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Quantum Fokker–Planck equation

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Abstract. The dynamics of quantum systems subject to dissipation is a subject of fundamental importance which has recently been of great interest due to its relation to macroscopic quantum phenomena. In particular the behaviour of the magnetic flux trapped in a SQUID is an example of this.

We derive the quantum mechanical analogue of the Fokker–Planck equation which describes such systems. The major difference between the quantum and classical Fokker–Planck equations arises from the presence of a quantum mechanical memory term.

Quantum Brownian motion is a subject which has been studied on account of its intrinsic and fundamental interest (Benguria and Kac 1981). Recently however, it has been of even greater interest due to its relation to macroscopic quantum phenomena. The example we have in mind is the behaviour of the magnetic flux trapped within a SQUID (Caldeira and Leggett 1983a) and this in fact provided the motivation for this work.

In this paper we derive the quantum mechanical generalisation of the Fokker–Planck (FP) equation. There exists a previous attempt at this (Iche and Nozières 1978) as well as high-temperature calculations relating to the FP equation (Caldeira and Leggett 1983b) and the Langevin equation (Schmid 1982).

We note here that the method we use to derive the quantum FP equation has an applicability much more general than the specific case considered.

A system composed of a single degree of freedom (the 'particle') interacting with a collection of harmonic oscillators (the 'environment') has been used as a model of dissipation (Caldeira and Leggett 1983a,b).

The Hamiltonian is‡

$$H = \frac{p^2}{2m} + V(q) + \sum_\alpha \left[\frac{\pi_\alpha^2}{2m_\alpha} + \frac{m_\alpha \omega_\alpha^2}{2}\left(x_\alpha - \frac{c_\alpha q}{m_\alpha \omega_\alpha^2}\right)^2\right]. \tag{1}$$

It describes the particle (coordinate q) moving in a potential $V(q)$ and interacting linearly with the harmonic oscillators (c_α being the coupling constants).

Using influence functional theory (Feynman and Vernon 1963) and making the assumptions: (1) only after time $t = 0$ were the particle and environment interacting

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‡ Note that we have explicitly included a counter-term in the Hamiltonian from the outset (Caldeira and Leggett 1983a).

(hence the density matrix factorised at $t=0$); (2) the environment was, at $t=0$, in thermal equilibrium at temperature $T=\hbar/k_B\tau$, Caldeira and Leggett (1983b) derived the time evolution equation for the reduced density matrix describing the particle alone:

$$\rho(q_1, q_2, t) = \int J(q_1 q_2 t | q_1' q_2' 0)\rho(q_1' q_2' 0)\, \mathrm{d}q_1'\, \mathrm{d}q_2' \tag{2}$$

with the propagator $J(q_1 q_2 t|q_1' q_2' 0)$ given by the path integral

$$J(q_1 q_2 t|q_2' q_2' 0) = \int_{q_1',0}^{-q_1,t} \mathrm{d}[q] \int_{q_2',0}^{-q_2,t} \mathrm{d}[r] \exp[\mathrm{i}(S[q,t] - S[r,t])/\hbar]\, F[q,r;t] \tag{3}$$

with

$$S[q,t] = \int_0^t \mathrm{d}u\, [(m\dot{q}^2/2) - V(q)] \tag{4}$$

and

$$\begin{aligned} F[q,r;t] = \exp &- (\mathrm{i}/\hbar)(q_1' + q_2') \int_0^t \mathrm{d}u\, Q_1(u)[q(u) - r(u)] \\ &\times \exp - (\mathrm{i}/\hbar) \int_0^t \mathrm{d}u \int_0^u \mathrm{d}v [q(u) - r(u)][\dot{q}(v) + \dot{r}(v)] Q_1(u-v) \\ &\times \exp - (1/\hbar) \int_0^t \mathrm{d}u \int_0^u \mathrm{d}v [q(u) - r(u)][q(v) - r(v)] Q_2(u-v). \end{aligned} \tag{5}$$

The functions $Q_1(u)$, $Q_2(u)$ are written in terms of the spectral density

$$J(\omega) \equiv \frac{\pi}{2} \sum_k \frac{c_k^2}{m_k \omega_k} \delta(\omega - \omega_k) \tag{6}$$

as

$$Q_1(u) \equiv \int_0^\infty \frac{\mathrm{d}\omega}{\pi} \frac{J(\omega)}{\omega} \cos \omega u \tag{7}$$

and

$$Q_2(u) \equiv \int_0^\infty \frac{\mathrm{d}\omega}{\pi} J(\omega) \coth\left(\frac{\omega\tau}{2}\right) \cos \omega u \qquad (\tau \equiv \hbar/k_B T). \tag{8}$$

We shall now present our own work.

Firstly we derive the equation of motion that the propagator obeys. Let us note that the group property for $J(q_1 q_2 t|q_1' q_2' 0)$ cannot be used in this derivation since for general temperatures and spectral densities it does not possess this property:

$$J(q_1 q_2 t|q_1' q_2' 0) \neq \int J(q_1 q_2 t|q_1'' q_2'' t_1) J(q_1'' q_2'' t_1|q_1' q_2' 0)\, \mathrm{d}q_1''\, \mathrm{d}q_2''. \tag{9}$$

We begin with equation (5). Time integrations are split into two parts $\int_0^{t-\varepsilon}$ and $\int_{t-\varepsilon}^t$. We quickly find that to order ε

$$F[q,r;t] = \Big(1 - (\mathrm{i}\varepsilon/\hbar)(q_1' + q_2')(q_1 - q_2)Q_1(t)$$

$$- (\mathrm{i}\varepsilon/\hbar)(q_1 - q_2)\int_0^t \mathrm{d}u\, Q_1(t-u)[\dot{q}(u) + \dot{r}(u)]$$

$$- (\varepsilon/\hbar)(q_1 - q_2)\int_0^t \mathrm{d}u\, Q_2(t-u)[q(u) - r(u)]\Big)\, F[q,r;t-\varepsilon]. \qquad (10)$$

In order to see the effects of varying the time period in the path integrals in equation (3) we consider the simpler object:

$$K(q_B, q_A; t) = \int_{q_A,0}^{q_B,t} \mathrm{d}[q]\, \exp(\mathrm{i}S[q,t]/\hbar)G[q;t] \qquad (11)$$

with G an arbitrary functional of q. Utilising the definition of the path integral as a multiple integral (Feynman and Hibbs 1965) we can write equation (11) as ($\varepsilon \to 0_+$)

$$K(q_B, q_A; t) = \int_{-\infty}^{\infty} \frac{\mathrm{d}q_{N-1}}{A} \exp\left\{\frac{\mathrm{i}\varepsilon}{\hbar}\left[\frac{m}{2}\left(\frac{q_B - q_{N-1}}{\varepsilon}\right)^2 - V(q_B)\right]\right\}$$

$$\times \int_{q_1,0}^{q_{N-1},t-\varepsilon} \exp(\mathrm{i}S[q,t-\varepsilon]/\hbar)G[q;t] \qquad (12)$$

with

$$A \equiv \left(\frac{2\pi\mathrm{i}\hbar\varepsilon}{m}\right)^{1/2}.$$

Noting that for any function $f(q)$,

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}q_{N-1}}{A} \exp\left[\frac{\mathrm{i}\varepsilon}{\hbar}\left(\frac{m}{2}\right)\left(\frac{q_B - q_{N-1}}{\varepsilon}\right)^2\right] f(q_{N-1})$$

$$= \left(1 + \frac{\mathrm{i}\varepsilon\hbar}{2m}\frac{\partial^2}{\partial q_B^2}\right) f(q_B) + \mathrm{O}(\varepsilon^2) \qquad (13)$$

we can write equation (12) as

$$K(q_B, q_A; t) = \left\{1 - \mathrm{i}\frac{\varepsilon}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q_B^2} + V(q_B)\right)\right\}$$

$$\times \int_{q_A,0}^{q_B,t-\varepsilon} \mathrm{d}[q]\, \exp(\mathrm{i}S[q,t-\varepsilon]/\hbar)G[q,t] + \mathrm{O}(\varepsilon^2). \qquad (14)$$

Equation (14) generalises in a straightforward way to apply to equation (3). Using, therefore, equations (3), (10) and (14) we obtain to $\mathrm{O}(\varepsilon)$

$$J(q_1 q_2 t|q_1' q_2' 0) = [1 - (\mathrm{i}\varepsilon/\hbar)(q_1' + q_2')(q_1 - q_2)Q_1(t) - (\mathrm{i}\varepsilon/\hbar)(H_{q_1} - H_{q_2})]$$

$$\times J(q_1 q_2 t - \varepsilon|q_1' q_2' 0) - \frac{\mathrm{i}\varepsilon}{\hbar}(q_1 - q_2)\int_0^t \mathrm{d}u\, Q_1(t-u)\int_{q_1,0}^{q_1,(t-\varepsilon)} \mathrm{d}[q]$$

$$\times \int_{q_2',0}^{q_2,(t-\varepsilon)} \mathrm{d}[r][\dot{q}(u) + \dot{r}(u)]\exp[\mathrm{i}(S[q,t-\varepsilon] - S[r,t-\varepsilon])/\hbar]$$

$$
\begin{aligned}
&\times F[q,r;t-\varepsilon] - \frac{\varepsilon}{\hbar}(q_1-q_2)\int_0^t \mathrm{d}u\, Q_2(t-u) \\
&\times \int_{q_1',0}^{q_1,(t-\varepsilon)} \mathrm{d}[q] \int_{q_2',0}^{q_2,t-\varepsilon} \mathrm{d}[r]\,[q(u)-r(u)] \\
&\times \exp[\mathrm{i}(S[q,t-\varepsilon]-S[r,t-\varepsilon])/\hbar]F[q,t;t-\varepsilon]
\end{aligned} \tag{15}
$$

where we have used the notation $H_q \equiv -(\hbar^2/2m)(\partial^2/\partial q^2) + V(q)$.

The time evolution for the propagator now follows from equation (15):

$$
\begin{aligned}
\mathrm{i}\hbar\frac{\partial}{\partial t}J(q_1q_2t|q_1'q_2'0) &= (H_{q_1}-H_{q_2})J(q_1q_2t|q_1'q_2'0) \\
&+ (q_1'+q_2')(q_1-q_2)Q_2(t)J(q_1q_2t|q_1'q_2'0) \\
&+ (q_1-q_2)\int_0^t \mathrm{d}u\, Q_1(t-u)\int_{q_1',0}^{q_1,t}\mathrm{d}[q]\int_{q_2',0}^{q_2,t}\mathrm{d}[r]\,[\dot{q}(u)+\dot{r}(u)] \\
&\times \exp[\mathrm{i}(S[q,t]-S[r,t])/\hbar]\,F[q,r;t] \\
&- \mathrm{i}(q_1-q_2)\int_0^t \mathrm{d}u\, Q_2(t-u)\int_{q_1',0}^{q_1,t}\mathrm{d}[q]\int_{q_2',0}^{q_2,t}\mathrm{d}[r]\,[q(u)-r(u)] \\
&\times \exp[\mathrm{i}(S[q,t]-S[r,t])/\hbar]\,F[q,r;t].
\end{aligned} \tag{16}
$$

Note that the boundary condition upon J is

$$
\lim_{t\to 0} J(q_1q_2t|q_1'q_2'0) = \delta(q_1-q_1')\delta(q_2-q_2'). \tag{17}
$$

Equation (16) holds for arbitrary spectral densities $J(\omega)$. In order to achieve the classical Brownian motion limit (friction force $= -\eta\dot{q}$) it is sufficient to take, for low frequencies, $J(\omega) = \eta\omega$ (Caldeira and Leggett 1983b). We take, for all frequencies

$$
J(\omega) = \eta\omega\exp(-\omega/\omega_c). \tag{18}
$$

Here ω_c is a high-frequency cut-off of the environment—assumed to be much larger than typical frequencies of the classical motion.

Let us note in passing that had we chosen $J(\omega) \propto \omega^3\exp(-\omega/\omega_D)$ with ω_D the Debye frequency, equation (16) would apply to tunnelling states in insulating glasses (Anderson *et al* 1972, Phillips 1972).

Equations (7) and (18) yield for $Q_1(u)$

$$
Q_1(u) = \eta\frac{1}{\pi}\frac{\omega_c^{-1}}{\omega_c^{-2}+u^2} \simeq \eta\delta(u). \tag{19}
$$

For $Q_2(u)$ we write

$$
\coth\frac{\omega\tau}{2} = \frac{2}{\omega\tau} + \left(\coth\frac{\omega\tau}{2} - \frac{2}{\omega\tau}\right)
$$

hence equation (8) gives

$$
Q_2(u) = \frac{2}{\tau}Q_1(u) + R(u) \tag{20}
$$

with

$$R(u) \equiv \int_0^\infty \frac{d\omega}{\pi}\, \eta\omega \exp(-\omega/\omega_c) \left(\coth\frac{\omega\tau}{2} - \frac{2}{\omega\tau}\right) \cos\omega u$$

$$\simeq \frac{\eta}{\pi}\left\{\frac{\omega_c^{-2} - u^2}{(\omega_c^{-2} + u^2)^2} - \frac{2}{\tau}\frac{\omega_c^{-1}}{\omega_c^{-2} + u^2} + \left[\frac{1}{u^2} - \left(\frac{\tau}{\pi}\sinh\frac{\pi u^2}{\tau}\right)^{-1}\right]\right\}. \qquad (21)$$

The last form for $R(u)$ is obtained by approximating $[\coth(\omega\tau/2)-1]\exp(-\omega/\omega_c) + \exp(-\omega/\omega_c)$ by $[\coth(\omega\tau/2) - 1] + \exp(-\omega/\omega_c)$ and hence holds for $\omega_{c\tau} \gg 1$.

To obtain the quantum Fokker–Planck equation from equation (16) we use equation (2) to 'fold in' an initial density matrix. Additionally we use the delta function approximation for $Q_1(u)$ in equations (19) and (20) and the initial condition given by equation (17). We obtain:

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\rho(q_1 q_2 t) &= (H_{q_1}(t) - H_{q_2}(t))\,\rho(q_1 q_2, t) + \eta(q_1^2 - q_2^2)\,\delta(t)\rho(q_1 q_2, t) \\ &\quad + \frac{\eta}{2m}(q_1 - q_2)(\hat{p}_1 - \hat{p}_2)\rho(q_1 q_2, t) - \frac{i\eta}{\tau}(q_1 - q_2)^2\rho(q_1 q_2, t) \\ &\quad - i(q_1 - q_2)\int_0^t du\, R(t-u)\frac{\hbar}{i}\frac{\delta}{\delta f(u)}\rho(q_1 q_2, t) \end{aligned} \qquad (22)$$

where $\hat{p}_1 \equiv (\hbar/i)(\partial/\partial q_1)$, and $-qf(u)$ is a time-dependent forcing term added to the Hamiltonian which will be set to zero in the end of the functional differentiation in the last term. Equation (22) is the central result of this work.

The last term in equation (22) can, in view of the external forcing term $\int_0^t du\, q(u)f(u)$ in the action, be written as

$$\begin{aligned} -i(q_1 - q_2)\int_0^t du\, R(t-u)\int dq_1'\int dq_2'\int_{q_1',0}^{q_1,t} d[q]\int_{q_2',0}^{q_2,t} d[r]\,(q(u) - r(u)) \\ \times \exp[i(S[q] - S[r])/\hbar]\, F[q,r]\,\rho(q_1', q_2', 0). \end{aligned} \qquad (23)$$

This can be most easily interpreted by taking a Wigner transform of equation (22). The classical FP equation is obtained plus terms of order $\hbar^2 V'''(q)$ in addition a contribution from the term of equation (23). At finite temperature, $R(u) \to 0$ as $\hbar \to 0$. We can thus give this term the interpretation of being a quantum memory effect corresponding to relatively long-ranged correlations in the environment. In comparison all classical memory effects are contained in the function $Q_1(u)$.

Let us briefly comment on the temperature regime where a classical description is valid. The Wigner function obeys the Wigner transform of equation (22). This function will obey a classical FP equation if the quantum memory term is negligible†. An analysis of the range of $R(u)$ enables us to estimate that for weak damping it is necessary to be at temperatures $T \gg \hbar\omega_S/k_B$ for this to be so (ω_s is a characteristic frequency of the classical motion).

In a recent work by Chakravarty and Leggett (1984) on the spin–boson system a 'dilute blip' approximation was used to obtain an exponential relaxation, in a certain regime of the parameter space, of a spin linearly coupled to a bosonic heat bath.

† We assume the $\hbar$-corrections arising from the potential terms are negligible.

From our understanding such an approximation corresponds to neglecting the quantum memory effect between the blips. To see this let us go back to equation (20). We can interpret it as a decomposition of $Q_2(u)$ into classical and quantum parts. From equations (2)–(5) we see that the only place where the quantum memory comes in is in the last term of equation (5). It is clear that for a spin system $q(u)$ and $r(u)$ take only two values, $q_0/2$ or $-q_0/2$. The last term of equation (5), with the boundary condition $q_1' = q_2' = q_1 = q_2 = q_0/2$, can be written as

$$\exp -\frac{\eta q_0^2}{\hbar}\sum_{i=1}^{n}\left(\frac{1}{\tau}(t_{2i}-t_{2i-1})+\frac{1}{\eta}\int_{t_{2i-1}}^{t_{2i}}\mathrm{d}u\int_{t_{2i-1}}^{-u}\mathrm{d}v\,R(u-v)\right)$$
$$\times\exp -\frac{q_0^2}{\hbar}\sum_{i>j}\left(\int_{t_{2i-1}}^{t_{2i}}\mathrm{d}u\int_{t_{2j-1}}^{t_{2j}}\mathrm{d}v\,R(u-v)\zeta_i\zeta_j\right) \tag{24}$$

where blips occur between each t_{2i} and t_{2i-1}, $\zeta_i = \pm 1$. The comparison between equation (25) and equation (5) of Chakravarty and Leggett (1984) indicates that the dilute blip approximation corresponds to neglecting the exponent of the second factor of equation (25) which is the quantum memory between blips. The classical part of $Q_2(u)$ gives rise to the term

$$\exp[-(\eta q_0^2/\hbar\tau)]\sum_i(t_{2i}-t_{2i-1})$$

which restricts the time scale of the blips to order τ/α, $\alpha = (\eta q_0^2/2\pi\hbar)$. The quantum correction to the self-energy, the exponent of the first term of equation (25), comes from the term

$$\frac{1}{\eta}\int_{t_{2i-1}}^{t_{2i}}\mathrm{d}u\int_{t_{2i-1}}^{u}\mathrm{d}v\,R(u-v)$$

which behaves as $\ln(\omega_c\tau)$ if $(t_{2i}-t_{2i-1})\gg\tau$ and $\ln(\omega_c\tau)+\ln[(t_{2i}-t_{2i-1})/\tau]$ if $(t_{2i}-t_{2i-1})\ll\tau$. Therefore, for all values of α the self-energy is dominated by the classical part. In the dilute blip approximation, τ/α is required to be much smaller than the decay time t_s. Thus for $\alpha<1$ the dilute blip approximation implies the classical limit†. For $\alpha>1$, t_s is found to be infinite (Chakravarty and Leggett 1984) and the condition for the classical limit is also satisfied. Of course, it is no surprise to see exponential decay in the classical limit.

We conclude by noting that the quantum Fokker–Planck equation we have holds under general conditions of temperature. We hope to discuss further our Fokker–Planck formalism for the spin–boson model elsewhere in the near future.

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† By classical limit we mean the effect of the environment instead of the system itself.

References

Anderson P W, Halperin B I and Varma C M 1972 *Phil. Mag.* **25**
Benguria R and Kac M 1981 *Phys. Rev. Lett.* **46** 1
Caldeira A O and Leggett A J 1983a *Ann. Phys., New York* **149** 374
—— 1983b *Physica* A**121** 587
Chakravarty S and Leggett A J 1984 *Phys. Rev. Lett.* **52** 5
Feynman R P and Hibbs A R 1965 *Quantum Mechanics and Path Integrals* (New York: McGraw–Hill)
Feynman R P and Vernon F L 1963 *Ann. Phys.* **24** 118
Iche G and Nozières P 1978 *Physica* A**91** 485
Phillips W A 1972 *J. Low Temp. Phys.* **7** 351
Schmid A 1982 *J. Low Temp. Phys.* **49** 609