langle H_{SR}^2\rangle = \sum_\alpha (|\lambda_\alpha^+|^2\langle a_\alpha^\dagger a_\alpha\rangle + |\lambda_\alpha^-|^2\langle a_\alpha a_\alpha^\dagger\rangle)\langle J_+J_-\rangle$$
$$+ \sum_\alpha (|\lambda_\alpha^-|^2\langle a_\alpha^\dagger a_\alpha\rangle + |\lambda_\alpha^+|^2\langle a_\alpha a_\alpha^\dagger\rangle)\langle J_-J_+\rangle\,, \tag{5.15}$$

and in the continuum limit

$$\langle H_{SR}^2\rangle \propto D\hbar\lambda_+^2 k_B T\omega_D j^2\,. \tag{5.16}$$

Then the Bornian weak coupling requires

$$\langle H_R^2\rangle + \langle H_S^2\rangle \gg \langle H_{SR}^2\rangle\,, \tag{5.17}$$

which is equivalent to

$$\frac{\hbar\lambda_+^2 j^2}{Dk_B T\omega_D^5} \ll 1\,. \tag{5.18}$$

This relation must be compared to the Markovian weak coupling (5.13b), which we may write as

$$\frac{\lambda_+^2 j^2 Dk_B T}{\hbar(\omega_D - B)} \ll 1\,. \tag{5.19}$$

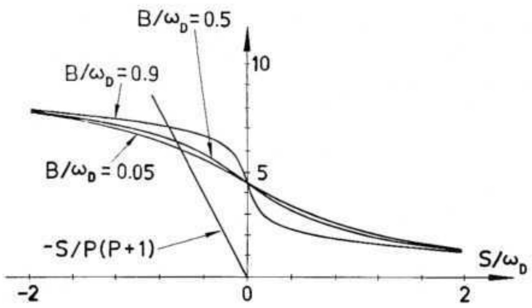

Fig. 3. Graphic solution of eq. (5.11). The function $\tilde{W}(s)$ (eq. (5.2′)) is plotted for different values of the relation B/ω_{D}.

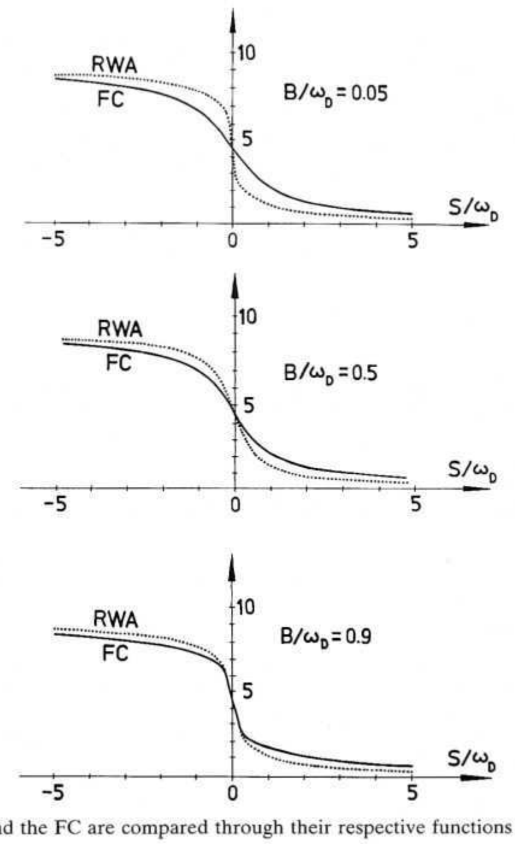

Fig. 4. The RWA and the FC are compared through their respective functions $\tilde{W}(s)$ (eq. (5.2)) for three values of B/ω_{D}.

Therefore, it becomes evident that (5.19) requires a much more weak interaction than (5.18). The Markovian relaxation frequencies are proportional to temperature and coupling strength (λ_+^2) as can be seen through eq. (5.13b).

If (5.19) is not fulfilled, the relaxation process is non-Markovian and its real frequencies can be graphically extracted through the intersections of the curve $\tilde{W}(s)$ (eq. (5.2′)) and the straight lines $-s/p(p+1)$ (eq. (5.11)). In fig. 3 we display this graphical method; thus the non-Markovian relaxation frequencies conserve the Markovian feature of being increasing functions of temperature, coupling strength and eigenvalue $[p(p+1)]$. However, the memory gives rise to a new effect: the frequencies increase with the parameter B/ω_D. In other words, the non-Markovian relaxation process is faster for a stronger magnetic field. We believe that this effect is closely related to the more rapid oscillations of the ITRs observed in fig. 1 for a higher B/ω_D. This fact is reflecting an interesting feature of the non-Markovian regime: the interplay between the correlation and the relaxation dynamics.

Let us finally test the validity of the RWA. In fig. 4 we have plotted $\tilde{W}(s)$ (eq. (5.2)) in the RWA ($\lambda_-^2 = 0$) and also for the proper FC ($\lambda_-^2 = \lambda_+^2$). Focusing upon the weak non-Markovian region $|s| \ll \omega_D$, we can appreciate that the RWA is very acceptable for strong magnetic fields ($B/\omega_D = 0.9$) and becomes poor for low ones ($B/\omega_D = 0.05$) as expected (cf. the discussion below eq. (5.5)).

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Appendix

Diagonalization of the collision matrix for $j = \frac{1}{2}, 1, \frac{3}{2}$.

a) $j = \frac{1}{2}$

$$\tilde{\phi}_0(0^+) = \begin{pmatrix} \tilde{W}_+ & -\tilde{W}_- \\ -\tilde{W}_+ & \tilde{W}_- \end{pmatrix};$$

then the eigenvalues are 0, $\tilde{W}_+ + \tilde{W}_-$. The respective eigenvectors (unnormalized) are

$$\begin{pmatrix} \beta \\ 1 \end{pmatrix}, \quad \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

and those of $[\tilde{\phi}_0(0^+)]^+$ are

$$\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \begin{pmatrix} 1 \\ -\beta \end{pmatrix},$$

where $\beta = \tilde{W}_-/\tilde{W}_+$. Notice that $\beta \cong 1$ corresponds to the high temperature limit (eq. (2.4)).

b) $j = 1$

$$\tilde{\phi}_0(0^+) = 2\begin{pmatrix} \tilde{W}_+ & -\tilde{W}_- & 0 \\ -\tilde{W}_+ & (\tilde{W}_+ + \tilde{W}_-) & -\tilde{W}_- \\ 0 & -\tilde{W}_+ & \tilde{W}_- \end{pmatrix}.$$

Eigenvalues: 0, $2(\tilde{W}_+ + \tilde{W}_- - \sqrt{\tilde{W}_+\tilde{W}_-})$, $2(\tilde{W}_+ + \tilde{W}_- + \sqrt{\tilde{W}_+\tilde{W}_-})$, with respective eigenvectors

$$\begin{pmatrix} \beta^2 \\ \beta \\ 1 \end{pmatrix}, \quad \begin{pmatrix} \sqrt{\beta} \\ 1-\sqrt{\beta} \\ -1 \end{pmatrix}, \quad \begin{pmatrix} \sqrt{\beta} \\ -1-\sqrt{\beta} \\ 1 \end{pmatrix}.$$

and for the adjoint matrix

$$\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad \begin{pmatrix} 1 \\ \sqrt{\beta}-\beta \\ -\beta\sqrt{\beta} \end{pmatrix}, \quad \begin{pmatrix} 1 \\ -\sqrt{\beta}-\beta \\ \beta\sqrt{\beta} \end{pmatrix}.$$

c) $j = \frac{3}{2}$

$$\tilde{\phi}_0(0^+) = \begin{pmatrix} 3\tilde{W}_+ & -3\tilde{W}_- & 0 & 0 \\ -3\tilde{W}_+ & 3\tilde{W}_- + 4\tilde{W}_+ & -4\tilde{W}_- & 0 \\ 0 & -4\tilde{W}_+ & 4\tilde{W}_- + 3\tilde{W}_+ & -3\tilde{W}_- \\ 0 & 0 & -3\tilde{W}_+ & 3\tilde{W}_- \end{pmatrix}.$$

General expressions are not readily available for this case; however in the high-temperature limit ($\tilde{W}_+ \cong \tilde{W}_- \equiv \tilde{W}$) it is easy to obtain eigenvalues 0, $2\tilde{W}$, $6\tilde{W}$, $12\tilde{W}$, with respective eigenvectors

$$\begin{pmatrix}1\\1\\1\\1\end{pmatrix}, \quad \begin{pmatrix}3\\1\\-1\\-3\end{pmatrix}, \quad \begin{pmatrix}1\\-1\\-1\\1\end{pmatrix}, \quad \begin{pmatrix}-1\\3\\-3\\1\end{pmatrix}.$$

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