A study of matter-wave diffraction for particle in the near field regime under the influence of a uniform electric field

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Abstract. For various experiments to investigate quantum effects, matter-wave diffraction is an apparent example. Particle diffractions have been measured even at the large molecular level, such as the C_{60} molecules. In order to describe the matter-wave diffraction of C_{60} beam, we assume the initial wave functions behind a grating in form of the Fourier series with a Gaussian distribution function. By applying the Feynman path integral, the exact wave functions of the molecule diffraction in the near-field regime can be derived analytically. The obtained probability density distributions are corresponding to interference fringes as found in the Fresnel diffraction. The probability of finding C_{60} molecules, behind the grating at the Talbot length, consistency with the mentioned experimental data of C_{60} diffractions.

1. Introduction

Diffraction phenomena in the near-field regimes are based on Fresnel diffraction theory, and the Talbot effect is a renowned optical example. The Talbot effect, discovered by Henry Fox Talbot in 1836, was found when the plane-wave light passes a diffraction grating, it produces a periodic interference pattern. The shape has the periodicity similar to grating itself, so-called self-image, observed by locating the screen behind the grating at a certain distance called the Talbot length (L_T) [1]. The Talbot effect has been widely applied in many studies and applications, such as a study of optical vortices [2], high-contrast optical vortex detection using the Talbot effect [3], elastic wave in solid [4], x-ray Talbot interferometry [5], and distance measurement [6]. In addition, the Talbot effect applications have been used to study a quantum phenomenon, opening a new framework between the foundation of physics, quantum optics, and physical chemistry [7].

Matter-wave diffraction is one of the important tools and becomes the useful approaches to investigate quantum effects. There were many successfully proven matter-wave experiments, which had been performed with electrons [8], neutrons [9], He atom [10], and molecular I_2 [11]. Not only the matter-wave experiments of small particle have been achieved, the diffractions have been measured even at the large molecular level. Such as the fullerene molecule C_{60} which have been considered the pattern diffraction under influence of an electric field for estimating the scalar polarizability of molecules [12].

In this study, we present a simple description of the matter-wave diffraction of the C_{60} molecules in the near-field regime. We assume an initial wave function behind the diffraction grating in form of the Fourier series modulated by a Gaussian distribution function. By applying the theory of the Feynman path integral [13], we calculate the exact wave functions of the molecule diffraction. Finally, we evaluate

the probability of finding C_{60} molecules behind the mask grating at two Talbot length and compare our calculations to the experimental data [12].
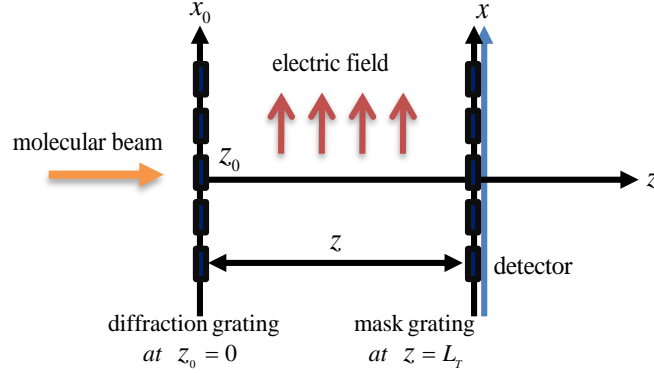
Figure 1. The coherent molecular beam passes through a diffraction grating at $z_0 = 0$, a mask grating at $z = L_T$, and then a detector. The two gratings are separated by one or multiples of the Talbot length $L_T = d^2/\lambda_{dB}$, where λ_{dB} is the de Broglie wavelength. The probability density of molecules is found with the detector behind the mask. The influence of an electric field between the gratings leads to a transverse shift of the diffraction pattern.

2. Theory and method

In this section, we present a brief derivation of the matter-wave diffraction. A molecular beam was prepared for a coherent source by passing through a grating or a single slit. Therefore, we assume that the coherent molecular source with a Gaussian beam shape spreads along x_0 axis and travels along z axis through the diffraction grating. The diffraction grating is placed at $z_0 = 0$, as shown in figure 1, the initial wave function may be assumed in form of the Fourier series modulated by a Gaussian distribution function as

$$\psi_0(x_0, z_0, t=0) = C\sum_n A_n \exp\left\{ink_d x_0 - \frac{x_0^2}{\beta_x^2}\right\}\exp\left\{ikz_0 - \frac{z_0^2}{\beta_z^2}\right\}, \tag{1}$$

where C is the normalized factor, and $k_d = 2\pi/d$ with d is the grating period. The wave vector k is corresponding to λ_{dB}. The factor $A_n = \sin(n\pi f)/n\pi$ is the components of the Fourier decomposition of the periodicity for the grating with an opening fraction f, where $n = 0, \pm 1, \pm 2, \dots$ [14]. The parameters β_x and β_z denote the full width at half maximum (FWHM) of the Gaussian distribution of the molecular beam. At a later time $t > 0$ behind the diffraction grating, the time evolution of ψ is described by

$$\psi(x, z, t) = \int dx_0 \int dz_0 K(x, z, t; x_0, z_0, 0)\psi_0, \tag{2}$$

where

$$K(x, z, t; x_0, z_0, 0) = \frac{M}{2\pi i\hbar t}\exp\left\{\frac{iM}{2\hbar t}(z - z_0)^2\right\}\exp\left\{\frac{i}{\hbar}\left[\frac{M}{2}\frac{(x-x_0)^2}{t} + \frac{F_x(x+x_0)t}{2} - \frac{F_x^2 t^3}{24M}\right]\right\} \tag{3}$$

is the propagator for a particle mass M moving in xz plane along z axis under the influence of an electric force F_x along x axis. Since the initial wave has been written in the exponential form, the integral in equation (2) can be done analytically. Consequently, the exact wave function can be obtained as

$$\psi(x, z, t) = C_t^2 \exp\left[R(z,t)\right]\sum_n A_n \exp\left\{P_n(x,t) + iQ_n(F_x, z, x, t)\right\}, \tag{4}$$

where

$$R(z,t) = -\frac{1}{\beta_z^2 \gamma_z}\left(z - \frac{k\hbar t}{M}\right)^2, \tag{5}$$

$$P_n(x,t) = -\frac{1}{\beta_x^2 \gamma_x}\left(x - \frac{F_x t^2}{2M} - \frac{nk_d \hbar t}{M}\right)^2, \tag{6}$$

and

$$Q_n(F_x, x, z, t) = \left(-\frac{F_x k_d n t^2}{2M} - \frac{F_x^2 t^3}{6M\hbar} + \frac{F_x tx}{\hbar} + nk_d x - \frac{n^2 k_d^2 \hbar t}{2M}\right) + \left(kz - \frac{k^2 \hbar t}{2M}\right) \tag{7}$$

with $C_t = \sqrt{C^2 / \gamma_x \gamma_z}$ with $\gamma_x = 1 + 2i\hbar t / M\beta_x^2$ and $\gamma_z = 1 + 2i\hbar t / M\beta_z^2$.

In order to describe the molecules detecting behind the mask grating (figure 1), we multiply the probability density $|\psi(x,z,t)|^2$ with a step function which is corresponding to the mask grating. Therefore, the probability of finding the molecules behind the mask grating can be represented as

$$I(x,z) = \sum_j F_j(x-\delta)|\psi(x,z,t)|^2. \tag{8}$$

Here, the step function $F_j(x)$ is given by

$$F_j(x) = \begin{cases} 1 & ; \ jd - \dfrac{fd}{2} < x < jd + \dfrac{fd}{2}, \\ 0 & ; \ \text{otherwise} \end{cases} \tag{9}$$

where $j = 0, \pm 1, \pm 2, \ldots$ and δ is the transverse shift, along x-axis, between the two gratings [15].

3. Results and Discussions

We demonstrate the theoretical simulations of the molecule C_{60} diffraction from the obtained wave function. The molecular beams move through the diffraction grating with the average velocity $v = 117$ m/s, then pass through the mask grating which is able to move transversely in the x-axis, as shown in figure 1. The two gratings with the period of $d = 911$ nm and the opening fraction of $f = 0.45$, are separated by two Talbot length $2L_T = 2d^2/\lambda_{dB} = 41.7$ cm. Since the molecules move freely along z-axis behind the diffraction grating, the corresponding probability density distribution can be simulated by using the absolute modulus of equation (4) with substituting time $t = z/v$ and the Gaussian radius $\beta_x \gg d$ and $\beta_z \gg \lambda_{dB}$, as shown in figure 2.
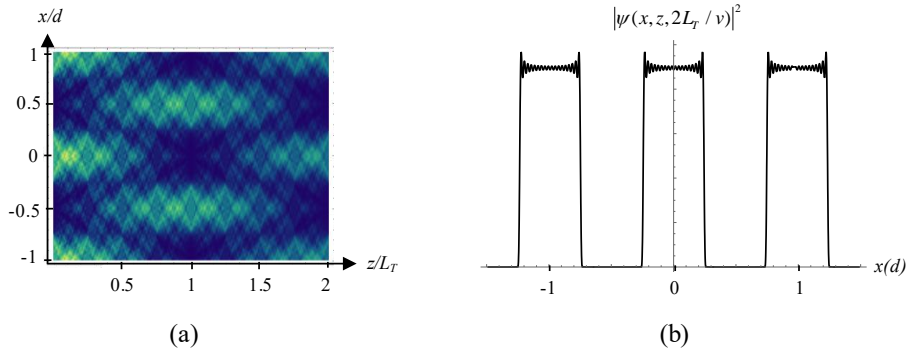
Figure 2. The probability density $|\psi(x,z,t = z/v)|^2$ at $z = 2L_T$, according to equation (4) without the electric field on **(a)** the xz-plane and **(b)** the distribution along x-axis.

To compare our simulations to the experimental data of the molecule counting in the Ref. [12], the probability density of the molecule diffractions is simulated by applying equation (8). Scanning the mask grating in steps of 20 nm can be involved in the theoretical calculation by changing the transverse shift with the same range, about $0 \le \delta \le 2d$, as done in the experiment [12]. Figure 3 shows the theoretical calculations in comparison to the experimental data. Both graphs express a consistent trend. The shifted pattern due to the electric field can be obtained by using the transverse force $F_x \simeq 9.4 \times 10^{-26}$ N.
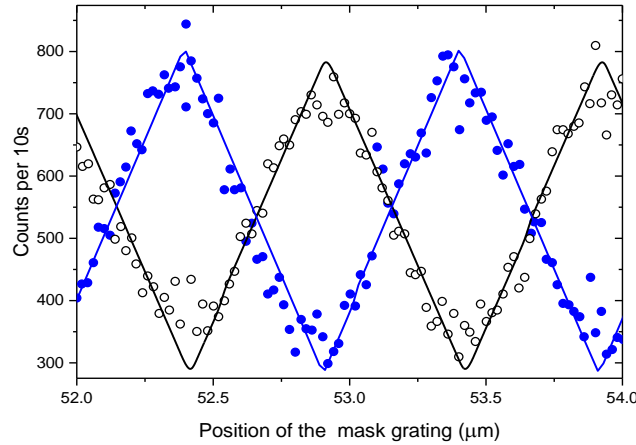
Figure 3. The simulation versus the experiment of the probability density of finding C_{60} molecules at $z = 2L_T$. The full circles and the open circles are the experimental graph of the molecule counting behind the mask with and without electric field, respectively [12]. The solid lines represent the theoretical calculations equation (8) with transverse force $F_x \simeq 9.4 \times 10^{-26}$ N and $F_x = 0$, respectively.

4. Conclusions

This theoretical study presents a practical analytical and simulation scheme for matter-wave diffraction in the near-field regime. We applied the Feynman path integral to calculate the exact wave function. In addition, we considered the C_{60} molecules pass through a grating diffraction. Finally, the probability density distribution of finding the molecules behind the mask grating gave the theoretical results in accordance with the molecules detecting as found in the experimental data.

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