DIFFERENT-TIME DECOUPLINGS FOR A MODEL ELECTRON-PHONON HAMILTONIAN

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Abstract

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It is known that time correlation functions contain sufficiently complete information about the properties of many-particle systems. Since for any real system their exact calculation is impossible, one studies a set of coupled equations containing higher correlation functions. The usual methods of decoupling higher correlation functions (or Green' s functions) in the theory of kinetic coefficients, ferromagnetism, etc., as is known ([1], [2]), lead to exponential damping for the corresponding correlation functions. In the theory of kinetic coefficients we thus arrive at a generalized kinetic equation, and the chosen approximation corresponds to the random-phase approximation.

A situation may arise, however, in which, in the sense of the problem, simple exponential damping is insufficient and a stronger dependence of $G(t)$ on t is required, for example a Gaussian-type dependence. It is well known ([3]) that in considering kinetic coefficients one can in principle distinguish two limiting cases: 1) the stochastic case, to which the generalized kinetic equation corresponds and, consequently, the above-mentioned method of decoupling higher correlation functions; and 2) the case in which dynamical coupling predominates. The second case corresponds to the main contribution at small times and can practically be realized, for example, for impurity conductivity, spin diffusion, and a broad class of transport phenomena in molecular crystals. In the case of electron-phonon interaction, a strong nonadiabatic coupling facilitates the realization of this type. In the simplest case we arrive at the so-called semiclassical approximation ([4]) (see also ([5])).

Recently Matsubara ([6]), by the method of functional derivatives, taking into account an infinite number of coupled equations for a model Hamiltonian, indeed obtained in the limiting case of high temperatures a Gaussian-type dependence. Matsubara' s method is rather complicated and does not lend itself to a simple generalization to other, more realistic Hamiltonians. Therefore the problem arises of obtaining a more convenient practically (and therefore less exact) way of improving the usual equal-time decoupling.

In the present work a so-called different-time decoupling is proposed, which, as it seems to us, satisfies the requirements stated above and in principle leads to more complete information than the corresponding equal-time decoupling. It is known (3) that the correlation function $\langle x(t) \mid x(0)\rangle$, where $x(t)$ obeys the equation

$$\dot{x} = i(\omega_0 + \omega'(t))x,$$

in the case of a Gaussian process is entirely determined by the behavior of $\langle \omega'(t) \mid \omega'(0)\rangle$. In equal-time decouplings this dependence is clearly not taken into account. One may hope that explicit allowance for this dependence in some form will have advantages in comparison with equal-time decouplings.

In the present work we take this dependence into account in the simplest form, carrying out a different-time decoupling in the second equation for the correlation function. Different-time decouplings are studied using the example of the simplest model Hamiltonian (6), which also admits an exact solution of the problem. Thus, in addition to estimating the accuracy of different-time decouplings, we obtain the possibility of investigating also the quality of the usual equal-time decouplings.

Consider the model Hamiltonian (6)

$$H = \omega_0 a^+ a + \omega \sum_q b_q^+ b_q + \sum_q A_q (b_q + b_q^+) a^+ a, \tag{1}$$

which describes the interaction of an electron with a set of harmonic oscillators of the same frequency. In formula (1), a^+, a are electron operators; b_q^+, b_q are the creation and annihilation operators of a phonon with momentum $\mathbf{q}$; ω is the frequency; A_q is the interaction constant. Instead of the phonon operators b_q, b_q^+, it is convenient to introduce the operators B and C, defined by the relations

$$B = \sum_q A_q (b_q + b_q^+), \qquad C = \sum_q A_q (b_q - b_q^+). \tag{2}$$

Equations of motion for the operators:

$$\begin{aligned} i\, da/dt &= \omega_0 a + Ba, \\ i\, dB/dt &= \omega C, \\ i\, dC/dt &= \omega B + 2A^2 a^+ a, \qquad A^2 = \sum_q A_q^2. \end{aligned} \tag{3}$$

The correlation function $\langle a^+(t) a(t')\rangle$ is to be calculated, where the operators are taken in the Heisenberg representation, and the symbol $\langle ... \rangle$ denotes averaging over the Gibbs canonical ensemble.

$$i\,\frac{d}{dt}\langle a^+(t)a(t')\rangle = -\omega_0\langle a^+(t)a(t')\rangle - \langle Ba^+|a\rangle, \tag{4}$$

$$i\,\frac{d}{dt'}\langle Ba^+|a\rangle = \omega_0\langle Ba^+|a\rangle + \langle Ba^+|Ba\rangle. \tag{5}$$

We use the decoupling

$$\langle Ba^+|Ba\rangle \simeq \langle B(t)B(t')\rangle\langle a^+(t)a(t')\rangle. \tag{6}$$

Denoting, for brevity, $\langle a^+(t)a(0)\rangle = e^{i\omega_0 t}G(t)$, we obtain for $G(t)$ the equation

$$\frac{d^2}{dt^2}G(t) + \langle B(t)B(0)\rangle G(t) = 0. \tag{7}$$

To calculate $\langle B(t)B(0)\rangle$, we introduce the Green function (^{1})

$$D = \langle\langle B(t)B(t')\rangle\rangle, \qquad \eta = -1, \tag{8}$$

$$i\,dD/dt = \delta(t-t')\,2\langle B^2\rangle + \omega\langle\langle C|B\rangle\rangle,$$

$$i\,\frac{d}{dt}\langle\langle C|B\rangle\rangle = \omega D + i\theta(t-t')\cdot 8A^4/\omega^2. \tag{9}$$

In writing (9) we have used the property of the model Hamiltonian: $a^+(t)a(t) = a^+(0)a(0)$. From (9) it follows that

$$\langle B(t)B(0)\rangle = 4A^4/\omega^2 + A^2\{\bar{n}e^{i\omega t} + (1+\bar{n})e^{-i\omega t}\}, \tag{10}$$

where $\bar{n} = 1/(\exp\beta\omega - 1)$.

Then equation (7) takes the form

$$G''(t) + G\left\{\frac{4A^4}{\omega^2} + A^2\left[\bar{n}e^{i\omega t} + (1+\bar{n})e^{-i\omega t}\right]\right\} = 0. \tag{11}$$

This is Mathieu’ s equation, and its solution in terms of known functions can be obtained in two limiting cases: $\omega t \ll 1$ and $\bar{n} \ll 1$. At short times and high temperatures the solution of equation (11) can be written in the form

$$G(t) = e^{-bt^2/2}\left\{{}_1F_1\left(\frac{b-a}{4b}, \frac{1}{2}, bt^2\right) + i\,\frac{2A^2}{\omega}\,t\,{}_1F_1\left(\frac{3b-a}{4b}, \frac{3}{2}, bt^2\right)\right\}; \tag{12}$$

here ${}_1F_1(...)$ is the confluent hypergeometric function; $a = 2A^2\bar{n}$; $b^2 = A^4\omega^2\bar{n}$.

In writing (12) the initial conditions were taken into account

$$G(0) = 1, \qquad iG'\big|_{t=0} = 2A^2/\omega. \tag{13}$$

The second of conditions (13) follows from the equations of motion (3). In the case of low temperatures the solution of (11) is a linear combination of the Bessel functions $J_{4iA^2}(2iAe^{-i\omega t/2}/\omega)$ and $J_{-4iA^2}(2iAe^{-i\omega t/2}/\omega)$. The unknown coefficients can again be found from (13).

As was already indicated, Hamiltonian (1), by virtue of its simplicity, makes it possible to obtain an exact expression for $G(t)$. Indeed, since $a^2 = 0$, $a^{+2} = 0$, $\langle a^+a\rangle = 1$, $\langle aa^+\rangle = 0$, we have

$$G(t) = \left\langle \exp itH \cdot \exp\left[-i\omega t\sum_q b_q^+ b_q\right]\right\rangle,$$

where by H we mean the expression $H = \omega\sum_q b_q^+ b_q + \hat{B}$. Expanding the operator expressions and carrying out the averaging (7), we obtain

$$G(t) = \exp\frac{A^2}{\omega^2}\left[\bar{n}e^{i\omega t} + (\bar{n}+1)e^{-i\omega t} - i\omega t\right] / \exp -\frac{A^2}{\omega^2}(2\bar{n}+1). \tag{14}$$

The exact correlation function sought satisfies the differential equation

$$G''(t) + G(t)\Big\{A^2[\bar{n}e^{i\omega t} + (\bar{n}+1)e^{-i\omega t}] + \frac{A^4}{\omega^2}[\bar{n}^2e^{2i\omega t} + (\bar{n}+1)^2e^{-2i\omega t} -$$

$$-2\bar{n}(\bar{n}+1) - 2\bar{n}e^{i\omega t} + 2(\bar{n}+1)e^{-i\omega t}]\Big\} = 0. \tag{15}$$

Comparison of (15) with (11) shows that, at high temperatures and strong coupling, different-time decouplings lead, for the Fourier transform of the correlation function sought, to a completely exact result. This becomes obvious if, in calculating the Fourier transform of (14), one uses the saddle-point method. At high temperatures the first saddle point, which determines the principal contribution, corresponds to the value $t \approx 0$; in the neighborhood of the saddle point, equations (15) and (11) coincide. Since the initial conditions (13) are specified at the same point, it follows that in this case different-time decouplings lead to a result coinciding with the exact one.

It is of interest to compare the results obtained with the results of equal-time decouplings for the same Hamiltonian. Constructing the equations for the correlation function with the aid of (3) and carrying out the decoupling $\langle Ba^+|a\rangle \approx \langle B\rangle\, a^+|a\rangle$, we obtain only one exponential

$$G^0(t) = \exp\left[-i\,\frac{2A^2}{\omega}\,t\right]. \tag{16}$$

Carrying out the decoupling at the next stage,

$$\langle BBa^+|a\rangle \approx \langle B^2\rangle\langle a^+|a\rangle, \qquad \langle Ca^+|a\rangle \approx \langle C\rangle\langle a^+|a\rangle,$$

we obtain already two exponentials

$$2G^0(t) = \left(1 + \frac{A^2}{\omega\Delta}\right)e^{i\Delta t} + \left(1 - \frac{A^2}{\omega\Delta}\right)e^{-i\Delta t}, \qquad \Delta = \langle B^2\rangle^{1/2}. \tag{17}$$

It is evident that simultaneous decoupling at any finite stage cannot lead, for example, to an expression of type (12).

Comparison of (17) with (12), and also comparison of both of them with (14), attests to the advantages of decouplings at different times. Of course, the results obtained are determined in many respects by the character of the Hamiltonian, and for real systems the situation for simultaneous decouplings will be more favorable. However, one may hope that for systems whose Hamiltonians are to some extent close to (1), the results obtained retain their meaning also for real systems. It is evident that Hamiltonian (1) is a limiting case of the Fröhlich Hamiltonian for semiconductors as the band width tends to zero. There are quite a few physical problems of this type. These include, for example, kinetic phenomena in molecular crystals, etc. Similar decouplings can also be applied in those cases where simultaneous ones are doomed in advance to failure. As an example one may cite the signal of free nuclear induction in a solid.

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Note: Figure translations are in progress. See original paper for figures.

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