КОМПЬЮТЕРНЫЕ ТЕХНОЛОГИИ ФИЗИКИ

QUANTUM DECOHERENCE
IN THE THEORY OF OPEN SYSTEMS

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Within the framework of the Lindblad theory for open quantum systems, we determine the degree of quantum decoherence of a harmonic oscillator interacting with a thermal bath. It is found that the system manifests a quantum decoherence which is more and more significant in time. We also calculate the decoherence time scale and analyze the transition from quantum to classical behaviour of the considered system.

В рамках теории Линдблада для открытых квантовых систем мы изучаем квантовую декогеренцию для гармонического осциллятора, взаимодействующего со своим окружением (тепловым резервуаром). Мы нашли, что данная система проявляет квантовую декогеренцию, усиливающуюся с течением времени. Мы определили также порядок времени декогеренции и рассмотрели переход от квантового к классическому поведению для рассмотренной системы.

INTRODUCTION

The quantum-to-classical transition and classicality of quantum systems continue to be among the most interesting problems in many fields of physics, for both conceptual and experimental reasons [1, 2]. Two conditions are essential for the classicality of a quantum system [3]: a) quantum decoherence (QD), that means the irreversible, uncontrollable and persistent formation of a quantum correlation (entanglement) of the system with its environment [4], expressed by the damping of the coherences present in the quantum state of the system, when the off-diagonal elements of the density matrix decay below a certain level, so that this density matrix becomes approximately diagonal, and b) classical correlations, expressed by the fact that the quantum state becomes peaked along a classical trajectory. Classicality is an emergent property of open quantum systems, since both main features of this process — QD and classical correlations — strongly depend on the interaction between the system and its external environment [1, 2]. In this work, we study QD and analyze quantum-classical transition of a harmonic oscillator interacting with an environment, in particular with a thermal bath, within the framework of the Lindblad theory for open quantum systems.

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1. MASTER EQUATION AND DENSITY MATRIX

In the Lindblad axiomatic formalism based on quantum dynamical semigroups, the irreversible time evolution of open system is described by the following general quantum Markovian master equation for the density operator $\rho(t)$ [5]:

$$\frac{d\rho(t)}{dt} = -\frac{i}{\hbar}[H, \rho(t)] + \frac{1}{2\hbar}\sum_j([V_j\rho(t), V_j^\dagger] + [V_j, \rho(t)V_j^\dagger]). \tag{1}$$

The harmonic oscillator Hamiltonian H is chosen of the general quadratic form

$$H = H_0 + \frac{\mu}{2}(qp + pq), \quad H_0 = \frac{1}{2m}p^2 + \frac{m\omega^2}{2}q^2 \tag{2}$$

and the operators V_j, $V_j^\dagger$, which model the environment, are taken as linear polynomials in coordinate q and momentum p. Then the master equation (1) takes the following form [6]:

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H_0, \rho] - \frac{i}{2\hbar}(\lambda + \mu)[q, \rho p + p\rho] + \frac{i}{2\hbar}(\lambda - \mu)[p, \rho q + q\rho] -$$
$$- \frac{D_{pp}}{\hbar^2}[q, [q, \rho]] - \frac{D_{qq}}{\hbar^2}[p, [p, \rho]] + \frac{D_{pq}}{\hbar^2}([q, [p, \rho]] + [p, [q, \rho]]). \tag{3}$$

The diffusion coefficients D_{pp}, D_{qq}, D_{pq} and the dissipation constant λ satisfy the fundamental constraints: $D_{pp} > 0, D_{qq} > 0$ and $D_{pp}D_{qq} - D_{pq}^2 \geqslant \lambda^2\hbar^2/4$. In the particular case when the asymptotic state is a Gibbs state $\rho_G(\infty) = \exp\left(-\frac{H_0}{kT}\right)/\text{Tr}\exp\left(-\frac{H_0}{kT}\right)$, these coefficients become

$$D_{pp} = \frac{\lambda + \mu}{2}\hbar m\omega\coth\frac{\hbar\omega}{2kT}, \quad D_{qq} = \frac{\lambda - \mu}{2}\frac{\hbar}{m\omega}\coth\frac{\hbar\omega}{2kT}, \quad D_{pq} = 0, \tag{4}$$

where T is the temperature of the thermal bath. In this case, the fundamental constraints are satisfied only if $\lambda > \mu$ and

$$(\lambda^2 - \mu^2)\coth^2\frac{\hbar\omega}{2kT} \geqslant \lambda^2 \tag{5}$$

and the asymptotic values $\sigma_{qq}(\infty), \sigma_{pp}(\infty), \sigma_{pq}(\infty)$ of the dispersion (variance), and respectively correlation (covariance) of the coordinate and momentum, reduce to [6]

$$\sigma_{qq}(\infty) = \frac{\hbar}{2m\omega}\coth\frac{\hbar\omega}{2kT}, \quad \sigma_{pp}(\infty) = \frac{\hbar m\omega}{2}\coth\frac{\hbar\omega}{2kT}, \quad \sigma_{pq}(\infty) = 0. \tag{6}$$

We consider a harmonic oscillator with an initial Gaussian wave function ($\sigma_q(0)$ and $\sigma_p(0)$ are the initial averaged positions and momentum of the wave packet)

$$\Psi(q) = \left(\frac{1}{2\pi\sigma_{qq}(0)}\right)^{1/4}\exp\left[-\frac{1}{4\sigma_{qq}(0)}\left(1 - \frac{2i}{\hbar}\sigma_{pq}(0)\right)(q - \sigma_q(0))^2 + \frac{i}{\hbar}\sigma_p(0)q\right], \tag{7}$$

representing a correlated coherent state (squeezed coherent states) with the variances and covariances of coordinate and momentum

$$\sigma_{qq}(0) = \frac{\hbar\delta}{2m\omega}, \quad \sigma_{pp}(0) = \frac{\hbar m\omega}{2\delta(1 - r^2)}, \quad \sigma_{pq}(0) = \frac{\hbar r}{2\sqrt{1 - r^2}}. \tag{8}$$

Here δ is the squeezing parameter which measures the spread in the initial Gaussian packet and r, with $|r| < 1$, is the correlation coefficient. The initial values (8) correspond to a minimum uncertainty state, since they fulfil the generalized uncertainty relation $\sigma_{qq}(0)\sigma_{pp}(0) - \sigma_{pq}^2(0) = \hbar^2/4$. For $\delta = 1$ and $r = 0$ the correlated coherent state becomes a Glauber coherent state.

From Eq. (3) we derive the evolution equation in coordinate representation:

$$
\frac{\partial \rho}{\partial t} = \frac{i\hbar}{2m}\left(\frac{\partial^2}{\partial q^2} - \frac{\partial^2}{\partial q'^2}\right)\rho - \frac{im\omega^2}{2\hbar}(q^2 - q'^2)\rho -
$$

$$
- \frac{1}{2}(\lambda + \mu)(q - q')\left(\frac{\partial}{\partial q} - \frac{\partial}{\partial q'}\right)\rho + \frac{1}{2}(\lambda - \mu)\left[(q + q')\left(\frac{\partial}{\partial q} + \frac{\partial}{\partial q'}\right) + 2\right]\rho -
$$

$$
- \frac{D_{pp}}{\hbar^2}(q - q')^2\rho + D_{qq}\left(\frac{\partial}{\partial q} + \frac{\partial}{\partial q'}\right)^2\rho - 2iD_{pq}\hbar(q - q')\left(\frac{\partial}{\partial q} + \frac{\partial}{\partial q'}\right)\rho. \quad (9)
$$

The first two terms on the right-hand side of this equation generate the usual Liouvillian unitary evolution. The third and the forth terms are the dissipative terms and have a damping effect (exchange of energy with the environment). The last three terms are noise (diffusive) terms and produce fluctuation effects in the evolution of the system. D_{pp} promotes diffusion in momentum and generates decoherence in coordinate q — it reduces the off-diagonal terms, responsible for correlations between spatially separated pieces of the wave packet. Similarly, D_{qq} promotes diffusion in coordinate and generates decoherence in momentum p. The D_{pq} term is the so-called «anomalous diffusion» term and it does not generate decoherence.

The density matrix solution of Eq. (9) has the general Gaussian form

$$
\langle q|\rho(t)|q'\rangle = \left(\frac{1}{2\pi\sigma_{qq}(t)}\right)^{1/2}\exp\left[-\frac{1}{2\sigma_{qq}(t)}\left(\frac{q + q'}{2} - \sigma_q(t)\right)^2 - \right.
$$

$$
\left. - \frac{\sigma(t)}{2\hbar^2\sigma_{qq}(t)}(q - q')^2 + \frac{i\sigma_{pq}(t)}{\hbar\sigma_{qq}(t)}\left(\frac{q + q'}{2} - \sigma_q(t)\right)(q - q') + \frac{i}{\hbar}\sigma_p(t)(q - q')\right], \quad (10)
$$

where $\sigma(t) \equiv \sigma_{qq}(t)\sigma_{pp}(t) - \sigma_{pq}^2(t)$ is the Schrödinger generalized uncertainty function. In the case of a thermal bath we obtain the following steady state solution for $t \to \infty$ $\left(\epsilon \equiv \dfrac{\hbar\omega}{2kT}\right)$:

$$
\langle q|\rho(\infty)|q'\rangle = \left(\frac{m\omega}{\pi\hbar\coth\epsilon}\right)^{1/2}\exp\left\{-\frac{m\omega}{4\hbar}\left[\frac{(q + q')^2}{\coth\epsilon} + (q - q')^2\coth\epsilon\right]\right\}. \quad (11)
$$

2. DECOHERENCE AND QUANTUM-CLASSICAL TRANSITION

An isolated system has a unitary evolution and the coherence of the state is not lost — pure states evolve in time only into pure states. The QD phenomenon, that is, the loss of coherence or the destruction of off-diagonal elements representing coherences between quantum states in the density matrix, can be achieved by introducing an interaction between the system and the environment: an initial pure state with a density matrix which contains nonzero off-diagonal terms can non-unitarily evolve into a final mixed state with a diagonal density matrix.

Using new variables $\Sigma = (q + q')/2$ and $\Delta = q - q'$, the density matrix (10) becomes

$$\rho(\Sigma, \Delta, t) = \sqrt{\frac{\alpha}{\pi}} \exp\left[-\alpha\Sigma^2 - \gamma\Delta^2 + i\beta\Sigma\Delta + 2\alpha\sigma_q(t)\Sigma + \right.$$
$$\left. + i\left(\frac{\sigma_p(t)}{\hbar} - \beta\sigma_q(t)\right)\Delta - \alpha\sigma_q^2(t)\right], \quad (12)$$

with the abbreviations

$$\alpha = \frac{1}{2\sigma_{qq}(t)}, \quad \gamma = \frac{\sigma(t)}{2\hbar^2\sigma_{qq}(t)}, \quad \beta = \frac{\sigma_{pq}(t)}{\hbar\sigma_{qq}(t)}. \quad (13)$$

The representation-independent measure of the degree of QD [3] is given by the ratio of dispersion $1/\sqrt{2\gamma}$ of the off-diagonal element $\rho(0, \Delta, t)$ to dispersion $\sqrt{2/\alpha}$ of the diagonal element $\rho(\Sigma, 0, t)$:

$$\delta_{\text{QD}}(t) = \frac{1}{2}\sqrt{\frac{\alpha}{\gamma}} = \frac{\hbar}{2\sqrt{\sigma(t)}}. \quad (14)$$

The finite temperature Schrödinger generalized uncertainty function has the expression [7] (with the notation $\Omega^2 \equiv \omega^2 - \mu^2$, $\omega > \mu$)

$$\sigma(t) = \frac{\hbar^2}{4}\left\{ e^{-4\lambda t}\left[1 - \left(\delta + \frac{1}{\delta(1 - r^2)}\right)\coth\epsilon + \coth^2\epsilon\right] + \right.$$
$$+ e^{-2\lambda t}\coth\epsilon\left[\left(\delta + \frac{1}{\delta(1 - r^2)} - 2\coth\epsilon\right)\frac{\omega^2 - \mu^2\cos(2\Omega t)}{\Omega^2} + \right.$$
$$\left.\left. + \left(\delta - \frac{1}{\delta(1 - r^2)}\right)\frac{\mu\sin(2\Omega t)}{\Omega} + \frac{2r\mu\omega(1 - \cos(2\Omega t))}{\Omega^2\sqrt{1 - r^2}}\right] + \coth^2\epsilon\right\}. \quad (15)$$

In the limit of long times Eq. (15) yields $\sigma(\infty) = (\hbar^2\coth^2\epsilon)/4$, so that we obtain

$$\delta_{\text{QD}}(\infty) = \tanh\frac{\hbar\omega}{2kT}, \quad (16)$$

which for high T becomes $\delta_{\text{QD}}(\infty) = \hbar\omega/(2kT)$. We can see that δ_{QD} decreases, and therefore, QD increases with time and temperature, i.e. the density matrix becomes more and more diagonal at higher T and the contributions of the off-diagonal elements get smaller and smaller. At the same time, the degree of purity decreases and the degree of mixedness increases with T. For $T = 0$ the asymptotic (final) state is pure and δ_{QD} reaches its initial maximum value 1. $\delta_{\text{QD}} = 0$ when the quantum coherence is completely lost, and if $\delta_{\text{QD}} = 1$ there is no QD. For quite a long time the magnitude of the elements of the density matrix in the position basis are peaked preferentially along the diagonal $q = q'$. Then $\delta_{\text{QD}} < 1$ and we can say that the considered system interacting with the thermal bath manifests QD. Dissipation promotes quantum coherences, whereas fluctuation (diffusion) reduces coherences and promotes QD. The balance of dissipation and fluctuation determines the final equilibrium value of δ_{QD}. The initial pure state evolves approximately (following the classical trajectory) into phase space and becomes a quantum mixed state during the irreversible process of QD.

In the macroscopic limit, when $\hbar$ is small, compared to other quantities with dimensions of action, the term in Eq. (9) containing $D_{pp}/\hbar^2$ dominates and induces the following evolution:

$$\frac{\partial \rho}{\partial t} = -\frac{D_{pp}}{\hbar^2}(q - q')^2 \rho. \tag{17}$$

Thus, the density matrix loses off-diagonal terms in position representation, while the diagonal ($q = q'$) ones remain untouched. Quantum coherences decay exponentially and the decoherence time scale is of the order of

$$t_{\text{deco}} = \frac{\hbar^2}{D_{pp}(q - q')^2}. \tag{18}$$

In the case of a thermal bath, we obtain (see Eq. (4))

$$t_{\text{deco}} = \frac{2\hbar}{(\lambda + \mu)m\omega\sigma_{qq}(0)\coth\epsilon}, \tag{19}$$

where we have taken $(q - q')^2$ of the order of the initial dispersion in coordinate $\sigma_{qq}(0)$. As expected, the decoherence time t_{deco} has the same scale as the time after which thermal fluctuations become comparable with quantum fluctuations. In the macroscopic domain QD occurs very much faster than relaxation. When $t \gg t_{\text{rel}}$, where $t_{\text{rel}} \approx \lambda^{-1}$ is the relaxation time, which governs the rate of dissipation, the particle reaches equilibrium with the environment. Indeed, the uncertainty function $\sigma(t)$ (15) approaches $\sigma^{\text{BE}} = (\hbar^2 \coth^2 \epsilon)/4$, which is the Bose–Einstein relation for a system of bosons in equilibrium at temperature T. In the case of $T = 0$ we approach the limit of pure quantum fluctuations, $\sigma_0 = \hbar^2/4$, which is the quantum Heisenberg relation. At high temperatures T we obtain the limit of pure thermal fluctuations, $\sigma^{\text{MB}} = (kT/\omega)^2$, which is a Maxwell–Boltzmann distribution for a system approaching a classical limit. The regime where thermal fluctuations begin to surpass quantum fluctuations is regarded as the transition point from quantum to classical statistical mechanics and the high temperature regime of a system is considered as the classical regime. We have shown that these two criteria of classicality are equivalent: the time when the quantum system decoheres is comparable with the time when thermal fluctuations overtake quantum fluctuations. After the decoherence time, the system has to be described by non-equilibrium quantum statistical mechanics. After the relaxation time the system is treated by equilibrium quantum statistical mechanics, and only at a sufficiently high temperature, when the spin statistics is represented by the Maxwell–Boltzmann distribution function, it can be considered in a classical regime [7, 8].

3. SUMMARY AND CONCLUDING REMARKS

We have studied QD within the framework of the theory of open quantum systems in order to understand the quantum-classical transition for a harmonic oscillator in interaction with a thermal bath. The classicality is conditioned by QD, expressed by the loss of quantum coherence in the case of a thermal bath at finite temperature.

The role of QD became relevant to many interesting physical problems. In many cases, one is interested in understanding QD because one wants to prevent decoherence from damaging

quantum states and to protect the information stored in quantum states from the degrading effect of the interaction with the environment. Decoherence is also responsible for washing out the quantum interference effects which are desirable to be seen as signals in experiments. QD has a negative influence on many areas relying upon quantum coherence effects, in particular it is a major problem in the physics of quantum information and computation.

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