Quantum Effects in Matter-Wave Diffraction

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Abstract

Advances in micro-technology of the last years have made it possible to carry optics textbooks experiments over to atomic and molecular beams, such as diffraction by a double slit or transmission grating. The usual wave-optical approach gives a good qualitative description of these experiments. However, small deviations therefrom and sophisticated quantum mechanics yield new surprising insights on the size of particles and on their interaction with surfaces.

1 Introduction

The wave nature of subatomic particles was postulated by de Broglie in 1923 and this idea suffices to explain many diffraction experiments. Indeed, some people have argued that for matter diffraction a good optics book is sufficient. The aim of this contribution is to show that in many cases this is not so, and that full quantum mechanics may be necessary to describe and evaluate recent more sophisticated experiments. First of all it is clear from the statistical interpretation of quantum mechanics that a diffraction picture is build up slowly from individual particles each of which contributes a single dot on the screen. A single particle does not give an interference picture, only the complete particle beam does. This shows the wave property belongs to the beam and not the single particle.

Interestingly, for atoms the simple but fundamental double slit experiment has been just a thought experiment for a long time. This is due to their small de Broglie wavelengths $\lambda = H/p$, with $p$ the particle moment. For usual beam velocities of a few hundred meters per seconds this is only about 1 Å. Therefore very small slit widths and distances are needed to obtain observable diffraction angles. Only the recent advances in micro-technology have made atomic diffraction experiments possible.

Let us first consider wave optics and a transmission grating of period $d$ with $N$ slits of widths $s$. If a classical wave passes through a grating one observes behind it and outside the original direction an intensity with characteristic directional

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Figure 1: Diffraction pattern of helium atoms and molecules up to He$_{26}$ and thereby the first definite detection of these exotic molecules (cf. Refs. [3] and [4]).

The deflection angle $\theta$ of the planes $\{n\}$ with normal $\mathbf{n}$ is given by

$$\theta_n = n \lambda / d \quad (n = 0, \pm 1, \pm 2, \cdots) ,$$

where $\lambda$ is the wavelength of the incident particle and $d$ is the spacing between the planes. The intensity $I_n$ of the $n$th order diffraction is given by

$$I_n = I(\theta_n) \propto \frac{\sin^2(n \pi s_0 / d)}{(n \pi s_0 / d)^2} .$$

For many purposes this simple wave-optical approach gives a good description of matter diffraction also. However, in some cases effects from the full quantum theory may be important so that the simple wave picture is no longer appropriate. This will now be explained for recent experiments.

The typical experimental setup for atomic and molecular diffraction consists of a beam of particles with very small velocity distribution which pass through a
transmission grating or double slit [1, 2, 3]. The grating used by the Toennies group in Göttingen has a period of \( d = 100 \) nm. A beautiful diffraction pattern for a helium beam is shown in Fig. 1. In the inset in the upper right hand corner one observes the first helium diffraction order and left of it at half the angle another small maximum. The latter provided the first direct evidence of the exotic helium molecule \( ^4\text{He}_2 \). In the atomic beam there can be helium clusters, all moving with the same velocity. Therefore their de Broglie wavelengths and their diffraction angles are inversely proportional to their mass. The main part of the figure shows diffraction maxima of higher clusters up to \( \text{He}_{26} \). The Zeilinger group in Vienna recently observed diffraction of the fullerenes \( \text{C}_{60} \) and \( \text{C}_{70} \) [5].

Deviations from the simple wave-optical diffraction theory are expected to occur due to

- the inner structure of the particles and van der Waals potentials
- the spatial extent of the particles
- the breakup of weakly bound molecules.

Are these expected deviations just “dirt effects” or do they contain surprises with useful information? To investigate this question one needs the full quantum theory.

2 Quantum Theory of Matter-Wave Diffraction

First of all one has to realize that matter diffraction off a grating is not a classical wave phenomenon but a quantum mechanical scattering problem. The diffraction is not caused by the slits but by scattering of the particles off the grating bars. This is depicted in Fig. 2. In addition to the reflective particle-surface interaction one also has to take a attractive van der Waals surface interaction into account.

Starting from the Schrödinger equation and using Faddeev scattering theory in the formulation of Alt, Grassberger and Sandhas [7, 8] we have obtained a general expression for the diffraction intensity \( I_n \) of an extended molecule in the form

\[
I_n \propto e^{-\left(2\pi n s/d\right)^2} \left[ \frac{\sin^2(n\pi s_{\text{eff}}/d) + \sinh^2(n\pi \delta/d)}{(n\pi s_{\text{eff}}/d)^2 + (n\pi \delta/d)^2} \right]
\]

where \( s_{\text{eff}} \) denotes an effective slit width which is smaller than \( s \). The term \( \delta \) diminishes the contrast and the exponential term takes into account that the number of molecules in the individual diffraction orders may decrease due to breakups at the bars and that small variations in the bar widths may occur. All these parameters may depend on the particle-grating interaction, on the spatial extent of the particles and on their velocity.
2.1 Surface Effects

During the passage through a slit an atom experiences an additional attractive surface van der Waals potential \( V = -C_3/l^3 \) where \( l \) denotes the distance from the surface of a grating bar and where \( C_3 \) depends on the particle species. Quite recently we have found the as yet unpublished result that for rare gas atoms \( s_{\text{eff}} \) behaves as \( s_{\text{eff}} \propto 1/\sqrt{v} \) where \( v \) is the particle velocity. Therefore we have plotted \( s_{\text{eff}}(v) \) obtained from experimental diffraction patterns for variable helium beam velocities as a function of \( 1/\sqrt{v} \) in Fig. 3. From the slope one can determine \( C_3 \). The intersection with the ordinate axis yields the true slit width. The result agrees with an alternative procedure we have used before [9]. The method is so sensitive that the geometrical trapeze form of the grating base has to be taken into account.

For the evaluation of these measurements one does indeed need quantum mechanics but qualitatively the difference to wave-optics is not so pronounced since an optical grating with a dielectric coating can produce similar effects. This however is no longer true in the following example.

2.2 Size of the Helium Dimer

The main difference to wave-optics occurs for excitations of higher levels [10] as for the helium trimer \( \text{He}_3 \) and for size and breakup effects [4]. The latter two effects are particularly interesting for the exotic \( \text{He}_2 \) which is fifty times larger than a hydrogen molecule and whose binding energy is a hundred million times smaller than that of an electron in a hydrogen atom. Therefore \( \text{He}_2 \) is extremely fragile and thus very difficult to investigate by conventional methods. But at
small diffraction angles most helium dimers arrive at the detectors unbroken so that deviations of the diffraction pattern from the predictions of wave-optics can be measured and analyzed.

In Ref. [11] experimental dimer diffraction intensities up to 7th order have been fitted to the expression $I_n$ from Eq. (4) and $s_{\text{eff}}$ was determined. By quantum mechanical multi-channel scattering theory we obtained a relation between $s_{\text{eff}}(v)$ and the inter-nuclear distance $\langle r \rangle$. A simplified result is $\langle r \rangle/2 = s_{\text{He}}^{\text{He}}(v) - s_{\text{eff}}^{\text{He}}(v)$, which gives $\langle r \rangle \approx 50 \, \text{Å}$. The more precise theory yields $\langle r \rangle = 52 \pm 4 \, \text{Å}$.

3 Conclusions

These examples show that refinements of a simple textbook experiment on matter diffraction can lead to new quantum mechanical applications in atomic and molecular physics. In particular we have discussed

- its use as a quantum mass spectrometer
- exploitation of quantum effects for
  - particle surface interaction

Figure 3: Plot of $s_{\text{eff}}$ over $1/\sqrt{v}$ for helium. From the slope of the straight line one can calculate $C_3$. The ordinate intersection gives the true slit width of $s = 71.2$ nm.
– influence of the particle size on the diffraction pattern: size determination
– detection of excited energy levels for He$_3$ (work in progress)

As a further development we mention the setup of an atom interferometer which, in a first approximation, can be understood similarly as in wave-optics, but to describe finer effects one needs full quantum mechanics.

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