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Dispersion and uncertainty in multislit matter wave diffraction

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Abstract

We show that single and multislit experiments involving matter waves may be constructed to assess dispersively generated correlations between the position and momentum of a single free particle. These correlations give rise to position dependent phases which develop dynamically as a result of dispersion and may play an important role in the interference patterns. To the extent that initial transverse coherence is preserved throughout the proposed diffraction setup, such interference patterns are noticeably different from those of a classical dispersion free wave.

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Fundamental aspects of quantum mechanics are revealed by diffraction experiments with particles. Much work has been devoted to the matter considering electron [1], neutron [2] and more recently large molecule [3,4] diffraction from multislit gratings. In the present contribution we are concerned with a double diffraction problem. The question to be addressed is how sensitive are the measured interference patterns to the dispersive dynamics of particle propagation *before* it reaches the grating and proceeds from there to the screen. We assume that a collimated beam with sufficiently large transverse coherence length γ is first sent through a narrow slit of width $\sigma_0 \ll \gamma$ after which it can be described by a fully coherent wave packet of initial transverse width σ_0 as described in detail below [5]. This wave packet subsequently goes through a second, multi-slit diffraction grating after a flight path sufficiently long to allow for the development of matter-wave dispersion effects. Also, as done in Ref. [7], we assume that the longitudinal (beam direction) wave packet localization is sharp enough compared with the flight path so that the time-of-flight approximation is valid. In other words, the flight paths involved in the problem are much larger than the position spread in longitudinal direction. Coherence loss mechanisms are neglected, since their effects are well known. In this idealized scenario a Gedanken experiment is described in terms of the time evolution of an initially Gaussian wave packet which travels freely from the first slit to the multislit grating.

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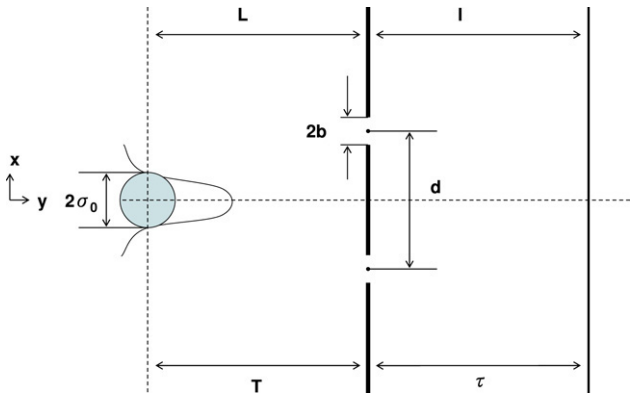

Fig. 1. Sketch of a double diffraction arrangement for a two-slit grating. Parameters: $\sigma_0 = 0.5 \times 10^{-5}$ m, $d = 10^{-7}$ m, $b = 1.8 \times 10^{-8}$ m, $L = 0.1$ m, $l = 1.25$ m, and $T = L/v$, $\tau = l/v$, where v is the velocity of the molecules.

This model sheds light on specific matter wave dispersion effects, notably the dynamic evolution of the position–momentum correlations. For a real initial Gaussian wave packet, these correlations appear in the form of a *position dependent* phase as soon as the particle leaves the first slit. The importance of this position dependent phase depends on the ratio between the time of flight and an intrinsic time $\tau = m\sigma_0^2/\hbar$, m being the particle mass and σ_0 is the initial width of the wave packet. Therefore if the particle travels long enough before it reaches the multislit grating, it will arrive at each slit with a different phase. As will be shown in what follows, this may radically alter the interference patterns observed on the screen.

In order to review the essential dispersive dynamic effects we discuss the time evolution in the transverse direction, from the first slit at $t = 0$ to the grating, of a Gaussian wave packet given by

$$\varphi(x, 0) = \left(\frac{1}{\sigma_0\sqrt{\pi}}\right)^{1/2} \exp\left(\frac{-x^2}{2\sigma_0^2}\right), \tag{1}$$

where x is the transverse direction (see Fig. 1) and the position in beam direction (y in Fig. 1) enters indirectly via the time coordinate. σ_0 is the width of the first slit. Its time evolution according to Schroedinger's equation will yield for the wave packet just before the grating [6]

$$\begin{aligned}\varphi(x, T) &= \left(\frac{1}{B(T)\sqrt{\pi}}\right)^{1/2} \exp\left[-\frac{x^2}{2B^2(T)}\left(1 - \frac{i\hbar T}{m\sigma_0^2}\right)\right] \\ &\equiv \widetilde{\varphi}(x, T)\exp(iS(x, T)),\end{aligned}$$

where

$$\begin{aligned}\widetilde{\varphi}(x, T) &= \left(\frac{1}{B(T)\sqrt{\pi}}\right)^{1/2} \exp\left[-\frac{x^2}{2B^2(T)}\right], \\ B^2(T) &= \sigma_0^2\left(1 + \frac{\hbar^2 T^2}{m^2\sigma_0^4}\right)\end{aligned} \tag{2}$$

and

$$S = \frac{x^2}{2B^2(T)}\frac{\hbar T}{m\sigma_0^2} \equiv \frac{x^2}{2B^2(T)}\frac{T}{\tau_0}. \tag{3}$$

Notice that the position dependent phase S contains the time scale $\tau_0 = \frac{m\sigma_0^2}{\hbar}$. The ratio T/τ_0 will determine the importance of this x-dependent phase to the interference pattern. In the experimental setups using fullerene molecules [3] $T/\tau_0 \approx 10^4$ which is also the condition for Frauhoffer diffraction (see Ref. [7]). The time scale τ_0 is fundamentally determined by Heisenberg's uncertainty relation, given the initial position dispersion $\Delta x(0) = \sigma_0/\sqrt{2}$.

In fact, the corresponding momentum dispersion is $\Delta p = \hbar/(\sigma_0\sqrt{2})$. Because the momentum is a constant of motion this momentum spread will be preserved in time. Both Δx and Δp constitute *intrinsic* properties of the initial wave packet, in terms of which the time scale τ_0 is expressed as [8]

$$\tau_0 = \frac{\Delta x(0)}{(\Delta p)/m}. \tag{4}$$

The numerator in the above relation represents the spatial dimensions of the initial wave packet, whilst the denominator stands for the scale of *velocity differences* enforced by the uncertainty principle. Therefore the time scale τ_0 corresponds essentially to the time during which a distance of the order of the wave packet extension is traversed with a speed corresponding to the dispersion in velocity. It can therefore be viewed as a characteristic time for the "aging" of the initial state, which consists in components with larger velocities (relatively to the group velocity of the wave packet) concentrating at the frontal region of the packet. This can be seen explicitly by deriving the velocity field associated with the phase S in Eq. (2), which reads

$$v(x, T) = \frac{\hbar}{m}\frac{\partial S}{\partial x} = \frac{Tx}{\tau_0^2 + T^2}. \tag{5}$$

This expression shows that for $T > 0$ the velocity field with the initial value $v(x, 0) = 0$ varies linearly with respect to the distance from centre of the wave packet ($x = 0$).

Next we relate quantitatively this "ageing" effect to position–momentum correlations. This is readily achieved using the generalized uncertainty relation devised by Schroedinger [9], which is expressed in this case in terms of the determinant of the covariance matrix Σ

$$\det \Sigma \equiv \det \begin{pmatrix} \Delta x^2 & \frac{1}{2}\langle \hat{x}\hat{p} + \hat{p}\hat{x}\rangle \\ \frac{1}{2}\langle \hat{x}\hat{p} + \hat{p}\hat{x}\rangle & \Delta p^2 \end{pmatrix} \geq \frac{\hbar^2}{4}.$$

For the minimumuncertainty wave packet of Eq. (2) we obtain, *at all times*,

$$\det \begin{pmatrix} \frac{B^2(T)}{2} & \frac{\hbar T}{2\tau_0} \\ \frac{\hbar T}{2\tau_0} & \frac{\hbar^2}{2\sigma_0^2} \end{pmatrix} = \frac{\hbar^2}{4}. \tag{6}$$

The Gaussian wave packet therefore saturates Schroedinger's uncertainty relation at all times. We can thus describe this result by saying that the time dependence of the *Heisenberg* uncertainty relation (obtained by dropping the off-diagonal elements of the covariance matrix) which is due, in this case, to the dispersive increase of the wave packet width in time, just reflects the $x - p$ correlation process. The relevant quantity in this connection is the correlation matrix element

$$\frac{\langle \hat{x}\hat{p} + \hat{p}\hat{x}\rangle}{2} = -\hbar\frac{T}{2\tau_0}. \tag{7}$$

Recently an interesting experiment [10] has been performed in order to study the Heisenberg uncertainty relation for fullerene molecules using the fullerene C_{70} and measuring the momentum spread after the passage through a narrow slit with a variable width (down to 70 nm). The results are interpreted in the light of Heisenberg's uncertainty relation. The results are summarized by the empirical relation

$$\Delta p = \frac{Ch}{\Delta x}, \tag{8}$$

where $C = 0.89$ and $h = 2\pi\hbar$. Having analytical expressions for each of the elements of the covariance matrix Σ and using the empirical value $\Delta x \Delta p = 0.89h$ we can evaluate $\langle xp + px\rangle$. Using the values of the experiment of Ref. [10] we get $\langle xp + px\rangle \approx 11.14\hbar$. This value is a measure of the $x - p$ correlation and thus of the dispersive increase of the wave-packet width.

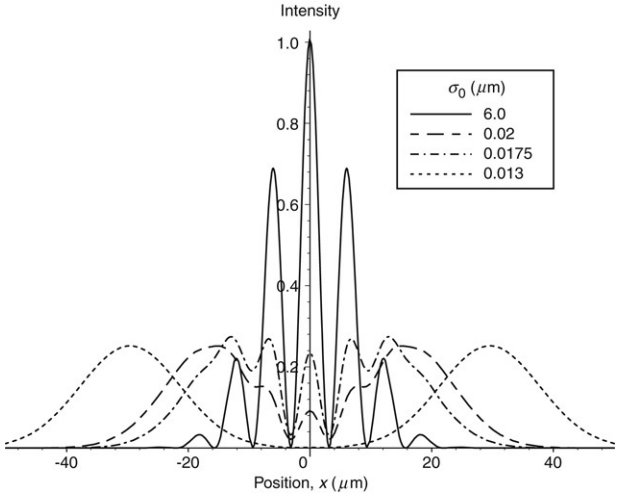

Fig. 2. Diffraction patterns for the arrangement of Fig. 1, for different values of the width of the first slit σ_0. As the intensity at $x = 0$ diminishes we have $\sigma_0 = 6.0$ μm, $\sigma_0 = 0.02$ μm, $\sigma_0 = 0.0175$ μm, $\sigma_0 = 0.013$ μm, respectively. Recall that the distance between two slits is ≈0.1 μm.

Two slit grating. We next consider the double diffraction experiment for a two-slit grating following the first slit (see Fig. 1). In this case the intensity at the screen is given by [7]

$$I(x) = |\Psi_+(x, T, \tau) + \Psi_-(x, T, \tau)|^2 \tag{9}$$

where

$$\Psi_\pm(x, T, \tau) = \int_{-\infty}^{+\infty} \mathrm{d}x_i \int_{-\infty}^{+\infty} \mathrm{d}w K(x, T + \tau; w, T) G(w \pm d/2) K(w, T; x_i, 0) \varphi(x_i) \tag{10}$$

and

$$K(z, t; w, t_0) = \sqrt{\frac{m}{2\pi i \hbar (t - t_0)}} \exp\left[i \frac{m(z - w)^2}{2\hbar(t - t_0)} \right], \tag{11}$$

$$G(w) = \exp\left[-\frac{w^2}{2b^2} \right], \quad \text{and} \tag{12}$$

$$\varphi(x_i) = \frac{1}{\sqrt{\sigma_0 \sqrt{\pi}}} \exp\left[-\frac{x_i^2}{2\sigma_0^2} \right]. \tag{13}$$

The kernel $K(z, t, w, t_0)$ is the free propagator for the particle, the functions $G(w \pm d/2)$ describe the double slit apertures which are taken to be Gaussian of width b separated by a distance d; the width of the first slit is σ_0, m is the mass of the particle, T (τ) is the time of flight from the first slit (double slit) to the double slit (screen). Parameter values are taken from Ref. [10].

Let us now allow for wave-packet "ageing", i.e. for significant transverse spreading with the accompanying $x - p$ correlation effects *before* reaching the two-slit grating. This can be achieved in a variety of ways, but we choose for simplicity to make σ_0 smaller while keeping the width just before the slits fixed at 1 μm. The result is shown in Fig. 2 for different values of σ_0, other parameters remaining unchanged. Note the qualitative changes of the interference pattern as the $x-p$ correlations grow, implying increasing phase difference between the contributions of the impinging wave packet at the two slits with decreasing σ_0.

Multislit grating. An alternate way to bring about the effects of quantum mechanical dispersion with fixed σ_0 is to consider diffraction by an increasing number of equally spaced diffraction slits instead of just two. In order to explore

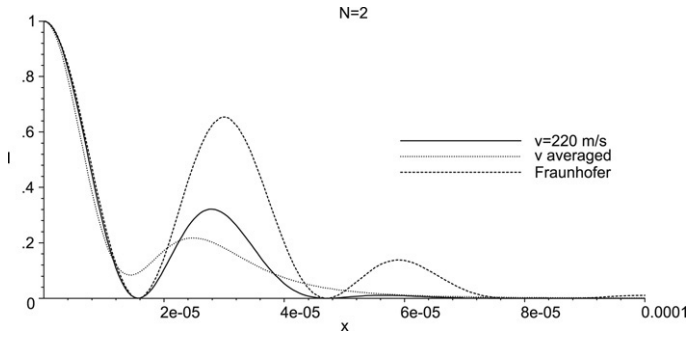

Fig. 3. Intensity pattern for two slits and parameters of Fig. 1.

this strategy we evaluate

$$I(x) = \left| \sum_{n=0}^{N-1} \Psi_n(x, T, \tau) \right|^2 \tag{14}$$

where

$$\Psi_n(x, T, \tau) = \int_{-\infty}^{+\infty} \mathrm{d}w \int_{-\infty}^{+\infty} \mathrm{d}x_i K(x, T+\tau; w, T) G(w - X_n) K(w, T; x_i, 0) \varphi(x_i) \tag{15}$$

with $X_n = X_0 - (N-1)\frac{d}{2} + nd$ for N slits centered around $X_0 = 0$. As discussed before, the wave function at the grating is given by

$$\Psi(x, t) \propto \exp\left[-\frac{x^2}{2B^2(t)} \left(1 - \frac{i\hbar t}{m\sigma_0^2} \right) \right] \tag{16}$$

where $B(t) = \sigma_0 \sqrt{1 + (\hbar^2 t^2)/(m^2 \sigma_0^4)}$. Note again the second term in the exponent giving rise to the quantum dispersive phase which will be different at each slit position. An estimate of the number of slits above which the effects of the phase in Eq. (16) become effective is

$$\frac{N^2 d^2}{2\sigma_0^2} \frac{\tau}{t} \geq 1. \tag{17}$$

With the parameter values of Ref. [10] and $\sigma_0 = 0.5 \times 10^{-5}$ m we obtain $N \sim 50$. The intensity $I(x)$ is depicted as a function of transverse position x in Figs. 3–5 for different values of the number of slits N (only half of the symmetrical interference pattern is shown). The parameters used correspond to the experimental setup for C_{60} molecules of Ref. [3]. In particular we take $\sigma_0 = 0.5 \times 10^{-5}$ m in the initial wave packet Eq. (13). The grating is characterized by the half width of the slits b and by the slit spacing d, the times T and τ in Eq. (2) are calculated from the velocity v of the molecules and the distance from the first slit to the grating and from there to the detector position respectively. Each figure shows the intensity for the most probable velocity $v = 200$ m/s (full line) and an incoherent sum over velocities (dotted line), which takes into account the experimental spread in the initial velocities of about 60% as parameterized in Ref. [3]. The dash-dotted lines exhibit the corresponding classical Fraunhofer interference pattern based on the de Broglie wavelength of the C_{60} molecule with $v = 220$ m/s.

The classical Fraunhofer expression for the intensity is very similar to the one with a definite velocity in the first case, $N = 2$. For the second case, $N = 30$, deviations from the classical Fraunhofer pattern can be seen. Note also that with such a large spread in the velocities this difference will not be experimentally accessible. For larger values of N as shown in Fig. 5 ($N = 100$), the difference between a matter wave and a classical wave becomes qualitative.

These are purely quantum effects; in fact they are quantum effects coming from the first stage of the experiment and the position dependent phase. Of course these effects could be observed for a smaller number of slits provided the x–p correlations in the first part of the experiment be large enough.

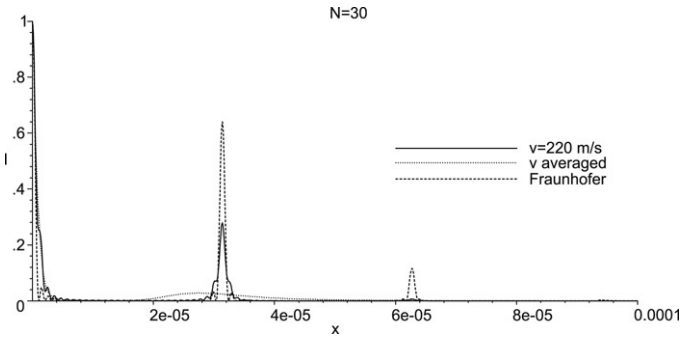

Fig. 4. Intensity pattern for thirty slits and parameters of Fig. 1.

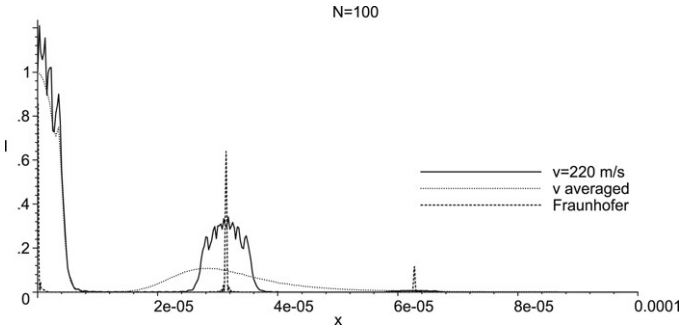

Fig. 5. Intensity pattern for a hundred slits and parameters of Fig. 1.

In summary, for multislit diffraction of matter waves we have shown that in an experiment with sufficiently monoenergetic trains of wave packets it is possible in principle to distinguish typical classical wave patterns from typical quantum matter wave patterns as a function of the number of slits. Decoherence and a spread in beam momentum will tend to obscure the effect we propose here. A possible way to circumvent this problem is to use paraxial light. When the conditions for this approximation to the Helmholtz equation are met there is a one-to-one correspondence between matter and light waves [11]. Besides, as extensively studied in Ref. [7], decoherence will not preclude the observation of interference fringes in the present experimental setup.

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