Decoherence in a Two Slit Diffraction Experiment with Massive Particles

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Abstract. Matter-wave interferometry has been largely studied in the last few years. Usually, the main problem in the analysis of the diffraction experiments is to establish the causes for the loss of coherence observed in the interference pattern. In this work, we use different type of environmental couplings to model a two slit diffraction experiment with massive particles. For each model, we study the effects of decoherence on the interference pattern and define a visibility function that measures the loss of contrast of the interference fringes on a distant screen. Finally, we apply our results to the experimental reported data on massive particles C_{70}.

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The wave-particle duality of material objects is a hallmark of quantum mechanics. Up to now, the wave nature of particles has been demonstrated for electrons, neutrons, atoms, and coherent atomic ensembles. Yet more important, many theoretical studies have been done around the mesoscopic systems [1, 2]. Mesoscopic objects are neither microscopic nor macroscopic. They are generally systems that can be described by a wavefunction, yet they are made up of a significant number of elementary constituents, such as atoms. Well-known examples these days are fullerene molecules C_{60} and C_{70}, which are expected to behave like classical particles. Nonetheless, the quantum interference of these molecules has been observed [3]. In particular, the advances with large molecules have stimulated the question what determines the limits to observe quantum delocalization with massive objects. Thus, there is a need to theoretically quantify the effect of decoherence (or dephasing) on the observed interference pattern in a double-slit experiment. It is quite intuitive that the resulting pattern shall be an interplay between the strength of the coupling to the environment, the slit separation and the distance the particle travels from the slit to the screen.

We shall study a two slit diffraction experiment with particles of mass M diffracted by a grating (in the x direction) and then detected on a distant screen (located a distance L in the y direction). Note that coherence in the x direction is required in order to observe an interference pattern on the screen, whereas the dynamics in the y direction can be that of a free non-interacting particle since it just serves to transport the particle from the grating to the screen. Initially, we may reasonably assume that the action of the grating is to prepare a superposition of two Gaussian wavepackets (which best describe a massive particle), centered at each location of the respective slits and factorized as [4, 5] $\Psi(\vec{x},0) = (\phi_1(x,0) + \phi_2(x,0))\chi(y,0) \otimes \zeta(\vec{X},0)$, where $|\phi_1|^2$ and $|\phi_2|^2$ correspond to the probability amplitudes for the particle to pass through slit 1 and slit 2 (in the x-axis), respectively, while $\chi(y,t)$ represents the Gaussian wave function in the y direction (where no superposition is needed) and $\zeta(\vec{X},t)$ describes the state of the environment coupled to the subsystem. Note that we are assuming translational invariance in the z-axis [5].

We shall consider the environment as a set of non-interacting harmonic oscillators and the dynamics of the particles modeled by a quantum brownian motion (QBM) [6]. This behavior can be imputed to the passing of the particles through the slits producing vibrations or any other kind of interactions with the walls of the grating able to corrupt the interference pattern. Moreover, also the finite size of the grating and the differences in the slit apertures can attenuate the visibility of the interference fringes, especially in the case of complex molecules such us C_{60} and C_{70} [7]. In order to study the interference pattern registered on the screen at a later time t_L, we need to obtain the evolution in time of the reduced density matrix $\rho_r(x,x',t)$, which is given by the following master equation

$$\frac{\partial\rho_r(x,x',t)}{\partial t} = \frac{i\hbar}{2M}\Big(\frac{\partial^2\rho_r}{\partial x^2} - \frac{\partial^2\rho_r}{\partial x'^2}\Big) - \frac{\mathcal{D}(t)}{4\hbar^2}(x-x')^2\rho_r - \gamma(t)(x-x')\Big(\frac{\partial\rho_r}{\partial x} - \frac{\partial\rho_r}{\partial x'}\Big) + 2f(t)(x-x')\Big(\frac{\partial\rho_r}{\partial x} + \frac{\partial\rho_r}{\partial x'}\Big), \quad (1)$$

where $\gamma(t)$ is the dissipative coefficient (proportional to the square of the coupling constant to the environment), $\mathcal{D}(t)$ the diffusive coefficient and $f(t)$ the coefficient responsible for the anomalous diffusion. Eq.(1) has been obtained by assuming the environment to be in equilibrium, at a temperature T. In the case that the system is coupled to an ohmic environment in the high temperature limit ($k_BT >> \hbar\omega$), these coefficients are constant $\gamma(t) = \gamma_0$, $\mathcal{D}(t) = 2M\gamma_0 k_BT$ and $f(t) \approx 1/k_BT$ in units of $\hbar = 1$ [6]. It is important to stress that the equation of movement for the generally used scattering model $i\frac{\partial\rho_r}{\partial t} = [H,\rho_r] - i\Lambda[x,[x,\rho_r]]$, where the effect of the environment is included in the collision term Λ, can be obtained from Eq.(1) in the high temperature limit (neglecting dissipation) for the markovian case if written in the Lindblad form. However, this master equation refers to a more general movement that can be used for all temperatures, even to study the dynamics of the test particle at zero temperature. Yet more interesting, this formulation includes the phenomenological scattering model and verifies the fluctuation-dissipation theorem for a general system in thermal equilibrium.

The interference pattern corresponds to the probability distribution of the time evolved wave function:

$$P(\vec{x},t) = |\Psi(\vec{x},t)|^2 = \Big(\phi_1(x,t)^*\phi_1(x,t) + \phi_2(x,t)^*\phi_2(x,t) + \phi_2(x,t)^*\phi_1(x,t) + \phi_1(x,t)^*\phi_2(x,t)\Big) \otimes \chi(y,t)^*\chi(y',t),$$

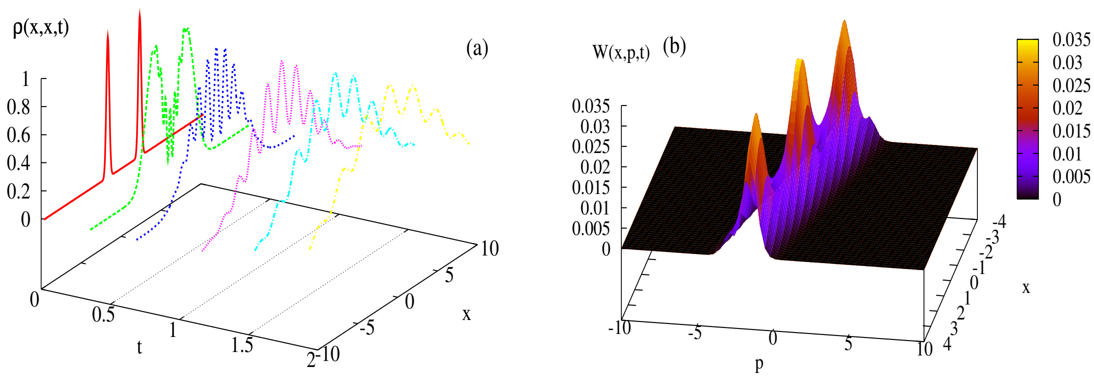

Figure 1. (a) Evolution in time for the interference pattern registered on the screen when the system is coupled to an environment. Parameters used: $L_0 = 2$, $\sigma_{x0} = 0.5$, $M = 1$, $\gamma_0 = 0.001$ and $k_BT = 300$. (b) For the same values the wigner function at $t = 2$ s shows that the interferences have disappeared since the wigner is positive.

which is proportional to the diagonal part of the density matrix defined as $\rho(\vec{x}, \vec{x}', t) = |\Psi(\vec{x}, t)\rangle\langle\Psi(\vec{x}', t)|$. In the case we are studying herein, i.e an open quantum system, the interference pattern at a given time t on the screen is given by:

$$P(\vec{x}, t) = \Big(|\phi_1(x,t)|^2 + |\phi_2(x,t)|^2 + 2\mathbf{\Gamma}(t)\mathrm{Re}(\phi_1^*(x,t)\phi_2(x,t))\Big)|\chi(y,t)|^2,$$

where the terms in brackets correspont to $\rho_r(x, x, t)$ and $\mathbf{\Gamma}(t)$ encodes the information about the statistical nature of noise since it is obtained after tracing out the degrees of freedom of the environment. $\Gamma(t)$ is an exponential decaying term which suppresses the interference terms in a decoherence time scale t_D. In the case of the QBM, $\Gamma(t) = e^{-\Delta x^2 \int_0^t \mathcal{D}(s)\mathrm{ds}}$ (with $\Delta x^2 = (x - x')^2$) represents the noise induced environmental effect on the system. In this framework, we numerically solved the master equation Eq.(1) for the reduced density matrix $\rho_r(x, x', t)$ of two well localized Gaussian wave packets initially given by

$$\Psi(\vec{x}, 0) = N\Big(\exp(\frac{(x - L_0)^2}{4\sigma_{x0}^2}) + \exp(\frac{(x + L_0)^2}{4\sigma_{x0}^2})\Big) \otimes \exp(-\frac{y^2}{4\sigma_{y0}^2} - ik_y y),$$

where $2L_0$ is the initial separation of the center of the wave packets, σ_{x0}^2 and σ_{y0}^2 are the initial width of the packet in the x and y-axis, respectively, and k_y the initial moment of the particle in the y direction. It is important to note that L_0, σ_{x0}, σ_{y0} and k_y are all free parameters that have to be tuned with the experimental data. In addition, we assume that $\Delta p_y << p_y$, so the moment component is sharply defined and the wave packet has a characteristic wavelength λ_{dB} associated $\lambda_{dB} \sim \hbar/p_y << \Delta y$ [8, 9]. Once the reduced density matrix is known for all time t, we know the dynamics of these two packets and can study the effects of decoherence on the interference pattern registered on the distant screen. In Fig.1(a) we present the time evolution for the interference pattern registered on the screen. We can there observe the two wave packets initially separated a distance

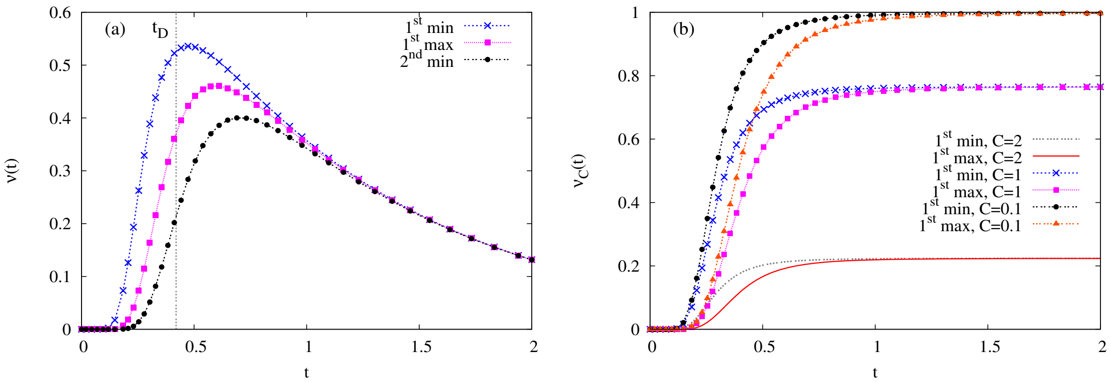

Figure 2. (a) Time evolution for the visibility fringe $\nu(t)$ for $k_BT = 300$, $\gamma_0 = 0.001$, $L_0 = 2$, $M = 1$ and $\sigma_{x0} = 0.5$. The estimation of the decoherence time $t_D \sim 1/(2M\gamma_0 k_B T L_0^2) = 0.41\ s$ coincides with the timescale at which the visibility starts to decrease towards a null value. (b) Time evolution for the visibility function $\nu_C(t)$ for neutrons ($C_{\rm N} = 0.1$) and fullerenes ($C_{\rm F} = 1$ and $C_{\rm F} = 2$) in the presence of an external classical time dependent electromagnetic field (incoherence effects). The curves are for the first minimum and maximum of the interference pattern and reach a different asymptotic value than in the case of $\nu(t)$.

$2L_0$ which start to spread as time increases. In a short timescale, interferences start to develop, however we can clearly observe that the minimum fringes of the interference pattern are not exactly zero. This means that there is a loss of contrast between theis case (an open system) with respect to the interference pattern of an unitary evolution. This means that decoherence is already playing a crucial role in determining the wave behavior of the massive particle. In Fig.1(b) we present the wigner function for the corresponding reduced density matrix at a fixed time $t = 2$ s. We can see that it is a completely positive function, which assures us that decoherence has been effective in this short timescale. We shall estimate the decoherence time t_D, i.e. the timescale for which the interferences are mostly destroyed (up to a 70 %) as $\Gamma_{\mathcal{D}}(t_D) = \exp(-\mathcal{D}\Delta x^2 t) \sim 1/e$. It is easily deduced that $t_D \approx 1/(\mathcal{D}\Delta x^2)$. A quantity of particular importance in matter wave interferometry is the fringe visibility $\nu(t)$. In order to study the role of decoherence on the fringe visibility, we define it as $\nu(t) \sim \frac{|\rho_{\rm int}(x,x,t)|}{\rho_{11}(x,x,t)+\rho_{22}(x,x,t)} = \frac{\Gamma(t)}{\rho_{11}(x,x,t)+\rho_{22}(x,x,t)}$ where $\rho_{ii} = |\phi_i(x,t)|^2$, with $i = 1, 2$ and $\rho_{\rm int}$ the interference terms.

Clearly, the visibility fringe goes down as t_L, i.e. the observation time, is larger than the decoherence time t_D. However, if we succeed in performing our two slit experiment in a time $t_L < t_D$ at a fixed room temperature k_BT, we can see that the visibility fringe decreases as the coupling to the environment (γ_0) increases. This is so, because the decoherence time depends inversely on the coupling constant: the bigger γ_0, the shorter the decoherence time. Not only can we check the dependence upon the coupling constant but also its time evolution. This behavior is shown in Fig.2(a). For short times, the visibility increases from zero to a maximum value because the interferences

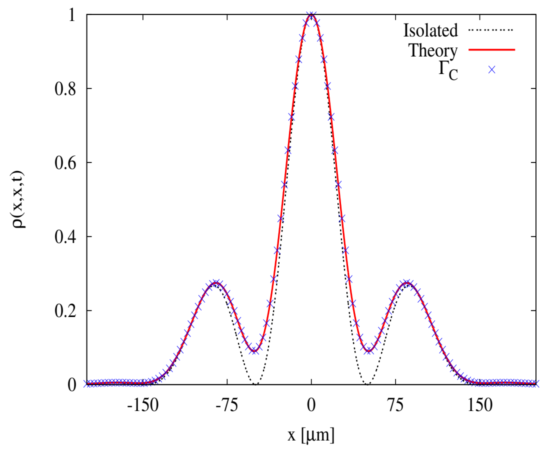

Figure 3. The interference pattern ($\nu \sim 0.62$) registered on the screen considering the incoherence (or dephasing) effects to model a two slit diffraction experiment with massive particles C_{70}. The curves are for the isolated case, the theoretical prediction using the experimental data reported in [3] and the incoherence model using Γ_C with $C = 1$.

start to develop at that short timescale but are not present at $t = 0$ (since the wave packets are initially separated and have to spread so as to generate the interferences see Fig.1(a)). This maximum value coincides with the estimated decoherence time t_D. Then, the visibility starts to decrease, since the destruction of the interferences is taking place. Note that the visibility is a quantity that measures the loss of contrast of the interference fringes. Then, it is expected that those with the bigger contrast suffer from this attenuation the more, as seen in Fig.2(a). Clearly, the observation time t_L must be shorter than the decoherence time in order to observe the interference pattern.

It shall also be interesting to study the visibility function for a model of incoherence such as the one presented by us in [10]. In particular, $\Gamma_C = J_0(|C|)$ is constant in time for the experimental data of neutrons and fullerenes [10]. Therein, we previously estimated the quantity C for these massive particles and observed that, contrary to might be naively expected, in thought and real experiments, $C_{\mathrm{F}} \sim \mathcal{O}(1)$. However, for neutral particles with permanent dipole moment this value is much lower $C_{\mathrm{N}} \sim \mathcal{O}(0.01)-\mathcal{O}(0.1)$. Therefore, we define the visibility function $\nu_C(t)$ as $\nu_C(t) = \frac{J_0(|C|)}{\rho_{11}(x,x,t)+\rho_{22}(x,x,t)}$ and show its time evolution for neutrons and fullerenes in Fig.2(b). We recall that this interaction is always present in charged and neutral particles with permanent dipole moment and can never be turned off. However, in the case of neutrons it has been shown in [10] that it can be neglected, whereas it is unexpectedly important for massive particles such as fullerenes.

Finally, we shall apply our models of decoherence and incoherence to the experimental data reported in [3] to reproduce the observed pattern for fullerenes C_{70}. In Fig.3, the interference pattern is shown. Therein, we have considered the unitary and nonunitary evolution of the particles. For these massive particles, we can see that the interference pattern is attenuated when the system is open. What is more important, is that the modeling of the incoherence effects through the overlap factor Γ_C is enough to reproduce the effects of the environment on the interference pattern of a real diffraction experiment with massive particles.

All in all, we have presented a fully quantum mechanical treatment using a microscopic model of environment and also a concrete example to include the incoherence effects. Therefore, we have studied the effects of decoherence on the interference pattern of thought diffraction experiments and presented an analysis of matter wave interferometry in the presence of a dynamical quantum environment such as the quantum brownian motion model. We have shown the interference patterns and visibility function $\nu(t)$ for thought diffracted free particles in the high temperature limit (assumption valid for massive particles diffracted at room temperature). Yet more important, we have defined the visibility function $\nu_C(t)$ for a model environment previously developed which describes the incoherence effects originated in the experimental difficulty of producing the same initial/final state for all particles (i.e the existence of a random variable such as the particle's emission time). We showed that it is qualitatively different than the one commonly found in the literature and very important in the case of diffraction experiments with massive particles such as fullerenes. In this case, the incoherence effects are enough to model the attenuation of the interference pattern observed in the real experiment, whereas in the case of cold neutrons the incoherence effects are not of such importance [11]. Therefore, in the latter case we must consider the decoherence effects by using the corresponding formulation (such us QBM). This result might have been expected since the interaction of more massive particles with the external classical field is more important than for those with a smaller mass where other kind of interactions (such as with the walls of the grating or the air molecules) seem to prevail.

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