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Superposition principle, spontaneous decoherence and C_{60} molecule interference*

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Abstract
A coherent superposition of two Gaussian wavepackets, which freely evolves in time, gives rise to an interference pattern similar to that of the single-particle double-slit Young's experiment. In this paper we show that fringe visibility can be reduced by spontaneous decoherence, which can also destroy quantum coherence when interaction between a system and its surroundings can be neglected. This decoherence is due to fluctuations in the evolution time and, in general, cannot be achieved when simple classical averages are considered. We compare our theoretical results with a C_{60} fullerenes interference experiment, where thermal decoherence is not relevant, but the fringe visibility is actually reduced.

Keywords: Quantum mechanics, interference, atomic and molecular physics

1. Introduction

Interference is one of the most amazing and puzzling fields of quantum mechanics. Feynman himself, speaking about Young's experiment with electrons, said that interference is '*the only mystery*' of the quantum mechanical world [1]. Double-slit experiments were used to give an example of the concept of quantum superposition and brought the scientists to the question of wave–particle duality: when it is possible to know the path of the interfering particles, quantum interference disappears. Furthermore, Scully *et al* [2] illustrated that the lost interference can be restored simply by erasing the *which-path* information. On the other hand, in this paper we consider a double-slit experiment from another point of view: a quantum Young's interference pattern is similar to that obtained when a superposition of two Gaussian wavepackets freely evolves in time. This analogy becomes clearer when the time t of the wavepacket time evolution is compared to the time $t = L/v$ that the particles of the Young's experiment moving at velocity v spend to reach a screen at a distance L [3]. We find that *spontaneous decoherence*, i.e. decoherence due to the system itself [4, 5] and not due to some interaction with the surroundings [6], reduces fringe visibility and we argue that this decoherence arises from velocity fluctuations of the interfering particles, as in cavity QED experiments [5], where they can destroy quantum coherence. Notice that in these experiments a simple classical average on velocity is not enough to describe the experimental results, as we show in the appendix of this paper. Finally, we compare our theoretical results with an interference experiment where C_{60} fullerenes are used as interfering particles [7]; here thermal decoherence and interaction with the surroundings are not relevant [7, 8], while velocity fluctuations are quite large.

2. Schrödinger spread and two-slit interference

A quantum superposition of two Gaussian wavepackets evolves in time giving rise to an interference pattern. We have discussed this effect in a previous paper, where we have shown that such interference is direct evidence of the Schrödinger spread and is described by the equation [3]

$$P(\bar{x},\bar{t}) \equiv |\Psi(\bar{x},\bar{t})|^2 \propto G_+ + G_- + 2\sqrt{G_+G_-}\cos[\omega(\bar{t})\bar{t}], \quad (1)$$

$\Psi(\bar{x},\bar{t})$ being the wavefunction of the system and

$$G_\pm = \exp\left\{-\frac{(\bar{x}\pm\bar{d})^2}{2(1+\bar{t}^2)}\right\}, \qquad \omega(\bar{t}) = \frac{\bar{x}\bar{d}}{1+\bar{t}^2}. \quad (2)$$

[*] This paper is dedicated to the memory of Luca Gardumi: I will never forget your friendship and kind hospitality.

In all the previous equations we used the scaling

$$\bar{x} = \frac{x}{\sigma_x}, \qquad \bar{d} = \frac{d}{\sigma_x}, \qquad \bar{t} = \frac{\sigma_v}{\sigma_x} t = \frac{\hbar}{2m\sigma_x^2} t \tag{3}$$

where σ_x is the width of the Gaussians, $\sigma_x \sigma_v = \hbar/2m$, m is the particle mass and equation (1) is obtained assuming the initial Gaussians centred in $x_1 = -x_2 = d$. Furthermore, under the condition

$$\bar{t} \gg \bar{d} \gg 1, \tag{4}$$

the time-dependent interference term $\cos[\omega(\bar{t})\,\bar{t}]$ is modulated by

$$\sqrt{G_+ G_-} \approx \exp\left\{-\frac{\bar{x}^2}{2\bar{t}^2}\right\}. \tag{5}$$

The link between what we said above and Young's interference experiment is achieved by taking into account the following considerations. We consider a beam of particles moving along the $\hat{z}$ axis with mean velocity $\bar{V}$ and with such a low intensity that one particle at a time arrives at a screen F where it passes through two slits (figure 1). In standard textbooks diffraction from a single slit is usually studied in momentum space, obtaining an angular distribution given by

$$\tilde{s}(k) = \frac{\sin(kb/2)}{kb/2} \equiv \mathrm{sinc}(kb/2) \tag{6}$$

where $k = 2\pi/\lambda$ is the wavevector and b is the slit width. Notice that the central peak of the sinc function can be well approximated by a Gaussian of width[1] $\sigma_k = \sqrt{2\pi}/b$. Moreover, a minimum uncertainty wavepacket is characterized by $\sigma_x \sigma_k = 1/2$, so that in the position space the diffraction is described by the Gaussian

$$g(x) \propto \exp\left\{-\frac{x^2}{2\sigma_x^2}\right\}, \tag{7}$$

where

$$\sigma_x = \frac{b}{2\sqrt{2\pi}}. \tag{8}$$

Now, in order to describe quantum double-slit interference, we assume as the initial wavefunction a superposition of two Gaussians with a width given by equation (8). Now the distribution $P(x,t)$ (coming from (1) using (3)) becomes the probability density of finding a particle on a screen S at distance L, such that $t = L/\bar{V}$, where $\bar{V}$ is the mean velocity perpendicular to the plane $\hat{x}$ of the slits (see figure 1); this is exactly the interference pattern one expects. In fact equation (5) can be written under the form of the diffraction envelope

$$\sqrt{G_+ G_-} \approx \exp\left\{-\frac{x^2 (2\sigma_x)^2}{2L^2 \lambdabar^2}\right\} = \exp\left\{-\frac{\vartheta^2}{2\vartheta_{\mathrm{diff}}^2}\right\}, \tag{9}$$

with $\lambdabar^2 = \lambda/2\pi \equiv \hbar/m\bar{V}$ (the *de Broglie wavelength*) and

$$\vartheta_{\mathrm{diff}} \equiv \frac{\lambda}{\sqrt{2\pi} b} \tag{10}$$

in agreement with the usual result.

[1] This condition is obtained by imposing that the sinc and Gaussian functions have the same height and area.

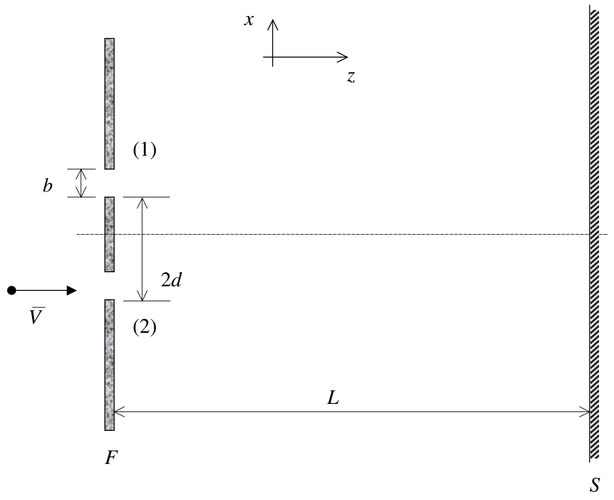

Figure 1. Set-up of a double-slit interference experiment.

3. Spontaneous decoherence and Young's interference

First of all we briefly summarize our model-independent formalism introduced in previous papers [5, 10, 11] to describe spontaneous decoherence due to fluctuations in the evolution time. The density matrix that takes into account these fluctuations is assumed to be the time average of the usual density matrix, i.e.

$$\bar{\rho}(t) = \int_0^\infty \mathrm{d}t'\, \mathcal{P}(t', t, \tau)\, \rho(t') \tag{11}$$

where the weight function is given by the Γ-distribution function

$$\mathcal{P}(t', t, \tau) = \frac{\exp(-t'/\tau)}{\tau} \frac{(t'/\tau)^{t/\tau - 1}}{\Gamma(t/\tau)}. \tag{12}$$

Such a choice was justified in [5] by imposing general conditions about the new density matrix $\bar{\rho}(t)$ and its time evolution. Here τ is a characteristic time which rules time fluctuations. Notice that τ can also be a function of t and can have experimental or intrinsic origin [5, 10].

In the interference case, since $t' = L/v$, time fluctuations are induced by velocity fluctuations as in the case of cavity QED studied in [5, 11]. Now, if the system is initially in a pure state, as assumed above, and we use the scaling (3), from equation (11) one obtains

$$\bar{P}(\bar{x}, \bar{t}) \equiv \langle \bar{x} | \bar{\rho}(\bar{t}) | \bar{x} \rangle = \int_0^\infty \mathrm{d}\bar{t}'\, \mathcal{P}(\bar{t}', \bar{t}, \bar{\tau}) P(\bar{x}, \bar{t}') \tag{13}$$

where the expression of $P(\bar{x}, \bar{t}')$ is given by (1) and $\bar{\tau}$ is

$$\bar{\tau} \equiv \frac{\sigma_v}{\sigma_x} \tau. \tag{14}$$

We argue that τ is the uncertainty in arrival time of particles at the screen, so that [3, 11, 12]

$$\bar{\tau} = a\bar{t} \qquad \text{with } a = \frac{\sqrt{\sigma_{\bar{V}}^2 + \Delta_{\bar{V}}^2}}{\bar{\mathcal{V}}}, \tag{15}$$

where $t = L/\bar{\mathcal{V}}$ and $\bar{\mathcal{V}}$ is the mean velocity of all the wavepackets along the $\hat{z}$ axis. Here we are assuming that particles along the $\hat{z}$ axis are described with minimum uncertainty wavepackets with mean velocity $\bar{V}$ and spread $\sigma_{\bar{V}}$. Moreover, if we note that each wavepacket can have a different mean velocity $\bar{V}$, then we define $\bar{\mathcal{V}}$ as the mean velocity of all the packets and $\Delta_{\bar{\mathcal{V}}}$ as the spread. In the limit $\bar{\tau}/\bar{t} = \tau/t = a \ll 1$ we can perform the average (13), obtaining

$$\bar{P}(\bar{x},\bar{t}) \propto G_+ + G_- + 2\sqrt{G_+G_-}\,\mathrm{e}^{-D}\cos\omega\bar{t} \qquad (16)$$

where, using equations (3) and (15),

$$D \approx \frac{\bar{x}^2\bar{d}^2}{2}\frac{\bar{\tau}}{\bar{t}^3} = \frac{1}{2}\frac{x^2(2d)^2}{L^2}\left(\frac{1}{\Lambda}\right)^2 a \qquad (17)$$

with

$$\frac{1}{\Lambda} \equiv \frac{m\bar{\mathcal{V}}}{\hbar}. \qquad (18)$$

The term e^{-D} is a *decoherence envelope not due to diffraction*, as in the case of equation (9), *but due to velocity spread*. It is very important and significative to note that it varies as $(2d)^2$, i.e. the square of the distance between slits, as is typical of all the decoherence phenomena [6].

One could think that this result could be easily reproduced just by performing an average on the classical velocity distribution along the $\hat{z}$ axis. However, this would give an expression of the decoherence exponent D similar to equations (17) but with two basic differences: (1) a^2 instead of a and (2) a will only be a function of the classical contribution $\Delta_{\bar{\mathcal{V}}}$, as shown in detail in the appendix. Hence, if $a < 1$, one will obtain a much smaller decoherence than in our approach.

4. Spontaneous decoherence and C_{60} interference

In a recent interference experiment, C_{60} fullerenes were produced in an oven, so that their velocity distribution had a most probable velocity $\bar{\mathcal{V}} = 220\ \mathrm{m\,s^{-1}}$ (corresponding to a de Broglie wavelength of 2.5 pm) and a spread $\Delta_{\bar{\mathcal{V}}}/\bar{\mathcal{V}} \approx 0.25$. They arrived at a grating and then a Channeltron electron multiplier counted their spatial distribution [7]. The interference pattern one expects can be well approximated by that from a double-slit experiment; as one can see in figure 2, the number of visible fringes is dramatically reduced and, in particular, the 'wings' of this interference pattern are not fitted by the standard Kirchhoff diffraction theory [13], which is only able to reproduce the central peak. Notice that this reduction of visibility cannot be associated with thermal decoherence, even if such molecules have an internal temperature as high as 900 K [8].

To fit the result displayed in figure 2, it is not enough to take into account the experimental velocity distribution. In fact, quoting [7] 'the agreement with the experimental results, including the 'wings', can be achieved allowing for a Gaussian variation of the slit widths over the grating, with a mean open gap width centred at $b = 38$ nm and with a full-width at half maximum of 18 nm'. The actual mean slit width (38 nm) is smaller than the width of 55 nm specified by the manufacturer, but this reduction can be justified if we consider the van der Waals potential which acts between the molecules and the slit

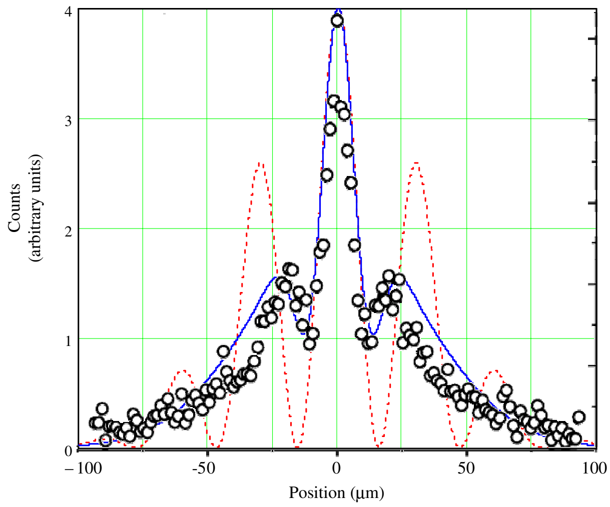

Figure 2. The dotted curve is a plot of equation (1), with the experimental parameters from [7]: $h/m\bar{\mathcal{V}} = 2.5$ pm, $2d = 100$ nm, $b = 38$ nm, $L = 1.25$ m, $\bar{\mathcal{V}} = 220\ \mathrm{m\,s^{-1}}$, $t = L/\bar{\mathcal{V}}$ and m is the particle mass. The solid curve is a plot of equation (16) with $a = 0.25$. Circles are experimental data from [7].

(This figure is in colour only in the electronic version)

edges and reduces the effective slit width of the grating [14]. However, the Gaussian variation of the width is not directly connected to the van der Waals potential, and could be due to the imperfections of the grating; these kinds of defects exponentially reduce the intensities of the maxima but also increase the diffuse background [15].

According to our formalism, we simply apply our theoretical results to the C_{60} interference experiment. In figure 2 we plot equations (1) and (16) using the experimental parameters from [7]. The dotted curve is the expectation of the quantum mechanical treatment of interference given by equation (1); the number of experimental fringes (circles) is actually reduced. Finally, the solid curve of the figure is a plot of equation (16) with $a = 0.25$ (we assumed $\Delta_{\bar{\mathcal{V}}} \gg \sigma_{\bar{V}}$). It is very interesting to note that our prediction only depends on the parameter τ, so that we must not invoke any kind of slit distribution to justify the experimental result. We think that the slight deviation from the data in figure 2 could be a consequence of other experimental errors which, at first approximation, we did not take into consideration (e.g. a classical average on the velocity distribution, which gives a second-order correction to the damping, see appendix).

Finally, from the point of view of equation (16), to increase the number of visible fringes and then the visibility of the interference pattern, one must reduce the width of the velocity distribution. This last assertion seems to be confirmed by the preliminary results of a new interference experiment, where the reduction of the velocity spread brings an increase in the visibility [8].

5. Conclusions

We have shown that interference fringe visibility can be reduced by *spontaneous decoherence*, i.e. a decoherence not due to interaction with the environment [4]. We argued that this kind of decoherence arises from fluctuations in the evolution time $t = L/v$, which, in this paper, are induced by particle velocity spread as already observed in cavity QED experiments [5].

Our theoretical results are in good agreement with a C_{60} fullerenes interference experiment, where extrinsic decoherence (thermal decoherence due to the internal vibrational states of the C_{60} molecules and their coupling with the surroundings) can be excluded [8]. In particular, our approach takes into account the presence of fluctuations in evolution time due to the velocity spread and this reproduces the experimental data, without any other assumption. In this way, our theory expects an increase of fringe visibility when the velocity spread is made narrower by a more efficient velocity selection, an expectation which is verified by the preliminary results of a new experiment [8].

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Appendix

We consider the effect of a simple average on a classical velocity distribution. For the sake of simplicity we assume a Gaussian velocity distribution:

$$P(v) = \frac{1}{\sqrt{2\pi}\,\Delta_{\bar{\mathcal{V}}}} \exp\left\{-\frac{(v-\bar{\mathcal{V}})^2}{2\Delta_{\bar{\mathcal{V}}}^2}\right\} \tag{19}$$

where $\bar{\mathcal{V}}$ is the mean wavepacket velocity and $\Delta_{\bar{\mathcal{V}}}$ is the spread. Furthermore, in the limit $\bar{t} \gg 1$, the interference term $\cos[\omega(\bar{t})\bar{t}]$ of equation (1) can be rewritten as

$$\cos[\omega(\bar{t})\bar{t}] \approx \cos\left(\frac{xd}{\sigma_x\sigma_v}\frac{v}{L}\right) \equiv \mathcal{I}(x, v) \tag{20}$$

where we used equations (2) and (3) and put $t = L/v$. Let us now perform the average of the interference term:

$$\langle\mathcal{I}(\omega, t)\rangle \equiv \int_{-\infty}^{\infty} \mathrm{d}v\, P(v)\mathcal{I}(x, v) = \mathrm{e}^{-A}\cos[\omega(\bar{t}_0)\bar{t}_0] \tag{21}$$

with $t_0 = L/\bar{\mathcal{V}}$ and

$$A \equiv \frac{\omega^2(\bar{t}_0)\,\bar{t}_0^2}{2}a^2 = \frac{1}{2}\frac{x^2(2d)^2}{L^2}\left(\frac{1}{\Lambda}\right)^2 a^2 \tag{22}$$

where $1/\Lambda \equiv m\bar{\mathcal{V}}/\hbar$.

Notice that in equation (22) $a \equiv \Delta_{\bar{\mathcal{V}}}/\bar{\mathcal{V}}$, so that the fluctuations in velocity have a simple *classical origin*, while in equation (15) the *quantum contribution* $\sigma_{\bar{\mathcal{V}}}$ due to the Heisenberg uncertainty principle is also present. Furthermore, one can observe that the exponential damping D of equation (17), coming from our theory, is a function of a, while in equation (22), due to a classical average, one finds a^2. When $a < 1$ the damping we obtain using our approach is greater than the damping due to the average of a velocity distribution. For this reason a classical average of velocity does not completely achieve for the 'wings' of figure 2.

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