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Energy absorption and dissipation in quantum systems

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Abstract

Stemming from the time-dependent Schrödinger equation, it is noted that any Hermitian form representing work done on a system yields a bounded expectation of energy. This expectation can be periodic, quasiperiodic or even chaotic. Such boundedness is unrealistic because energy may be added to or removed from the system. Thus, a complex non-Hermitian form is introduced into the Hamiltonian of a system which, when positive represents work being done on the system and gives an increasing energy expectation, and when negative represents a dissipation of energy from the system and gives a decreasing energy expectation. Two cases are studied. In the first, the perturbative term is purely time-dependent. In the second, it is also space-dependent. This latter case is applied to the kicked quantum rotor. A number of other applications of this formalism to systems of experimental and theoretical interest are noted.

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1. Introduction

In a number of works addressing the kicked quantum rotor [1–4], it is implied that for this system, the classical configuration gives an increasing average energy but the quantum system gives an expectation of energy that returns eventually to its starting value. In this work, we re-examine this problem and note that any Hermitian work function gives an oscillating expectation of energy. The paradoxical situation of a system with a bounded expectation of energy on which work is being done is resolved by the fact that the quantum system is not isolated. Thus, standard

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conservation laws cannot be applied and, e.g., the system's energy is not conserved. To correct this situation, a non-Hermitian component of the Hamiltonian is included that accounts for either energy being absorbed or dissipated.

2. Analysis

To more formally examine this question, consider a simple one-dimensional quantum system whose Hamiltonian includes a term, $i\hbar\alpha(x,t)$, corresponding to energy input ($\alpha > 0$) or dissipation ($\alpha < 0$). We consider two cases: (a) $\alpha = \alpha(t)$ and (b) $\alpha = \alpha(x,t)$.

2.1. Case a

For this case consider a system whose Hamiltonian is given by

$$H = \frac{p^2}{2m} + V(x) + i\hbar\alpha(t), \tag{1}$$

where the indefinite (Lebesgue) integral of $\alpha(t)$ exists. The dimension of the real parameter α is $1/t$. In addition, if $\alpha(t)$ is odd in t, then

$$H^*(-t) = H(t), \tag{2}$$

and $H(t)$ satisfies time reversibility. The complex work term of H renders H non-Hermitian. Furthermore, H is an explicit function of time, so the expectation of H is time-dependent [5]. The integral of $\alpha(t)$ is defined to be

$$\int_{-\infty}^{t} \alpha(\lambda)\,\mathrm{d}\lambda \equiv g(t) \equiv \ln\left[\left(1 + \frac{\Delta E}{E_0}\right)^{1/2}\right], \tag{3}$$

where $\Delta E = \Delta E(t)$ is the increment of energy absorbed ($\Delta E > 0$) or dissipated ($\Delta E < 0$) by the system at the time t and E_0 is the initial energy of the system. (For energy dissipation we also require that $|\Delta E| < E_0$ in order to guarantee that the argument of the logarithmic term is positive. The ln function in (3) was introduced for conciseness of formulas.) Additionally, the system is defined on a bounded spatial domain. We hence assume that the time-independent component, H_0, of the Hamiltonian, H, admits a discrete set of eigenenergies, as is the case in most circumstances.

Consider the Schrödinger equation for this system,

$$\frac{-\hbar^2}{2m}\varphi_{xx} + V(x)\varphi + i\hbar\alpha(t)\varphi = E\varphi. \tag{4}$$

Eigenfunctions and eigenvalues of the component H_0, independent of $\alpha(t)$, satisfy the equation

$$H_0\varphi_n = E_n^0\varphi_n \tag{5}$$

Substituting this form into (4) yields

$$H_0\varphi_n + i\hbar\alpha(t)\varphi_n = E_n\varphi_n, \tag{6}$$

where

$$E_n(t) = E_n^0 + i\hbar\alpha(t). \tag{7}$$

It follows that $\varphi_n(x)$ given by (5) are eigenstates of H given by (1). Now consider the time-dependent Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t} = H\Psi, \tag{8}$$

whose solution is given by

$$\Psi(t) = \exp\left[-\frac{i}{\hbar}\int_{-\infty}^{t} \mathrm{d}\lambda\, H(\lambda)\right]\Psi(0). \tag{9}$$

With the eigenstates (5), one may write the initial wavefunction as

$$\Psi(0) = \sum_n a_n\varphi_n, \qquad \sum_n |a_n|^2 E_n^0 = E_0, \tag{10}$$

where the expansion coefficients a_n are determined by initial data. Substituting the latter expression into (9) gives the general solution

$$\Psi(t) = \mathrm{e}^{g(t)}\sum_n a_n\varphi_n(t)\,\mathrm{e}^{-\mathrm{i}E_n^0 t/\hbar}, \tag{11}$$

where $g(t)$ is given by (3). We define the expectation of our non-Hermitian Hamiltonian, H, to be

$$\langle E\rangle \equiv \Re\langle\Psi|H\Psi\rangle = \Re\,\mathrm{e}^{2g(t)}\sum_n |a_n|^2 E_n(t) = \left(1+\frac{\Delta E(t)}{E_0}\right)\sum_n |a_n|^2 E_n^0 = E_0 + \Delta E(t), \tag{12}$$

which is the expectation of energy of the system at time t. Recall that $\Delta E > 0$ for energy absorption and $\Delta E < 0$ for energy dissipation.

This latter result indicates that an appropriate manner of describing energy absorption or dissipation in a quantum system is by the addition of a non-Hermitian term in the Hamiltonian. If, e.g., the i factor in the complex form (1) is replaced by 1, this form is Hermitian as is the Hamiltonian, and the expectation of energy, (12), becomes oscillatory. This behavior is not representative of a system that is absorbing or dissipating energy. We may conclude in general that a Hamiltonian with an imaginary component yields an expectation of energy that grows or decays in time. An alternative description of phenomena related to explicitly time-dependent Hamiltonians is given by the formalism of *quantum dissipation* [6,7], which embeds a dissipative system into a larger Hamiltonian system by explicitly incorporating a heat bath to account for dissipation or absorption. In many situations, this Hamiltonian embedding entails weak coupling between the system of interest to a heat bath whose thermal equilibrium is not noticeably altered by the system of interest. Descriptions similar to our own, which incorporate dissipation and absorption directly by adjusting the Hamiltonian, have been utilized in other disciplines (including optics and laser physics) [8].

2.2. Case b

For case (b), we write (for separable forms)

$$\alpha(x,t) = Z(x)\alpha_1(t), \tag{13}$$

and apply this formalism to a dissipative quantum kicked rotor, whose Hamiltonian is given by [1,3]:

$$H = \frac{p^2}{2m} - iZ(x)\sum_s \delta\left[s - \frac{t}{T}\right], \quad Z(x) \equiv \frac{Kx^2}{2}, \tag{14}$$

where, consistent with our formalism, a factor of i was inserted before the perturbative term. The summation in (14) is over positive integers s. Additionally, the parameter T represents the kicking period and K is the spring constant of the rotor. For simplicity, $Z(x)$ is averaged employing eigenstates of the harmonic oscillator. We label $\langle Z(x)\rangle \equiv \kappa$. If the rotor is frictionless, then α_1 is related to energy absorption of the rotor through (3). Eq. (6) now appears with $\alpha_1(t)$ replaced as follows:

$$\alpha_1(t) \to \frac{\kappa\alpha_1(t)}{\hbar}. \tag{15a}$$

Relation (12) requires evaluation of the integral g. This is obtained as follows. We write (with the factor $\kappa/\hbar$ tacitly included)

$$g(t) = \int_{-\infty}^{t} \sum_s \delta\left[s - \frac{\lambda}{T}\right] \mathrm{d}\lambda. \tag{15b}$$

Let

$$\xi \equiv s - \frac{\lambda}{T}, \tag{15c}$$

then

$$\delta(\xi) = \frac{\mathrm{d}G_s}{\mathrm{d}\xi} = \frac{\mathrm{d}G_s}{\mathrm{d}\lambda}\frac{\mathrm{d}\lambda}{\mathrm{d}\xi} = -T\frac{\mathrm{d}G_s}{\mathrm{d}\lambda}. \tag{15d}$$

Thus

$$g(t) = -T\sum_s \int_{-\infty}^{t} \frac{\mathrm{d}G_s}{\mathrm{d}\lambda}\mathrm{d}\lambda = -T\sum_s G_s\left(s - \frac{t}{T}\right) = -T\Phi\left(\frac{t}{T}\right), \tag{16a}$$

where $G_s(x)$ is the step function defined as: $G_s(x) = 1$, $x \geq 0$, $G_s(x) = 0$, $x < 0$. The value of the sum in (16a) is the number of s values $\geq t/T$, which we call, $\Phi(t/T)$. With (3) and (15a) we find that

$$\Delta E = E_0\left[\exp\left(-\frac{2\kappa T\Phi}{\hbar}\right) - 1\right] \leq 0 \tag{16b}$$

for the increment of energy dissipated by the system at t. Note in particular that the argument of the exponential function is dimensionless.

In addition to the dissipative kicked rotor, one may also apply this formalism to quantum billiards [9–11] with either stationary or oscillating boundaries in which particle collisions with walls are inelastic. (Here it is envisioned that energy loss to the walls is carried away to a temperature bath in which the billiard is adiabatically immersed.) For example, collisions in experimental billiards can take a finite amount of time, indicating an extended contact between an enclosed particle with the boundary as opposed to an instantaneous specular reflection. This application thus pertains to the study of dissipative quantum dots [12]. Other possible applications include spin-lattice relaxation in nuclear magnetic resonance [13] and superconducting quantum interference devices (SQUIDs) [14].

3. Conclusions

In conclusion, a formalism has been introduced to describe energy absorption and dissipation in quantum systems, in terms of which, e.g., work done on a frictionless system gives rise to a monotonic increase of the expectation of energy of the system. Specific application of the formalism was described in terms of a dissipative kicked quantum rotor. Possible application of the formalism was mentioned also to quantum billiards (and hence to quantum-well nanostructures) in which particle collisions with walls are inelastic.

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