# Stochastic symmetry breaking of time reversal invariance

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An equation for the time evolution of the density matrix for a nonrelativistic quantum mechanical system is presented. It involves a Hamiltonian which contains a stochastic contribution. Before stochastic averaging is performed, it is shown that the density matrix equation is time reversal invariant, whereas after stochastic averaging is performed, it is shown that the averaged density matrix equation is not time reversal invariant.

In a series of three papers[1,2,3] a new approach to the theory of non-equilibrium statistical mechanics has been presented. The approach is based upon the mathematical theory of multiplicative stochastic processes.[1] Within this context it has been possible to derive an averaged density matrix equation which shows time irreversible behavior,[1] to prove an H-theorem,[2] and to characterize the approach to equilibrium for microcanonical and canonical ensembles.[3] In this paper, the relationship between time reversible and time irreversible behavior will be considered from the viewpoint of the time reversal operation of quantum mechanics.

The Schrödinger–Heisenberg picture of quantum mechanics may be expressed by the equation

$$i\frac{d}{dt}C_\alpha(t)=\sum_\beta M_{\alpha\beta}C_\beta(t), \tag{1}$$

where $M^*_{\beta\alpha}=M_{\alpha\beta}$. In the following the repeated index summation convention will be used. When a stochastic contribution to the Hamiltonian is considered, (1) becomes

$$i\frac{d}{dt}C_\alpha(t)=M_{\alpha\beta}C_\beta(t)+\tilde{M}_{\alpha\beta}(t)C_\beta(t), \tag{2}$$

where $\tilde{M}^*_{\beta\alpha}(t)=\tilde{M}_{\alpha\beta}(t)$. The stochastic properties of $\tilde{M}_{\alpha\beta}(t)$ are those appropriate for a purely random, Gaussian stochastic matrix.[1] The first two averaged moments are given by

$$\langle\tilde{M}_{\alpha\beta}(t)\rangle=0, \tag{3}$$

$$\langle\tilde{M}_{\alpha\beta}(t)\tilde{M}_{\mu\nu}(S)\rangle=2Q_{\alpha\beta\mu\nu}\delta(t-s). \tag{4}$$

Equation (2) leads to a density matrix equation. The density matrix $\rho_{\alpha\beta}(t)$ is defined by

$$\rho_{\alpha\beta}(t)\equiv C^*_\alpha(t)C_\beta(t), \tag{5}$$

and (2) with (5) gives

$$i\frac{d}{dt}\rho_{\alpha\beta}(t)=L_{\alpha\beta\mu\nu}\rho_{\mu\nu}(t)+\tilde{L}_{\alpha\beta\mu\nu}(t)\rho_{\mu\nu}(t), \tag{6}$$

where $L_{\alpha\beta\mu\nu}$ and $\tilde{L}_{\alpha\beta\mu\nu}(t)$ are defined by

$$L_{\alpha\beta\mu\nu}\equiv\delta_{\alpha\mu}M_{\beta\nu}-\delta_{\beta\nu}M^*_{\alpha\mu}, \tag{7}$$

$$\tilde{L}_{\alpha\beta\mu\nu}(t)\equiv\delta_{\alpha\mu}\tilde{M}_{\beta\nu}(t)-\delta_{\beta\nu}\tilde{M}^*_{\alpha\mu}(t). \tag{8}$$

It has been proved[1] that stochastic averaging of (6) leads to

$$\frac{d}{dt}\langle\rho_{\alpha\beta}(t)\rangle=-iL_{\alpha\beta\mu\nu}\langle\rho_{\mu\nu}(t)\rangle-R_{\alpha\beta\mu\nu}\langle\rho_{\mu\nu}(t)\rangle, \tag{9}$$

where $R_{\alpha\beta\mu\nu}$ is defined by

$$R_{\alpha\beta\mu\nu}\equiv\delta_{\alpha\mu}Q_{\beta\theta\theta\nu}+\delta_{\beta\nu}Q_{\theta\alpha\mu\theta}-Q_{\beta\nu\mu\alpha}-Q_{\mu\alpha\beta\nu} \tag{10}$$

and $\sum_\alpha\langle\rho_{\alpha\alpha}(t)\rangle=1$ for all $t$. It has also been proved,[2] on the basis of the properties of $R_{\alpha\beta\mu\nu}$, that if $H(t)$ is defined by

$$H(t)\equiv\mathrm{Tr}\,[\langle\rho(t)\rangle\log_e\langle\rho(t)\rangle], \tag{11}$$

then

$$\frac{d}{dt}H(t)\leqslant 0. \tag{12}$$

While (12) clearly demonstrates the time irreversibility of (9), the time reversibility of (6) remains to be demonstrated.

## TIME REVERSAL INVARIANCE

If the Schrödinger equation for a single particle in a potential field is given by

$$ih\frac{\partial}{\partial t}\Psi(rt)=\left(-\frac{h^2}{2m}\nabla^2+V(r)\right)\Psi(r,t), \tag{13}$$

then the time reversal operation is accomplished by simultaneously complex conjugating every term in (13) and replacing all instances of $t$ by $-t$.[4] Doing this to (13) gives

$$-i\hbar\frac{\partial}{-\partial t}\Psi^*(r,-t)=\left(-\frac{\hbar^2}{2m}\nabla^2+V(r)\right)\Psi^*(r,-t). \tag{14}$$

It is seen that $\Psi^*(r,-t)$ also satisfies the original Schrödinger equation. This is the condition of time reversal invariance.

Suppose that a complete, orthonormal set of complex basis functions, $\varphi_k(r)$, are introduced satisfying the conditions

$$\int\varphi^*_k(r)\varphi_l(r)dr=\delta_{kl}. \tag{15}$$

By introducing the definitions

$$\Psi(r,t)\equiv\sum_l C_l(t)\varphi_l(r) \tag{16}$$

and

$$H_{kl}\equiv\int\varphi^*_k(r)\left[-\left(\frac{\hbar^2}{2m}\right)\nabla^2+V(\mathbf{r})\right]\varphi_l(r)dr, \tag{17}$$

Eq. (13) becomes, upon multiplication by $\varphi^*_k(r)$ and integration over all $r$,

$$i\hbar\frac{d}{dt}C_k(t)=H_{kl}C_l(t). \tag{18}$$

Generally, (17) also implies $H^*_{lk}=H_{kl}$.

When applied to (18), the time reversal operation leads to

$$-i\hbar\frac{d}{-dt}C^*_k(-t)=H^*_{kl}C^*_l(-t). \tag{19}$$

This is the same as the result achieved from (14) by multiplication by $\varphi_k(\mathbf{r})$ followed by integration over all $\mathbf{r}$. The complex conjugate of (17) provides for the $H^*_{kl}$ in (19).

Therefore, in matrix notation, the condition for time reversal invariance of (18) is that $C^*_k(-t)$ satisfies

$$i\frac{d}{dt}C^*_k(-t) = H^*_{kl}C^*_l(-t), \tag{20}$$

which is equivalent to (19). The presence of $H^*_{kl}$ in (20) instead of $H_{kl}$ should be noted, and reflects the antilinear character of the time reversal operation.

## KUBO OSCILLATOR

Before proceeding to the consideration of the time reversal properties of (6), it is instructive to consider a simple, special case, the Kubo oscillator[1]:

$$\frac{d}{dt}a(t) = i\,[\omega_0 + \tilde{\varphi}(t)]a(t), \tag{21}$$

where $a(t)$ is complex and $\tilde{\varphi}(t)$ is a purely random, Gaussian stochastic frequency fluctuation with average value zero and second moment given by

$$\langle\tilde{\varphi}(t)\tilde{\varphi}(s)\rangle = 2\lambda\delta(t-s). \tag{22}$$

The oscillator equation (21) is a one-component special case of (18). Because the $H_{kl}$ in (18) is Hermitian, in the one-component case $H_{kl}\to H$ which must be real. In (21) the analog of $H$ is $\omega_0 + \tilde{\varphi}(t)$ which is also real.

The time reversal operation applied to (21) gives

$$-\frac{d}{dt}a^*(-t) = -i\,[\omega_0 + \tilde{\varphi}(-t)]a^*(-t). \tag{23}$$

If the $\tilde{\varphi}(t)$ in (21) and the $\tilde{\varphi}(-t)$ in (23) were not present, then time reversibility of (21) would be proved by (23). However, because of the presence of $\tilde{\varphi}(t)$ in (21) and $\tilde{\varphi}(-t)$ in (23), it is necessary that $\tilde{\varphi}(t) = \tilde{\varphi}(-t)$ in order for time reversal invariance to obtain.

If $\tilde{\varphi}(t)$ were an ordinary, nonstochastic function, then $\tilde{\varphi}(t) = \tilde{\varphi}(-t)$ would require that $\tilde{\varphi}(t)$ be an even function of $t$. It will be shown that $\tilde{\varphi}(t)$ is not an even function of $t$, but that $\tilde{\varphi}(t) = \tilde{\varphi}(-t)$ anyway, because of the stochastic properties of $\tilde{\varphi}(t)$.

Consider the time interval from $-T$ to $+T$. $\tilde{\varphi}(t)$ may be given a Fourier representation in the interval $(-T, +T)$ by[5]

$$\tilde{\varphi}(t) = \sum_k\,[\tilde{a}_k\cos(\omega_k t) + \tilde{b}_k\sin(\omega_k t)], \tag{24}$$

where $\omega_k = k\pi/T$, and the $\tilde{a}_k$'s and $\tilde{b}_k$'s are all independent, Gaussianly distributed stochastic coefficients. Now, from (24) it is seen that

$$\tilde{\varphi}(-t) = \sum_k[\tilde{a}_k\cos(\omega_k t) - \tilde{b}_k\sin(\omega_k t)]. \tag{25}$$

Therefore, the equality $\tilde{\varphi}(t) = \tilde{\varphi}(-t)$ requires that $\tilde{b}_k = -\tilde{b}_k$.

For ordinary, nonstochastic variables, $X = -X$ implies $X = 0$. For stochastic variables other possibilities exist. The $\tilde{b}_k$'s are completely characterized by their Gaussian distribution functions:

$$W(b_k) = (1/\sqrt{4\pi\lambda})\exp(b_k^2/4\lambda). \tag{26}$$

Two stochastic variables are equal if and only if their distribution functions are equal. Clearly, for Gaussian distributions such as (26) it follows that $\tilde{b}_k = -\tilde{b}_k$, without $\tilde{b}_k = 0$ having to hold. Therefore

$$\tilde{\varphi}(t) = \tilde{\varphi}(-t) \tag{27}$$

and using (27) in (23) leads to

$$\frac{d}{dt}a^*(-t) = i[\omega_0 + \tilde{\varphi}(t)]a^*(-t), \tag{28}$$

which is a special case of (20), and confirms time reversal invariance of (21).

It should be observed that if (21) is averaged,[1] the result is

$$\frac{d}{dt}\langle a(t)\rangle = i\omega_0\langle a(t)\rangle - \lambda\langle a(t)\rangle, \tag{29}$$

which is definitely not time reversible since the time reversal operation leads to

$$\frac{d}{dt}\langle a(-t)\rangle^* = i\omega_0\langle a(-t)\rangle^* + \lambda\langle a(-t)\rangle^* \tag{30}$$

and $\langle a(-t)\rangle^*$ does not satisfy the appropriate time reversed equation because of the dissipative $\lambda$-dependent term.

## DENSITY MATRIX

The results for the Kubo oscillator may be straightforwardly generalized for the consideration of the density matrix as follows. The time reversal operation, when applied to (6), leads to

$$-i\frac{d}{-dt}\rho^*_{\alpha\beta}(-t) = L^*_{\alpha\beta\mu\nu}\rho^*_{\mu\nu}(-t) + \tilde{L}^*_{\alpha\beta\mu\nu}(-t)\rho^*_{\mu\nu}(-t). \tag{31}$$

If the stochastic terms in (6) and (31) are omitted, consideration of (5), (7), and (20) verifies time reversal invariance. However, the presence of the stochastic terms requires that

$$\tilde{L}^*_{\alpha\beta\mu\nu}(-t) = \tilde{L}^*_{\alpha\beta\mu\nu}(t) \tag{32}$$

in order for time reversal invariance to be satisfied. This is the density matrix analog of (27).

In order to check the validity of (32), (8) may be used to see that (32) is equivalent to

$$\tilde{M}_{\alpha\beta}(-t) = \tilde{M}_{\alpha\beta}(t). \tag{33}$$

Therefore, it remains to prove the validity of (33). Again consider the time interval $(-T, +T)$. A Fourier representation for $\tilde{M}_{\alpha\beta}(t)$ is possible:

$$\tilde{M}_{\alpha\beta}(t) \equiv \sum_k[\tilde{a}^k_{\alpha\beta}\cos(\omega_k t) + \tilde{b}^k_{\alpha\beta}\sin(\omega_k t)], \tag{34}$$

where $\omega_k = k\pi/T$, and the $\tilde{a}_{\alpha\beta}$'s and $\tilde{b}_{\alpha\beta}$'s are Gaussianly distributed stochastic matrix coefficients satisfying the conditions

$$\langle\tilde{a}^k_{\alpha\beta}\tilde{b}^l_{\mu\nu}\rangle = 0 \quad \text{for all } k, l, \alpha, \beta, \mu, \text{and } \nu, \tag{35}$$

$$\langle\tilde{a}^k_{\alpha\beta}\tilde{a}^l_{\mu\nu}\rangle = 2\delta_{kl}Q_{\alpha\beta\mu\nu}, \quad \langle\tilde{b}^k_{\alpha\beta}\tilde{b}^l_{\mu\nu}\rangle = 2\delta_{kl}Q_{\alpha\beta\mu\nu},$$

These conditions lead to (4). Returning to (34) we see that (33) will be satisfied if and only if

$$\tilde{b}^k_{\alpha\beta} = -\tilde{b}^k_{\alpha\beta}, \tag{36}$$

which is the analog of $\tilde{b}_k = -\tilde{b}_k$ in the Kubo oscillator case. Equation (36) is true because the $\tilde{b}^k_{\alpha\beta}$'s are Guassianly distributed. Therefore, it has been demonstrated that (31) leads to

$$i\frac{d}{dt}\rho^*_{\alpha\beta}(-t) = L^*_{\alpha\beta\mu\nu}\rho^*_{\mu\nu}(-t) + \tilde{L}^*_{\alpha\beta\mu\nu}(t)\rho^*_{\mu\nu}(-t), \quad (37)$$

which is the time reversal invariant equation corresponding with (6). Application of the time reversal operation to (9), however, leads to time reversal noninvariance because of the dissipative $R_{\alpha\beta\mu\nu}$ term in (9). Of course, the time irreversible nature of (9) is already evident in (12).

## SUMMARY

It has been proved that the addition of a purely random, Guassian stochastic contribution to the Hamiltonian of a quantum mechanical system leads to a density matrix equation which is time reversal invariant if stochastic averaging is not performed, but which is time reversal noninvariant if stochastic averaging is performed. The key reason behind this result is the special property of Gaussian stochastic variables that they are equal to their own negatives without having to be zero. This follows from consideration of the distribution function for a Gaussian stochastic variable.

The implications of this theory for nonequilibrium statistical mechanics have already been discussed in earlier publications.[1,2,3] Whether or not stochastic symmetry breaking of time reversal invariance has significance in relativistic quantum mechanics and particle physics invites consideration.

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