Search for a border between classical and quantum worlds

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The effects of environmental decoherence on a mass-center position of a body consisting of many atoms are studied using a kind of linear quantum Boltzmann equation. It is shown that under realistic laboratory conditions these effects can be essentially eliminated for dust particles containing 10^{15} atoms. However, the initial velocity distribution and certain geometrical conditions make standard interference-type measurements extremally difficult beyond the nanometer scale. The results are illustrated by the analysis of the recent experiments involving fullerenes. Applications of decoherence effects to precise monitoring of environment or to separation of molecules are suggested.

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I. INTRODUCTION

Despite its long history, the problem of transition between macroscopic and microscopic worlds remains a fundamental issue in the discussion of foundations of quantum mechanics [1,2]. The simplest model illustrating this topic is a macroscopic body moving in a slowly varying gravitational potential. To describe its motion we use the position of its mass center $\mathbf{x}(t)$ as a collective variable that is separated from the internal degrees of freedom. One expects that for all practical purposes $\mathbf{x}(t)$ is well localized and evolves according to the Newton equation

$$\frac{d^2}{dt^2}\mathbf{x}(t) = -\boldsymbol{\nabla} U(\mathbf{x}(t)), \tag{1}$$

while apparently quantum-delocalized states corresponding to macroscopically extended wave packets $\Psi(\mathbf{x},t)$ satisfying the Schrödinger equation

$$-i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{x},t) = -\frac{\hbar^2}{2M}\Delta\,\Psi(\mathbf{x},t) + V(\mathbf{x})\Psi(\mathbf{x},t), \tag{2}$$

do not appear $[V(\mathbf{x}) = MU(\mathbf{x})]$.

In the literature, there are discussed at least four types of mechanisms leading to localization phenomena (or wave-function collapse) of above.

(1) *Environmental decoherence.* Quantum coherence is destroyed by scattering processes with particles of an environment both massive and massless (photons) [3]. Emission and absorption of thermal photons must also be included.

(2) *Decoherence by bremsstrahlung.* Electric charges moving in a slowly varying potential decohere by emission of soft photons [4]

(3) *Wave-function collapse by gravity.* Here the exact mechanism is not known due to the absence of an ultimate theory of quantum gravity but several models were proposed [5].

(4) *Spontaneous localization theories.* Fundamental stochastic or/and nonlinear modifications of the Schrödinger equation are proposed that are neglible at the atomic scale but become relevant for macroscopic bodies [6].

II. MARKOVIAN MODEL OF ENVIRONMENTAL DECOHERENCE

In the following we propose a simple description of the first, most conventional mechanism, and the only one that is very sensitive to the temperature and the density of environmental particles. A generic model is a mass center of a body described by the Hamiltonian

$$H = \frac{1}{2M}\mathbf{P}^2 + V(\mathbf{X}), \tag{3}$$

where $\mathbf{X}$ and $\mathbf{P}$ are the operators of mass center and total momentum of the body. The body is immersed in a gas consisting of particles or quasiparticles (atoms, molecules, photons, phonons, etc.) and the interaction with such an environment can be reduced to processes of scattering, absorption, or emission. Guided by the classical theory of Markovian evolutions generated by combination of jump processes (e.g., linear Boltzmann equation) and diffusion ones (e.g., Fokker-Planck equation) we consider the quantum Markovian master equation for the reduced density matrix $\rho(t)$ of the body mass center

$$\frac{d}{dt}\rho = -\frac{i}{\hbar}[H,\rho] + L\rho. \tag{4}$$

However, in contrast to the classical theory where the corresponding evolution equation for the phase-space probability distribution can be easily constructed in the quantum case there exists no such generator L, which for a generic Hamiltonian satisfies the following conditions:

(a) preserves positivity and normalization of the density matrix,
(b) drives the system asymptotically to a proper equilibrium state,
(c) satisfies natural symmetry conditions and conservation laws.

The exceptions are the systems with pure point spectrum Hamiltonians and well-separated eigenvalues, weakly coupled to heat baths with appropriate decay of multitime correlations functions. Under these assumptions, one can derive the corresponding generators applying weak-coupling (van Hove) limit or alternatively low-density limit. The obtained generators possess the standard (Gorini-Kossakowski-Lindblad-Sudarshan) form

$$L\rho=\sum_{\alpha}([V_\alpha\rho,V_\alpha^\dagger]+[V_\alpha,\rho V_\alpha^\dagger]), \tag{5}$$

where the operators V_α depend on the interaction with an environment, the Hamiltonian of the body H and the environmental parameters [7]. In particular, the best-know example is a harmonic oscillator with operators V_α being linear combinations of $\mathbf{X}$ and $\mathbf{P}$. These derivation procedures do not apply to systems with continuous (or quasicontinuous) part of the Hamiltonian's spectrum including the case of free motion. The existing in the literature equations either violate positivity requirement (a) (e.g., Caldeira-Legget equation [8]) or does not satisfy (b) and (c) even for the free motion case [3,6,9]. It seems that generally we cannot have a fully quantum (i.e., described in terms of the reduced density matrix), Markovian, and valid for different time scales description of the equilibration process for an open system [10].

In the following we shall use a semiphenomenological construction of the generator similar to the classical derivation of the linear Boltzmann equation. The effect of a collision with a gas particle and emission, absorption, or scattering of a photon (or other quasiparticle) is a transfer of momentum $\hbar\mathbf{k}$ that changes the total momentum as described by the following transformation in the Heisenberg picture:

$$e^{i\mathbf{k}\cdot\mathbf{X}}\mathbf{P}e^{-i\mathbf{k}\cdot\mathbf{X}}=\mathbf{P}+\hbar\mathbf{k}, \tag{6}$$

independently of the detailed microscopic mechanism of energy redistribution. Assuming statistical independence of different momentum transfer events (called simply *collisions*) we propose the following form of the generator:

$$L\rho=\int d^3\mathbf{k}n(\mathbf{k})(e^{-i\mathbf{k}\cdot\mathbf{X}}\rho e^{i\mathbf{k}\cdot\mathbf{X}}-\rho), \tag{7}$$

where $n(\mathbf{k})$ is a density of collisions per unit time leading to the momentum transfer $\hbar\mathbf{k}$.

The generator (7) satisfies the condition (a) and partially (c), taking into account momentum conservation. Unfortunately, the average kinetic energy grows to infinity for $t\to\infty$ and hence the process of ultimate relaxation to equilibrium is not properly described. However, it is expected that in the limit of large mass M and for slowly varying potential $V(\mathbf{x})$ the decoherence time τ_D is much shorter than the energy dissipation time scale τ_E [3]. Therefore, the generator (7) is a good approximation for the study of pure decoherence in the relevant regime of large body at slowly varying potential and rare collisions.

Assuming rotational invariance, i.e., $n(\mathbf{k})=n(k), k=|\mathbf{k}|$ we can introduce the following parametrization:

$$4\pi k^2 n(k)=\mathcal{N}\nu(k),\quad \mathcal{N}=4\pi\int_0^\infty dk\, k^2\, n(k). \tag{8}$$

Here $\nu(k)$ is a probability density of collisions and $\mathcal{N}$ their total number per time unit.

The generator L in the position representation reads

$$(L\rho)(\mathbf{x}|\mathbf{y})=-\gamma(|\mathbf{x}-\mathbf{y}|)\rho(\mathbf{x}|\mathbf{y}), \tag{9}$$

where

$$\gamma(r)=\mathcal{N}\int_0^\infty dk\,\nu(k)\left(1-\frac{\sin kr}{kr}\right). \tag{10}$$

Introducing the average wave vector $\overline{k}$ defined by

$$\overline{k^2}=\int_0^\infty dk\,k^2\nu(k), \tag{11}$$

we obtain simple formulas for the decay rates of the off-diagonal matrix elements $\rho(\mathbf{x}|\mathbf{y})$ in two regimes:

$$\gamma(|\mathbf{x}-\mathbf{y}|)\simeq\mathcal{N}\quad\text{for}\quad|\mathbf{x}-\mathbf{y}|\gg\overline{\lambda}=2\pi\overline{k}^{-1}, \tag{12}$$

$$\gamma(|\mathbf{x}-\mathbf{y}|)\simeq\frac{\mathcal{N}\overline{k^2}}{6}|\mathbf{x}-\mathbf{y}|^2\quad\text{for}\quad|\mathbf{x}-\mathbf{y}|\ll\overline{\lambda}. \tag{13}$$

The magnitude of decoherence can be characterized by the decoherence time

$$\tau_D=\mathcal{N}^{-1}. \tag{14}$$

In order to analyze an experiment that takes time t between the preparation of a quantum state and its measurement it is convenient to introduce the total number of collisions $\overline{n}=\mathcal{N}t$ and the coherence length

$$l_{coh}=\frac{\overline{\lambda}}{\pi}\sqrt{\frac{3}{2t\mathcal{N}}}\approx\frac{\overline{\lambda}}{\sqrt{\overline{n}}}, \tag{15}$$

which, according to Eq. (13) gives the maximal distance $|\mathbf{x}-\mathbf{y}|$ such that the corresponding off-diagonal elements decohere less than by a factor e^{-1}. The parameter l_{coh} puts an upper bound on the dimensions of diffraction grating (slit width and period) that can produce interference patterns.

One should mention that the regime given by Eq. (13) can be approximatively described by the generator of the form

$$L'\rho=-\frac{\mathcal{N}\overline{k^2}}{6}[\mathbf{X},[\mathbf{X},\rho]], \tag{16}$$

which often appears in the literature on decoherence [3,6,8,9].

III. THREE EXAMPLES OF DECOHERENCE REGIMES

We shall discuss three cases of environmental decoherence regime that are important for the topic of experimental search for the mechanisms of decoherence and the transition between classical and quantum worlds.

A. Macroscopic black body

To estimate the effect of thermal photons absorption (or emission) for a macroscopic body of a radius R treated as a black body we calculate $\mathcal{N}$ as a number of photons with Planck density entering a surface of a ball per unit time

$$\mathcal{N}=\frac{1}{4}(4\pi R^2 c)\frac{1}{\pi^2}\int_0^\infty \frac{k^2 dk}{e^{c\hbar k/k_B T}-1}\simeq 0.8R^2 c\left(\frac{k_B T}{\hbar c}\right)^3. \tag{17}$$

The corresponding decoherence time $\tau_D=\mathcal{N}^{-1}$ is given by

$$\tau_D[\mathrm{s}]\approx 10^{-17}(R[\mathrm{m}])^{-2}(T[\mathrm{K}])^{-3}. \tag{18}$$

It follows from Eq. (18) that the 3 K background radiation alone washes out all quantum-coherence effects for macroscopic bodies. The related estimations of the decoherence effects in this regime were already performed but with a simplified model described by the Eq. (16) containing a different parameter called ‘‘localization rate’’ and essentially equal to $\mathcal{N}\overline{k^2}/6$ [3].

B. Laboratory experiment with dust particles

Consider now a laboratory experiment performed at temperatures of the order of $T\approx 1$ K, high vacuum of $n_0\approx 10^9$ particles/m^3 (mass of the gas particle $m\approx 10^{-25}$ kg) and with a ‘‘small macroscopic’’ body, say a metallic ball of a radius $a=10^{-5}$ m containing $\approx 10^{15}$ atoms. Because at low temperatures the metallic body is almost a perfect conductor and its radius is much smaller than the thermal radiation wavelength the leading decoherence factors are the scattering of low-density gas particles and the Rayleigh scattering of thermal photons. A number of collisions per unit time for the former is given in terms of the average thermal velocity $v_{th}=\sqrt{8k_B T/\pi m}$,

$$\mathcal{N}_{gas}=\frac{1}{2}(4\pi a^2 v_{th})n_0=4\sqrt{2\pi}a^2 n_0\sqrt{k_B T/m}. \tag{19}$$

The Rayleigh scattering is characterized by the k-dependent cross section [11],

$$\sigma(k)=\frac{10\pi}{3}k^4 a^6, \tag{20}$$

and leads to

$$\mathcal{N}_R=\frac{1}{2}\left(\frac{10\pi}{3}a^6 c\right)\frac{1}{\pi^2}\int_0^\infty \frac{k^6 dk}{e^{c\hbar k/k_B T}-1}\simeq 380ca^6\left(\frac{k_B T}{\hbar c}\right)^7. \tag{21}$$

A straightforward calculation with the parameters of above yields

$$\tau_D^{gas}\approx 0.05[\mathrm{s}],\quad \tau_D^R\approx 0.002[\mathrm{s}]. \tag{22}$$

Both contributions are comparable in this regime and display quite different temperature and radius dependence. Hence, in principle, the onset of environmental decoherence might be observed and well separated from the other hypothetical mechanisms such as *gravitational collapse* and *spontaneous localization*, which incidentally are supposed to be of the comparable magnitude for a body containing 10^{15} atoms [5,6] (the mass-center motion of an electrically neutral body should not produce *bremsstrahlung*).

Unfortunately, the main obstacle is now a possibility of preparing and detecting quantum delocalized states. The difficulties are illustrated, for example, by the proposal of *free-orbit experiment with laser-interferometry x rays* [5]. Other geometrical obstacles for interference experiments with macromolecules are discussed in the next section.

C. Experiments on fullerenes

The recent successful experiments involving C_{60} [12], the molecules with $a\simeq 0.5$ nm, pushed substantially the border between classical and quantum worlds towards macroscopic objects. The authors rightfully argued that decoherence effects can be neglected under the conditions of their experiments. We can quite precisely estimate the decoherence magnitude using their data. First, we have to compute the total number of collisions $\overline{n}$ during the time of flight t of a fullerene due to emission, absorption and Rayleigh scattering of radiation and scattering of gas particles. For the emission the authors estimate $\overline{n_1}\approx 3.5$. As the environment temperature $T_1\approx 300$ K is much lower than the temperature of the fullerene molecule $T_2\approx 900$ K then due to Eq. (17) absorption can be neglected. The same holds due to Eq. (21) for the Rayleigh scattering because the radius a is much smaller than the average radiation wavelength $\lambda_{T_1}\approx 10$ μm. The number of collisions with gas particles is estimated to be $\overline{n_2}\approx 10^{-2}$ and can be neglected also. As $\overline{\lambda}\approx 10$ μm the coherence length (15) $l_{coh}\approx 1$ μm—the value that is still essentially larger than the width of the slits (50 nm) and their separation (100 nm). It follows that the diffraction picture is not destroyed by decoherence.

IV. GEOMETRICAL LIMITS FOR INTERFERENCE EXPERIMENTS

Any interference-type experiment demands that the de Broglie wavelength $\Lambda=2\pi\hbar/MV$ is comparable with the width of the slits d. In all existing experiments starting from the historical Young's experiment till the recent ones performed by Zeilinger group [12] the ratio $\delta=\Lambda/d$ is between $10^{-4}-1$. Obviously, for standard (material) diffraction gratings we have a geometrical condition

$$d\geqslant 2a. \tag{23}$$

On the other hand, V cannot be much smaller than the thermal velocity $V_{th}=\sqrt{8k_B T/\pi M}$ what gives

$$\Lambda\leqslant\frac{2\pi\hbar}{MV_{th}}=\frac{(\pi)^{3/2}\hbar}{\sqrt{(2Mk_B T)}}. \tag{24}$$

Putting $M=(4/3)\pi a^3\kappa$, where the density of the body $\kappa\approx 10^4$ kg/m^3 and a rather optimistic value for $\delta=10^{-5}$ we obtain from Eqs. (23),(24) the first condition for the successful interference type experiment,

$$a \leqslant \delta^{-2/5}(\hbar^2/\kappa k_B T)^{1/5} \approx 10(T[\mathrm{K}])^{-1/5} \ \ \mathrm{nm}. \qquad (25)$$

The second geometrical condition is related to the resolution of the interference picture, i.e., the distance D between the interference fringes on the "screen" which is placed at the distance L from the grating. Introducing the time of flight $t = L/V$ and adding another reasonable assumption that the resolution cannot be finer than the atomic scale,

$$D \geqslant D_0 = 0.1 \ \ \mathrm{nm}, \qquad (26)$$

we finally obtain the second condition

$$a \leqslant (\hbar t/\kappa D_0)^{1/4} \approx 100(t[\mathrm{s}])^{1/4} \ \ \mathrm{nm}. \qquad (27)$$

The very weak temperature and the time of flight dependence of the right-hand sides of Eqs. (25),(27) make rather impossible to go essentially far beyond the *nanometer* scale with traditional interference measurements satisfying the geometrical constraints (23),(26). It would be extremally difficult to overcome conditions (23) and (26) because a mass center does not couple to external fields except the case of uniform gravitational one. As a consequence, the new idea of using optical diffraction structures [13] ("made of" standing light waves) to overcome (23) is unlikely to work as the electromagnetic field will couple to a local atomic structure increasing decoherence and the net effect on a mass center will be averaged out. For the same reason, lacking a direct access, it would be difficult to localize the center of mass position with better accuracy than given by Eq. (26).

V. CONCLUSIONS

It was shown that under realistic laboratory conditions the environmental decoherence of the center-of-mass position can be eliminated on the time scale of *miliseconds* for macroscopic dust particles containing 10^{15} atoms—the regime that is relevant for testing different theories of decoherence. Nevertheless, the emerging quantum coherence effects are extremally difficult to observe at least in standard diffraction-interference type experiments. Therefore, only completely new ideas concerning preparation and measurement of spatially extended quantum states might push the border between quantum and classical worlds far beyond the scale of *nanometers*. On the other hand, the experiments involving large molecules of a diameter less than 10 nm are feasible and can provide interesting information concerning the detailed mechanism of environmental decoherence. In particular, the basic Eq. (7) is appropriate for precise quantitative description of environmental decoherence at laboratory. It will allow to use the interference of large molecules as a precise device to determine the parameters of environment. On the other hand, the presented examples show very sensitive dependence of decoherence on the size of molecule and its internal temperature. The same will be true for its shape, emissivity, etc. Hence, the interference devices might provide new techniques for separation of molecules.

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