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Friction and Dissipative Phenomena in Quantum Mechanics

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Frictional and dissipative terms of the Schrödinger equation are studied. A proof is given showing that the frictional term of the Schrödinger–Langevin equation causes the quantum system to lose energy. General expressions are derived for the frictional term of the Schrödinger equation.

KEY WORDS: Quantum statistical mechanics; dissipative phenomena; Schrödinger–Langevin equation; energy dissipation operator; friction.

1. INTRODUCTION

In classical mechanics, the fundamental equations of motion may be taken to be Newton's laws. In quantum mechanics, the fundamental equation may be taken to be the Schrödinger equation,

$$i\hbar\, \partial\psi/\partial t = -(\hbar^2/2m)\, \nabla^2\psi + V(\mathbf{r})\psi(\mathbf{r}, t) \tag{1}$$

It is well known that Newton's equations can be derived from the Schrödinger equation:

$$d\langle \mathbf{p}\rangle/dt = \langle \mathbf{F}\rangle \tag{2}$$

$$m\, d\langle \mathbf{r}\rangle/dt = \langle \mathbf{p}\rangle \tag{3}$$

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where the expectation value of the force is equal to the negative of the expectation value of the gradient of the potential

$$\langle \mathbf{F} \rangle = -\langle \nabla V \rangle \tag{4}$$

One of the basic equations of classical mechanics in which frictional forces are present is Langevin's equation. Expressed in terms of expectation values, this equation has the form

$$d\langle \mathbf{p} \rangle/dt = -\gamma\langle \mathbf{p} \rangle + \langle \mathbf{F} \rangle + \langle \mathbf{F}_s \rangle \tag{5}$$

where γ is the friction constant and $\mathbf{F}_s$ is a stochastic force. It has been shown that the Schrödinger–Langevin equation[1]

$$i\hbar\, \partial\psi/\partial t = -(\hbar^2/2m)\, \nabla^2\psi + V\psi + V_s\psi + (\hbar\gamma/2i) \ln(\psi/\psi^*)\psi \tag{6}$$

entails the Langevin equation (5), the momentum condition (3), and the normalization condition

$$d(\psi, \psi)/dt = 0 \tag{7}$$

The stochastic force $\mathbf{F}_s$ is the negative of the gradient of the stochastic potential V_s.

The frictional force of the Langevin equation is proportional to the negative of the momentum. However, studies of the slowing down of electrons, protons, and other atomic particles under a wide variety of conditions have shown that the friction force has many different functional dependences on momentum.[2] The energy dissipation operator $K(\psi)$ of the Schrödinger equation

$$i\hbar\, \partial\psi/\partial t = H\psi + V_s\psi + K(\psi) \tag{8}$$

causes the slowing down of the particle. All possible wave functions of the Schrödinger equation (8) should satisfy the normalization condition

$$d(\psi, \psi)/dt = 0 \tag{9}$$

the momentum condition

$$(\psi, \mathbf{p}\psi) = m\, d(\psi, \mathbf{r}\psi)/dt \tag{10}$$

and the energy dissipation condition, namely that $K(\psi)$ causes the quantum system to lose energy. In the phenomenological approach one asks what forms of $K(\psi)$ satisfy the normalization, momentum, and energy dissipation conditions. Previous attempts from the phenomenological point of view to answer this question have not been entirely successful.[3–6] It is the purpose of this paper to derive general forms of $K(\psi)$ which satisfy the normalization, momentum, and energy dissipation conditions.

2. DISSIPATION OF ENERGY

The change in the energy of a quantum system as a result of its interaction with a surrounding dissipating system is

$$\langle E(t)\rangle - \langle E(0)\rangle = [\psi(t), H\psi(t)] - [\psi(0), H\psi(0)] \tag{11}$$

For an infinitesimal time of interaction, expression (11) becomes

$$d\langle E\rangle/dt = (\psi, H\,\partial\psi/\partial t) + (\partial\psi/\partial t, H\psi) \tag{12}$$

If the stochastic potential V_s is neglected, then the energy of the quantum system will either remain the same or decrease:

$$d\langle E\rangle/dt \leqslant 0 \tag{13}$$

The special case where $d\langle E\rangle/dt = 0$ will be discussed later in this section. Substituting (8) into (12), neglecting V_s, and using the fact that the operator H is Hermitian, we obtain

$$d\langle E\rangle/dt = (1/i\hbar)\{[\psi, HK(\psi)] - [K(\psi), H\psi]\} \leqslant 0 \tag{14}$$

Thus the energy dissipation operator K must satisfy the energy dissipation condition (14) for all possible wave functions ψ.

The energy dissipation operator K must also be such that all possible wave functions of the Schrödinger equation satisfy the normalization condition (9). Substituting (8) into (9) gives us

$$[\psi, K(\psi)] = [K(\psi), \psi] \tag{15}$$

Thus the energy dissipation operator K must satisfy the normalization condition (15) for all possible wave functions.

In addition, the momentum condition (10) must hold. Combining (8) and (10) yields

$$[\psi, \mathbf{r}K(\psi)] = [K(\psi), \mathbf{r}\psi] \tag{16}$$

Condition (16), derived from the momentum condition (10), must be valid for all possible wave functions ψ.

An example of an energy dissipation operator which satisfies the energy dissipation condition (14), the normalization condition (15), and the momentum condition (16) for all possible wave functions is the operator of the Schrödinger–Langevin equation (6)

$$K(\psi) = (\hbar\gamma/2i)\ln(\psi/\psi^*)\psi \tag{17}$$

Substituting (17) into (14) with

$$H = -(\hbar^2/2m)(\partial^2/\partial x^2) + V(x) \tag{18}$$

we obtain

$$\frac{d\langle E\rangle}{dt} = \frac{\gamma\hbar^2}{4m}\int \psi^*\left\{\frac{\partial^2[\psi \ln(\psi/\psi^*)]}{\partial x^2} - \ln\left(\frac{\psi}{\psi^*}\right)\frac{\partial^2\psi}{\partial x^2}\right\}dx \tag{19}$$

Integrating by parts gives us

$$\frac{d\langle E\rangle}{dt} = -\frac{\gamma\hbar^2}{4m}\int \frac{\partial \ln(\psi/\psi^*)}{\partial x}\left(\psi\frac{\partial\psi^*}{\partial x} - \psi^*\frac{\partial\psi}{\partial x}\right)dx \tag{20}$$

which can be written in the form

$$\frac{d\langle E\rangle}{dt} = -\frac{\gamma\hbar^2}{4m}\int \left|\psi\frac{\partial \ln(\psi/\psi^*)}{\partial x}\right|^2 dx \tag{21}$$

Therefore the energy dissipation operator (17) satisfies the energy dissipation condition (14). The special case of $d\langle E\rangle/dt = 0$ arises when the quantum system is in a pure state with a wave function of the form

$$\psi(x, t) = [\exp(-iE_n t/\hbar)]u_n(x)$$

where E_n is the energy eigenvalue of the nth state and $u_n(x)$ is real. However, it should be noted that the stochastic potential V_s will cause the pure state to change to a mixed state, in which state the energy dissipation operator then tends to decrease the energy.

Next, by substituting (17) into (15) and (16), we readily confirm that the energy dissipation operator of the Schrödinger–Langevin equation also satisfies the normalization and momentum conditions.

3. DISSIPATION OPERATORS

It is our aim to derive other forms of $K(\psi)$ which satisfy the energy dissipation, momentum, and normalization conditions. Let us consider expressions of the type

$$K(\psi) = \epsilon g(\theta)\psi \tag{22}$$

where ϵ is a coupling constant and $g(\theta)$ is a real function of the real variable θ:

$$\theta = (1/2i)\ln(\psi/\psi^*) \tag{23}$$

For example, the operator (17) of the Schrödinger–Langevin equation is a member of this class with $\epsilon = \hbar\gamma$ and $g(\theta) = \theta$.

Substituting (22) into (14) and integrating by parts, we have

$$\frac{d\langle E\rangle}{dt} = -\frac{\hbar\epsilon}{2im}\int \frac{dg}{d\theta}\frac{\partial\theta}{\partial x}\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right)dx \tag{24}$$

Noting that

$$\frac{\partial\theta}{\partial x} = \frac{1}{2i}\left(\frac{1}{\psi}\frac{\partial\psi}{\partial x} - \frac{1}{\psi^*}\frac{\partial\psi^*}{\partial x}\right) \tag{25}$$

we find that (24) becomes

$$d\langle E\rangle/dt = -(\hbar\varepsilon/m)\int g'(\theta)|\psi\,\partial\theta/\partial x|^2\,dx \tag{26}$$

A similar result can be derived for higher dimensional problems. We obtain

$$d\langle E\rangle/dt = -(\hbar\varepsilon/m)\int g'(\theta)|\psi|^2\,\nabla\theta\cdot\nabla\theta\,d\mathbf{r} \tag{27}$$

Therefore, if the first derivative of g is positive, then the energy dissipation condition (14) is satisfied. By substituting (22) into (15) and (16), we confirm that (22) also satisfies the normalization and momentum conditions. Thus we have shown that any expression of the form (22) where the first derivative of g is positive leads to frictional or dissipative effects where the quantum system tends to lose energy.

Are there other general expressions for $K(\psi)$ which produce frictional or dissipative effects? Let us investigate expressions of the form

$$K(\psi) = \kappa T(t)S(x, t)\psi \tag{28}$$

where κ is a coupling constant, T is a real function of time, and S is a real function of space and time. Is there any relationship between S and T so that the energy dissipation condition (14) is satisfied? Combining (28) with (14) and integrating by parts yields

$$\frac{d\langle E\rangle}{dt} = -\frac{\hbar\kappa T(t)}{2im}\int\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right)\frac{\partial S}{\partial x}\,dx \tag{29}$$

Making use of the expression for the probability current density j, we find that (29) simplifies to

$$d\langle E\rangle/dt = -\kappa T(t)\int j(\partial S/\partial x)\,dx \tag{30}$$

where

$$j = \frac{\hbar}{2im}\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right) \tag{31}$$

Thus, according to (30), if we take for $T(t)$

$$T(t) = \int j(\partial S/\partial x)\,dx \tag{32}$$

then $K(\psi)$ of (28) will satisfy the energy dissipation condition (14). It is easily confirmed that (28) also satisfies the normalization condition (15) and the momentum condition (16).

The energy dissipation operator (28) for one spatial dimension can be generalized to treat higher dimensional problems. We consider expressions of the form

$$K(\psi) = \kappa T(t)\cdot \mathbf{S}(\mathbf{r}, t)\psi \tag{33}$$

where T and S are now vector functions. Substituting (33) into (14) and integrating by parts gives us

$$d\langle E\rangle/dt = -\kappa \mathbf{T}(t)\cdot \int (\mathbf{j}\cdot\nabla)\mathbf{S}(\mathbf{r}, t)\,d\mathbf{r} \tag{34}$$

where

$$\mathbf{j} = (\hbar/2im)(\psi^*\,\nabla\psi - \psi\,\nabla\psi^*) \tag{35}$$

Therefore the energy dissipation condition (14) is satisfied by taking for the vector function $\mathbf{T}(t)$

$$\mathbf{T}(t) = \int (\mathbf{j}\cdot\nabla)\mathbf{S}(\mathbf{r}, t)\,d\mathbf{r} \tag{36}$$

For example, if we let the vector function $\mathbf{S}(\mathbf{r}, t)$ be equal to $\mathbf{r}$,

$$\mathbf{S}(\mathbf{r}, t) = \mathbf{r} \tag{37}$$

then the energy dissipation operator (33) becomes

$$K(\psi) = \kappa \mathbf{r}\cdot\bar{\mathbf{j}}\psi \tag{38}$$

where

$$\bar{\mathbf{j}} = \int \mathbf{j}\,d\mathbf{r} = \langle\mathbf{p}\rangle/m \tag{39}$$

It is not difficult to show that the Schrödinger equation

$$i\hbar\,\partial\psi/\partial t = H\psi + V_s\psi + K(\psi) \tag{40}$$

with the energy dissipation operator (38) satisfies the Langevin equation

$$d\langle\mathbf{P}\rangle/dt = \langle\mathbf{F}\rangle + \langle\mathbf{F}_s\rangle - (\kappa/m)\langle\mathbf{p}\rangle \tag{41}$$

In summary, we have studied quantum systems where friction or other dissipative effects occur. The energy dissipation, normalization, and momentum conditions for such systems have been discussed. General expressions have been derived for the energy dissipator operator of the Schrödinger equation which satisfy these conditions for all possible wave functions.

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