Dynamical Decomposition of a Large System

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The equations for the statistical matrix ρ_θ and the correlation matrix $\rho_\theta(t_1,t_2)$ of a large system subject to time-dependent external forces are cast in a new form based on a continuation of Schrödinger's equation to complex times. It is shown that these equations also apply when the time dependence of the Hamiltonian is due to a coupling with another system (heat bath) which is at equilibrium at a temperature θ', but that such time dependence must be expressed in terms of random functions of the complex argument $z'=t-i/2\theta'$. A generalization to the case that the external time-dependent fields and the coupling with a heat bath exist simultaneously is straightforward and leads to a Schrödinger-type equation with non-Hermitian Hamiltonian which describes the dynamical and statistical aspects of the motion.

THE long-time behavior of a large system with time-independent Hamiltonian $\mathcal{H}$ is characterized by the statistical matrix

$$\rho_\theta=\exp(-\mathcal{H}/\theta). \tag{1}$$

The average of any operator F is given by

$$\langle F\rangle_\theta=\mathrm{Tr}F\rho_\theta/\mathrm{Tr}\rho_\theta. \tag{2}$$

The spontaneous fluctuations of the system are expressed by the correlation matrix

$$\rho_\theta(t_1,t_2)=W(t_1)\exp[-\mathcal{H}/\theta]W^\dagger(t_2), \tag{3}$$

where $W(t)$ is the unitary time-evolution matrix satisfying

$$i\partial W/\partial t=\mathcal{H}W(t),\quad W(0)=1. \tag{4}$$

The quantity

$$\langle F(t_1,t_2)\rangle_\theta=\mathrm{Tr}F\rho_\theta(t_1,t_2)/\mathrm{Tr}\rho_\theta(t_1,t_2) \tag{5}$$

will be called the correlation function of F.

As $\mathcal{H}$ is independent of t Eq. (4) gives $W=\exp(-i\mathcal{H}t)$ and therefore

$$\rho_\theta(t_1,t_2)=\exp[i(t_2-t_1)-1/\theta]\mathcal{H}. \tag{6}$$

It is useful to write this in terms of the complex variable

$$z=t-i/2\theta: \tag{7}$$

$$\rho_\theta(t_1,t_2)=W(z_1)W^\dagger(z_2^*), \tag{8}$$

$$idW(z)/dz=\mathcal{H}W(z),\quad W(0)=1. \tag{9}$$

The Eqs. (8) and (9) can be generalized readily to the case that the system is subject to time-dependent external forces. Let the Hamiltonian be of the form

$$\mathcal{H}(t)=\mathcal{H}+h(t),\quad h(t)=0(t\leqslant 0). \tag{10}$$

The statistical matrix satisfies

$$i\partial\rho_\theta/\partial t=[\mathcal{H}(t),\rho_\theta(t)]_-, \tag{11}$$

$$\rho_\theta(0)=\exp(-\mathcal{H}/\theta). \tag{12}$$

Equation (11) is solved by the matrix $\rho_\theta(t,t)$ obtained from Eq. (8) with Eq. (9) being replaced by

$$idW(z)/dz=\mathcal{H}(t)W(z), \tag{13}$$

$$W(0)=1. \tag{14}$$

The initial condition (14) differs from (12) because the intergral of Eq. (13) from $z=0$ $(t=i/2\theta)$ to $z=-i/2\theta$ $(t=0)$ contains contributions from $h(t)$. We are, however, interested in Eq. (11) in cases for which, after the transients near $t=0$ have died out, $\rho(t)$ is quasisteady for a long time. (Eventually, $h(t)$ will cause heating to indefinite temperatures.) For this purpose, $\mathcal{H}$ must belong to a system which includes a heat bath so large that, at the temperature θ, the absorption of energy from $h(t)$ during the transcient period causes a negligible rise in temperature. In this situation, Eqs. (14) and (12) give the same result beyond the transient region. The advantage of Eq. (14) will become evident in the following.

The corresponding unequal time operator $\rho_\theta(t_1,t_2)$ will be used as correlation matrix.

The question is now posed to what extent the exact value of quantities such as $\langle F\rangle_\theta$ and $\langle F(t_1,t_2)\rangle_\theta$ can be obtained from a calculation with a decomposed Hamiltonian. Let the dynamical variables of the system be separated in two groups, $p_i'q_i'$ and $p_k''q_k''$ (e.g., the spin and lattice variables of a magnetic system). A decomposition of $\mathcal{H}$ is here defined as the replacement:

$$\mathcal{H}(p'q'p''q'')\rightarrow\mathcal{H}'(p'q'\alpha_m')+\mathcal{H}''(p''q''\alpha_n''). \tag{15}$$

α_m' and α_n'' are suitably chosen parameters. As a correlation between the single and double primed variables is lacking in such a decomposed Hamiltonian, one can at most demand a faithful reproduction of operators which are likewise separated:

$$F(p,q)=F'(p'q')+F''(p''q''). \tag{16}$$

The case of a time-independent Hamiltonian will be considered first. An equal-time average $\langle F_\theta\rangle$ can be reproduced after a separation with constant values of α' and α''. The conditions are that, for all F' and F''

$$\langle F'+F''\rangle_\theta=\langle F'\rangle_{\theta,s}+\langle F''\rangle_{\theta,s}, \tag{17}$$

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where, e.g.,

$$\langle F'\rangle_{\theta,s}=\mathrm{Tr}F'\rho_\theta'/\mathrm{Tr}\rho_\theta', \tag{18}$$

$$\rho_\theta'=\exp(-\mathcal{H}'/\theta). \tag{19}$$

Values of α' and α'' which satisfy Eq. (17) can be found in principle, provided that their number is sufficiently large and that $\mathcal{H}'$ and $\mathcal{H}''$ are suitably chosen.

In order to obtain a faithful presentation of the correlation functions $\langle F(t_1,t_2)\rangle_\theta$, α' and α'' must be allowed to be random functions of time. In applying Eqs. (17) and (18), one has to replace Eq. (19) by an expression for $\rho_\theta'(t_1,t_2)$ valid for a randomly time-dependent $\mathcal{H}'$. The Eqs. (8) and (13) are not applicable in this case. They lead to a correlation matrix which contain t and θ separately, whereas the exact averages, according to Eq. (6), depend only on the variable $z_1-z_2^*$. This property can be retained after decomposition by making α' and α'' functions of the complex variable z:

$$\alpha'=\alpha'(z),\quad \alpha''=\alpha''(z). \tag{20}$$

This gives, e.g.,

$$\rho_\theta'(t_1,t_2)=\{W'(z_1)W'^\dagger(z_2^*)\}_{\mathrm{av}}, \tag{21}$$

$$idW'(z)/dz=\mathcal{H}'(z)W'(z),\quad W(0)=1. \tag{22}$$

"av" indicates the long time average with constant t_1-t_2 which is needed on account of the random changes of $\alpha'(z)$ and which makes ρ_θ' a function of $z_1-z_2^*$ only. Equations (17), (21), and (22) give a set of relations from which one may hope that the random functions $\alpha'(t)$ and $\alpha''(t)$ can be determined.

The appearance of $\mathcal{H}(t)$ in the coupling with external fields, Eq. (13), and of $\mathcal{H}(t-i/2\theta)$ in the coupling with another system with temperature θ, Eq. (22), in otherwise identical equations, allows for an interesting interpretation. The application of external fields, e.g., of frequency ω, is by and large equivalent to coupling the system with another system of a very high temperature, through a filter which, e.g., passes only the frequency ω, the temperatures being such that the blackbody radiation at frequency ω has the same intensity as the applied field. Equations (13) and (22) can be unified to

$$idW(z)/dz=\mathcal{H}(z')W(z), \tag{23}$$

$$z'=z-i/2\theta'+i/2\theta, \tag{24}$$

where θ' is the temperature of the system causing the time dependence of $\mathcal{H}$ and θ is the initial temperature of the system described by Eq. (23).

This interpretation shows how to decompose a system in the presence of time-dependent forces, acting, e.g., on the primed variables. The Hamiltonian

$$\mathcal{H}(t)=\mathcal{H}(p'q'p''q'')+h'(p'q't) \tag{25}$$

is replaced by

$$\mathcal{H}(t)\to\mathcal{H}'(p'q'\alpha'(z))+h'(p'q't)+\mathcal{H}''(p''q''\alpha''(z)). \tag{26}$$

The statistical matrix for the primed system is obtained from Eq. (21) with

$$idW'/dz=(\mathcal{H}'(z)+h'(t))W'(z), \tag{27}$$

showing the coupling with the double primed system which has the temperature θ, and with a fictitious system at $\theta=\infty$. But Eq. (27) will be valid only if the applied fields do not destroy the thermal equilibrium (at temperature θ) of the double primed system. This imposes a restriction which, though clear from a physical point of view, may be involved mathematically.

Finally, it is of interest to obtain the high-θ approximation of Eqs. (21) and (27). One has:

$$W'(z)=W'(t)-(i/2\theta)\partial W'/\partial t+\cdots, \tag{28}$$

$$i\partial W'/\partial t=(\mathcal{H}'(t)+h'(t)+(i/2\theta)dh'/dt+\cdots)W'(t). \tag{29}$$

Therefore, to first order in $1/\theta$

$$\begin{aligned}\rho_\theta'(t_1,t_2)\approx\langle&\exp\{-[\mathcal{H}'(t_1)+h'(t_1)]/2\theta\}W'(t_1)W'^\dagger(t_2)\\&\times\exp\{-[\mathcal{H}'(t_2)+h'(t_2)]/2\theta\}\rangle_{\mathrm{av}}.\end{aligned} \tag{30}$$

Owing to the anti-Hermitian term in Eq. (29), W' is nonunitary, and the (approximate) equal time value of ρ_θ' obtained from Eq. (30) does not reduce to $\exp[-(\mathcal{H}'+h')/\theta]$. The term idh'/dt corresponds to absorption, while the change in the form of ρ_θ' corresponds to a deviation from equilibrium of the primed system.

In the following paper Eq. (30) is used to derive the modified Bloch equations for a spin system. An application to the Overhauser effect is in progress.

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