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Atom diffraction from magnetic gratings in the thin phase-grating approximation

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Abstract. The problem of atom diffraction from a reflecting magnetic diffraction grating is solved in the thin phase-grating approximation. The general problem for scalar diffraction is modelled using a semi-classical method in which the grating potential is separated into a reflecting term and a diffracting term. The trajectory of the atom in the reflecting potential is solved classically and the atom wave function in the diffracting potential found by integrating the phase change along the classical trajectory. The diffraction orders are obtained after Fourier transforming the result. This can be done independently of the grating potential resulting in a general formula for the diffraction efficiencies. The general result is applied to the problem of atom diffraction from a magnetic grating. Several approximations are required to reduce the problem to a form amenable to analytic solution. The results are compared with an accurate numerical method.

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1 Introduction

Current research into optical elements for the control and manipulation of slow-moving atoms has been driven by the development of laser techniques for creating clouds of ultra-cold atoms. Both evanescent wave and magnetic mirror technology have become well established but there has only been limited success in making and demonstrating diffraction gratings for atoms. A reflecting diffraction grating for atoms can be made from an evanescent standing wave of light [1] and evidence of diffraction has been observed at grazing incidence [2–4] and at normal incidence [5] although the diffraction orders in the latter were not resolved. Another method for producing reflecting diffraction gratings for atoms has been proposed based on periodic arrays of permanent magnetisation or current-carrying wires [6]. These structures form magnetic fields that fall off rapidly with distance to create magnetic mirrors that reflect [7–17] or deflect paramagnetic atoms [18,19] (also see the review [20]). The diffraction grating is formed by applying an appropriate uniform magnetic field to the mirror field. This produces a periodic variation in the strength of the magnetic field [6]. The periodicity of the grating formed by this method is equal to the periodicity of the magnetisation of the mirror. Such devices have potential application in the coherent splitting of atomic de Broglie waves as required in matter wave interferometers.

Conventional laser-cooling techniques produce atoms with wavelengths of the order of 100 nm and below. Most of the magnetic mirrors produced to date have a periodicity greater than 10 μm, which is generally too large to be used as diffraction gratings for atoms. However, recent developments using microlithography have led to the production of mirrors formed from permanent magnet arrays with sub-micron periodicity [21]. To be used efficiently to diffract atoms it is important to have an understanding of the factors that affect the diffraction efficiencies. In this regard analytical models of the diffraction process are important. In this paper we develop an approximate method for calculating the diffraction efficiency of atoms from a magnetic diffraction grating. The method that we present is similar to that of Henkel *et al.* [22] who model the diffraction of atoms from both Gaussian standing waves and evanescent standing waves of light. A review of the theory of diffraction of atoms from evanescent waves is given in [23]. The models require an approximation that is valid for weak potentials that do not change rapidly. In this regard the potentials act as thin phase-gratings and the approximation is referred to as the thin phase-grating approximation (TPGA).

The general problem of diffraction within the TPGA is formulated in Section 2. This yields an expression for the reflectance of a diffracting order from any thin grating. By limiting this to a potential with a single spatial frequency we obtain a general formula for the diffraction efficiencies, defined as the relative flux of atoms in a particular diffraction order. In Section 3 the general formula is applied to

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the magnetic diffraction grating. Then in Section 4, the approximate analytical result is compared with an accurate numerical method [24] for calculating the diffraction of atoms from any reflecting periodic potential.

2 Thin phase-grating approximation

2.1 General reflecting diffraction grating

The wave properties of matter are described by the time-independent Schrödinger equation

$$\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r}) + (E - V(\mathbf{r}))\Psi(\mathbf{r}) = 0 \tag{1}$$

where E is the energy of the atom of mass m, V is the potential energy with $\hbar$ Planck's constant divided by 2π. We express the atom energy in terms of its kinetic energy at a point far from the grating, $E = \hbar^2k^2/2m$, where k is the wave number of the incident atom, and re-scale the potential $U(\mathbf{r}) \equiv (2m/\hbar^2)V(\mathbf{r})$, which enables us to write (1) in the form

$$\nabla^2\Psi(\mathbf{r}) + (k^2 - U(\mathbf{r}))\Psi(\mathbf{r}) = 0. \tag{2}$$

With these units, k is equivalent to the momentum and k^2 is equivalent to kinetic energy. We shall take the interaction described by (2) to be independent of the internal degrees of freedom of the atom so that the wave function as a scalar quantity. It then follows that the present theory is only applicable to scalar diffraction problems.

The potential U is associated with the diffraction grating. It is responsible for reflecting the atoms as well as causing diffraction. In the following derivation we shall assume that the diffraction grating lies in the x–z-plane and is periodic in x with the upwards direction along the y-axis. The potentials that we consider are independent of z so that the problem is essentially two-dimensional. The problem is simplified by separating out the part of the wave function associated with the "mirror" or reflecting potential from that due to diffraction. We do this by writing the wave function in (2) as a product

$$\Psi(\mathbf{r}) = \Psi_{\mathrm{m}}(\mathbf{r})\Psi_{\mathrm{g}}(\mathbf{r}) \tag{3}$$

where the mirror function satisfies

$$\nabla^2\Psi_{\mathrm{m}}(\mathbf{r}) + (k^2 - U_{\mathrm{m}}(\mathbf{r}))\Psi_{\mathrm{m}}(\mathbf{r}) = 0 \tag{4}$$

and where U_{m} is that part of the potential responsible for reflection. The potential responsible for diffraction is then $U_{\mathrm{g}} = U - U_{\mathrm{m}}$. From (2–4) we find that the grating wave function is given by

$$\nabla^2\Psi_{\mathrm{g}}(\mathbf{r}) + 2\mathrm{i}\mathbf{p}(\mathbf{r})\cdot\nabla\Psi_{\mathrm{g}}(\mathbf{r}) - U_{\mathrm{g}}(\mathbf{r})\Psi_{\mathrm{g}}(\mathbf{r}) = 0 \tag{5}$$

where $\mathbf{p}(\mathbf{r}) \equiv -\mathrm{i}\nabla\Psi_{\mathrm{m}}(\mathbf{r})/\Psi_{\mathrm{m}}(\mathbf{r})$ represents the momentum (or strictly wave number) of the atom wave at $\mathbf{r}$ in the mirror potential. To enable us to solve the problem analytically, we shall replace this by the classical momentum at each point on the trajectory of the atom in the mirror potential. Since we are mixing classical and quantum concepts the method becomes a semi-classical one. Note that far from the mirror $\mathbf{p} = \mathbf{k}$, the incident wave vector.

To solve (5) we assume that $\nabla^2\Psi_{\mathrm{g}}(\mathbf{r})$ is sufficiently small that it can be ignored, *i.e.* $|\nabla^2\Psi_{\mathrm{g}}(\mathbf{r})| \ll |2\mathbf{p}(\mathbf{r})\cdot\nabla\Psi_{\mathrm{g}}(\mathbf{r})|$. As we discuss below, this requires the diffracting potential to vary slowly over a distance of the order of the atom wavelength and for the strength of the potential to be much smaller than the kinetic energy of the atom. In this regard the diffraction grating behaves as a thin phase-grating. The approximation is referred to as the thin phase-grating approximation (TPGA).

If we let $p_x(\mathbf{r}) = -\mathrm{i}(\partial\Psi_{\mathrm{m}}(\mathbf{r})/\partial x)/\Psi_{\mathrm{m}}(\mathbf{r})$, do likewise for $p_y(\mathbf{r})$ and ignore $\nabla^2\Psi_{\mathrm{g}}(\mathbf{r})$, then (5) becomes a first-order partial differential equation

$$p_x(\partial\Psi_{\mathrm{g}}/\partial x) + p_y(\partial\Psi_{\mathrm{g}}/\partial y) = (-\mathrm{i}/2)U_{\mathrm{g}}\Psi_{\mathrm{g}}. \tag{6}$$

(A similar reduction to a first-order equation was done by Henkel *et al.* [25] to model diffraction from a time-modulated evanescent wave mirror.) From the theory of partial differential equations [26], we find that the solution to (6) lies along characteristic curves. If we use the classical momentum for $\mathbf{p}$, the characteristics are the set of trajectories of the atom in the mirror potential determined by $\mathrm{d}y/\mathrm{d}x = p_y/p_x$. At this stage we do not need to specify these characteristics so that $\mathbf{p}$ may be either the quantum mechanical or the classical momentum. The general solution to (6) is found by introducing an integral operator L whose inverse is a differential operator defined by $L^{-1} \equiv 2\mathbf{p}(\mathbf{r})\cdot\nabla$. Then (6) can be written in the form

$$L^{-1}\Psi_{\mathrm{g}}(\mathbf{r}) = -\mathrm{i}U_{\mathrm{g}}(\mathbf{r})\Psi_{\mathrm{g}}(\mathbf{r}) \tag{7}$$

which has a solution

$$\Psi_{\mathrm{g}}(\mathbf{r}_{\mathrm{f}}) = \exp(-\mathrm{i}LU_{\mathrm{g}}(\mathbf{r})) \tag{8}$$

normalised to unit amplitude. The vector $\mathbf{r}_{\mathrm{f}}$ is the end point of the integration and it is associated with the characteristic curves of the integral operator L. In this formula, the atom wave function is determined by the phase change, arising from the grating potential, accumulated along the characteristic curves. If the classical momentum is used for $\mathbf{p}$ then the characteristic curves are the classical trajectories of the atom in the mirror potential. For any specified starting momentum at a given height there is a whole class of characteristics corresponding to different starting positions in x. Each of these characteristics is symmetrical about a point $x = x_0$ corresponding to the x-position of the classical turning point associated with the trajectory. If we shift the x-axis origin for each characteristic to x_0, then the integral operator L is independent of the particular characteristic in the class. This also has the advantage of making the symmetry in the x-direction explicit, so that terms in U_{g} that are anti-symmetric about $x = 0$ will integrate to zero. Assuming that the grating potential is independent of z, we expand U_{g} in a Fourier series across the grating of period a with

spatial frequency $\kappa = 2\pi/a$

$$U_{\rm g}(x,y) = \sum_m u_m(y)\exp({\rm i}m\kappa(x+x_0)) \tag{9}$$

where the x-origin is now at x_0. Since x_0 is a constant for a given trajectory, it is not operated on by L. Thus with (9) in (8) we have

$$\Psi_{\rm g}(x_{\rm f},y_{\rm f}) = \exp\left(-{\rm i}\sum_m \exp({\rm i}m\kappa x_0)L(u_m(y)\exp({\rm i}m\kappa x))\right). \tag{10}$$

The diffraction orders associated with the wave function in the TPGA can be obtained from a Fourier transform across the line at a constant height $y_{\rm f}$ after interaction with the grating [22]. Since the final x-position $x_{\rm f}$ is linearly related to x_0, we can replace $x_{\rm f}$ by x_0 in the Fourier transform. The consequence is a constant phase difference that does not affect the diffraction efficiencies. The reflectance of the grating for diffraction order n is then the Fourier transform of (10)

$$R_n = \frac{1}{a}\int_0^a \exp\Bigg(-{\rm i}\sum_m \exp({\rm i}m\kappa x_0) \times L(u_m(y)\exp({\rm i}m\kappa x)) - {\rm i}n\kappa x_0\Bigg){\rm d}x_0 \tag{11}$$

where the integration is over the period of the grating. If we let $L_m = L(u_m(y)\exp({\rm i}m\kappa x))$ be the number obtained from the integral operator, and re-scale the co-ordinates so $\tilde{x} = \kappa x_0$ then (11) takes a simpler form

$$R_n = \frac{1}{2\pi}\int_0^{2\pi} \exp\left(-{\rm i}n\tilde{x} - {\rm i}\sum_m L_m\exp({\rm i}m\tilde{x})\right){\rm d}\tilde{x}. \tag{12}$$

This is the main result of this section. Equation (12) is a general expression for the reflectance R_n of order n of the diffraction grating. It represents the amplitude of the plane wave component propagating in direction θ_n with respect to the grating surface normal. Since the x-component of the momentum or wave vector of the atom is given by $k_{xn} = k_{x0} + n\kappa$, where k_{x0} is the initial x-component of the momentum, we can derive an expression for θ_n

$$\sin\theta_n = \sin\theta + n\kappa/k. \tag{13}$$

This is the well-known grating equation. Here k is the initial wave number of the atom, θ is the incidence angle with respect to the grating surface normal and θ_n the angle of diffraction. Depending on the form of the grating potential and the form of $\mathbf{p}$, the integral in (12) can be evaluated either analytically or numerically. In the following section an analytical result is obtained for a grating with a single harmonic.

2.2 Single harmonic diffraction grating

We consider the special case of a grating with a single harmonic and write the grating potential in the form

$$U_{\rm g}(x,y) = 2u_1(y)\cos\kappa x \tag{14}$$

where $u_{-1} = u_1$. This simplifies (12) to

$$R_n = \frac{1}{2\pi}\int_0^{2\pi} \exp\left(-{\rm i}n\tilde{x} - {\rm i}L_1\cos\tilde{x}\right){\rm d}\tilde{x} \tag{15}$$

where $L_1 = L(2u_1(y)\cos\kappa x)$ and where an anti-symmetric term operated on by L has been omitted since it integrates to zero. The integral in (15) can be evaluated directly [27], with the result

$$R_n = \exp({\rm i}n\pi/2)J_n(L_1) \tag{16}$$

where J_n is a Bessel function of the first kind of order n. The diffraction efficiency is defined by

$$e_n = (\cos\theta_n/\cos\theta)R_n^* R_n. \tag{17}$$

This represents the fraction of the total atom flux or wave energy that is diffracted into order n. For energy conservation, or particle conservation in the case of matter waves, the sum of the diffraction efficiencies over all orders should be [28]

$$\sum_n e_n = 1. \tag{18}$$

Violation of this condition is a sign that the diffraction theory is either wrong, or at least inaccurate. The diffraction efficiency in the thin phase-grating approximation is

$$e_n = (\cos\theta_n/\cos\theta)J_n^2(L_1). \tag{19}$$

This is a general result for a diffraction grating with a sinusoidal profile, *i.e.* with a single harmonic. The variation of the potential with height y and the reflecting properties of the grating determine the value of the argument of the Bessel function and therefore determine the diffraction pattern. Note that this is a generalisation of Henkel *et al.* [22] and it is similar to the result from the distorted-wave Born approximation [23] for orders -1 and $+1$ if we take the first term in a series expansion of J_1.

We can make contact with the Lagrangian formulation of Henkel *et al.* [22] if we use the classical momentum for $\mathbf{p}$. In classical mechanics $\mathbf{p}$ is proportional to the velocity $({\rm d}r/{\rm d}t)$ so that $L^{-1} \to 2({\rm d}r/{\rm d}t)\partial/\partial r$ and then $L \to {\rm d}r/(2{\rm d}r/{\rm d}t) = {\rm d}t/2$ which is equivalent to a time derivative. Then L acts as a time integral in the classical regime and (8) is equivalent to the equations (2, 6b) given in [22].

2.3 Validity conditions

At this point we consider the range of validity of (12). It was derived assuming that $|\nabla^2\Psi_{\rm g}(\mathbf{r})| \ll |2\mathbf{p}(\mathbf{r})\cdot\nabla\Psi_{\rm g}(\mathbf{r})|$. From the solution (8), this condition becomes

$$|\nabla^2 LU_{\rm g} + \nabla(LU_{\rm g})\cdot\nabla(LU_{\rm g})| \ll |U_{\rm g}|. \tag{20}$$

Since L is an integral operator involving the inverse of $\mathbf{p}$ then its derivative is approximately $|\nabla L| \sim 1/p$ where p is the magnitude of $\mathbf{p}$. To obtain estimates of the terms in (20) we shall consider each term on the left side of (20) independently and shall treat p as slowly varying. The first term becomes

$$|\nabla U_{\rm g}/U_{\rm g}| \ll p \tag{21}$$

which tells us that the fractional change in the potential with distance must be much less than the wave number of the mirror wave. If Δr is the typical distance over which the potential changes at some point and λ is the wavelength at this point then (21) is equivalent to $\Delta r \gg \lambda$. A typical distance for a grating with a single harmonic is its period a, which implies that the atom wavelength must be much smaller than the grating period, or $\lambda/a \ll 1$.

The second term leads to the condition

$$|U_{\rm g}| \ll p^2. \tag{22}$$

Note that in our units, p^2 represents the kinetic energy of the atom. Far from the grating, $p^2 = k^2$ but it decreases as the atom approaches the classical turning point in the mirror potential. The problem here is that for normal incidence, the kinetic energy of the atom is zero at the classical turning point so that (22) will never be satisfied, in the classical sense, for normal incidence. We get a more accurate evaluation of criterion (22) if we use $p(\mathbf{r}) = |\nabla \Psi_{\rm m}(\mathbf{r})/\Psi_{\rm m}(\mathbf{r})|$ obtained from the quantum mechanical solution to the reflection problem. To continue further requires specific knowledge of the mirror potential. An example of this is given in Section 3 when we discuss the magnetic grating.

3 TPGA for a magnetic grating

In this section we derive a formula for the diffraction efficiencies in the thin phase-grating approximation (TPGA) using the classical trajectory of the atom in the mirror potential. The classical trajectories are found from the characteristic curves associated with equation (6) where we use the classical momentum for $\mathbf{p}$. In addition, we linearise the grating potential to reduce it to a single harmonic which adds an additional approximation to the formula.

The magnetic diffraction grating can be formed from an array of permanent magnets or current carrying wires, periodic in x, and by applying an appropriate uniform magnetic field in the x–y-plane. In the adiabatic approximation, a paramagnetic atom has an induced magnetic moment that maintains the same orientation with respect to the direction of the local magnetic field. In this situation, the potential energy of the atom is proportional to the magnitude of the magnetic field. The adiabatic state can be enforced in regions where the mirror or grating fields are zero by applying a uniform quantizing magnetic field in the z-direction. Following Opat *et al.* [29] we can write the magnetic field from the array of magnets up to the first spatial harmonic as this dominates the field away from the surfaces of the magnets. Since the energy of the atom is proportional to the magnitude of the field, then the potential takes the form

$$U(x,y) = \sqrt{U_0^2 + 2U_{\rm a}U_B \exp(-\kappa y)\cos\kappa x + U_B^2\exp(-2\kappa y)} \tag{23}$$

where U_B is the potential associated with the magnet array, $U_{\rm a}$ the potential arising from the uniform magnetic field applied in the x–y-plane, $U_0 = \sqrt{U_{\rm a}^2 + U_z^2}$ with U_z the potential arising from the uniform magnetic field applied in the z-direction and $\kappa = 2\pi/a$ where a is the period of the grating. The potential associated with the reflecting part of the potential is

$$U_{\rm m}(x,y) = \sqrt{U_0^2 + U_B^2\exp(-2\kappa y)}. \tag{24}$$

The vertical component of the momentum $p_y(y)$ of the atom (or its wave number) as a function of y can be obtained from (24) using energy conservation. Here we define the incident kinetic energy associated with the vertical motion of the atom to be k_y^2 in the region where $U_{\rm m} = U_0$; *i.e.* far above the grating. The total energy in this region is then $k_y^2 + k_x^2 + U_0$ where the component in the x-direction k_x is constant. If the incident angle is θ and the wave number is k then $k_y = k\cos\theta$ and $k_x = k\sin\theta$. It is convenient to shift the y co-ordinate origin to coincide with the classical turning point of the atom in the mirror potential. This point y_0 is obtained from the conservation of energy $k_y^2 + U_0 - U_{\rm m} = 0$, which for $U_B\exp(-\kappa y) \gg U_0$ becomes

$$U_B\exp(-\kappa y_0) = k_y^2 + U_0. \tag{25}$$

To use (19) we need to reduce (23) to a single harmonic. As it stands, (23) contains a large number of spatial harmonics on account of the square root. The square root can be represented to first order in $\cos\kappa x$ by the first two terms of a series expansion. There are two regions we consider that allow this: $U_B\exp(-\kappa y) \gg U_0$ and $U_B\exp(-\kappa y) \ll U_0$. This naturally leads to simple representations of (23, 24) in two regions:

(i) $y \le y_{\rm c}$:

$$U_{\rm m} \approx (k_y^2 + U_0)\exp(-\kappa y) \tag{26}$$

$$U \approx (k_y^2 + U_0)\exp(-\kappa y) + U_{\rm a}\cos\kappa x \tag{27}$$

(ii) $y \ge y_{\rm c}$:

$$U_{\rm m} \approx U_0 \tag{28}$$

$$U \approx U_0 + (U_{\rm a}/U_0)(k_y^2 + U_0)\exp(-\kappa y)\cos\kappa x \tag{29}$$

where (25) has been used to shift the co-ordinate origin so that $y = 0$ corresponds to the classical turning point. The cross-over point $y_{\rm c}$ between the two regions is

$$y_{\rm c} = \frac{1}{\kappa}\ln\left(\frac{k_y^2 + U_0}{U_0}\right). \tag{30}$$

Note that condition (i) is valid close to the grating whereas (ii) is valid far from the grating. The momentum $p_y(y)$ in these two regions is obtained from energy conservation. We find that

(i) $y \leq y_c$:

$$p_y(y) = (k_y^2 + U_0)^{1/2}(1 - \exp(-\kappa y))^{1/2}, \qquad (31)$$

(ii) $y \geq y_c$:

$$p_y(y) = k_y = k\cos\theta. \qquad (32)$$

The error in the grating potential associated with the approximation is largest at y_c where the amplitude of the first harmonic $\cos\kappa x$ is too large by a factor of $\sqrt{2}$. This overestimates the strength, or effective "groove depth" of the grating in this region. An example of this is given in Section 4 below. The actual effect on the diffraction efficiencies of this approximation is difficult to quantify.

We need to evaluate the integral $L_1 = L(2u_1\cos\kappa x)$ in (19). Since the momentum in the x-direction is constant it is simpler to use x as the independent variable. The integration follows the trajectory of the atom from the starting point above the grating, down to the classical turning point and then back up again. Since the reflection process is symmetrical, we need only integrate from the turning point upwards and then multiply the result by 2. In addition, $2u_1\cos\kappa x$ is the grating potential $U_g = U - U_m$. Thus we have

$$L_1 = \frac{1}{k\sin\theta}\int_0^\infty [U(y(x)) - U_m(y(x))]\mathrm{d}x. \qquad (33)$$

The integral is divided into two parts corresponding to the two regions (i) and (ii) above. In the first region the grating potential is independent of y so that the integral is trivial. In the second region it depends on y so that we need to find $y(x)$. Since the x-momentum is constant we have that

$$x = k_x\int_0^y p_y^{-1}(y)\mathrm{d}y \qquad (34)$$

which follows from (6). However from (32) the vertical momentum is constant here also so that y is simply related to x by

$$y = y_c + (x - x_c)\mathrm{cotan}\,\theta \qquad (35)$$

where x_c is the cross-over point in x corresponding to y_c and $\mathrm{cotan}\,\theta$ is the ratio of the y-momentum to the x-momentum in this region. With substitution (35) and (26–29) in (33) the integral is

$$L_1 = \frac{1}{k\sin\theta}\int_0^{x_c} U_a\cos\kappa x\mathrm{d}x + \left(\frac{U_a}{U_0}\right)\left(\frac{k_y^2+U_0}{k\sin\theta}\right) \times \int_{x_c}^\infty \exp(-\kappa(y_c + (x-x_c)\mathrm{cotan}\,\theta))\cos\kappa x\,\mathrm{d}x \qquad (36)$$

which has a solution

$$L_1 = \frac{U_a}{k\kappa}\left\{\frac{\sin\kappa x_c}{\sin\theta} + \left(\frac{U_a}{U_0}\right)\cos(\kappa x_c + \theta)\right\}. \qquad (37)$$

To relate x_c to y_c, we use (34) with (31) and $k_x = k\sin\theta$. Then

$$x_c = \frac{k\sin\theta}{\sqrt{k_y^2+U_0}}\int_0^{y_c}\frac{\mathrm{d}y}{\sqrt{1-\exp(-\kappa y)}}. \qquad (38)$$

The integral can be evaluated by a change of variable to $s = 1 - \exp(-\kappa y)$. After some effort and on substituting (30) for y_c and (32) for k_y we finally obtain

$$\kappa x_c = \frac{k\sin\theta}{\sqrt{k^2\cos^2\theta + U_0}}\ln\left(\frac{\sqrt{k^2\cos^2\theta+U_0}+k\cos\theta}{\sqrt{k^2\cos^2\theta+U_0}-k\cos\theta}\right). \qquad (39)$$

Note that, although (37) appears to diverge for waves at normal incidence where $\theta = 0$, we find that the ratio remains finite

$$\lim_{\theta\to 0}\frac{\sin\kappa x_c}{\sin\theta} = \frac{k}{\sqrt{k^2+U_0}}\ln\left(\frac{\sqrt{k^2+U_0}+k}{\sqrt{k^2+U_0}-k}\right). \qquad (40)$$

The diffraction efficiencies associated with the magnetic grating are obtained from (19) with (37, 39). These equations represent the TPGA formula for a magnetic grating. Note that both (37) and (39) can be expressed in terms of ratios U_0/k^2 and $\kappa/k = \lambda/a$ so that the diffraction pattern with the TPGA depends only on the angle of incidence, the wavelength to period ratio and the ratio of the mirror potential to the atom kinetic energy.

In the following section we wish to compare the results from this approximate formula with an accurate numerical procedure. Before this, we need to consider the range of parameters for which the TPGA formula is valid. As discussed in Section 2.3, we require the atom wavelength to be much smaller than the grating period

$$\lambda/a \ll 1 \qquad (41)$$

which characterises the distance over which the potential varies. The other criterion (22) is more difficult. This requires the momentum calculated from the quantum mechanical solution to the problem. Near the classical turning point, the mirror potential is described by (26) which decays exponentially with height. Henkel *et al.* [30] have solved the quantum mechanical problem for this potential in terms of modified Bessel functions of the first kind $I_{i2\nu}(\alpha)$ that depend on $\nu = k\cos\theta/\kappa$ and where α is a function of y. Evaluating the fractional derivative of this at the turning point gives an estimate of the momentum $p_y(0)$ there (this is discussed in the appendix). This is a non-zero complex number. Although the solution is complicated we find that for $\lambda/a \ll 1$ and hence $\nu \gg 1$ the magnitude of this momentum can be fitted by a simple function $p_y(0) \approx 0.690(\lambda/a\cos\theta)^{0.32}k\cos\theta$. Taking account of both vertical and horizontal components of momentum leads to the condition

$$U_a \ll k^2\left(0.476(\lambda/a)^{0.64}\cos^{1.36}\theta + \sin^2\theta\right). \qquad (42)$$

4 Comparison between TPGA and a numerical model

An accurate numerical procedure for calculating the diffraction efficiencies of atoms from reflecting diffraction gratings has been discussed by Davis [24]. This is based on the rigorous coupled-wave analysis (RCWA) method developed for light diffraction from dielectric gratings [31,32]. In this section we compare results from the RCWA method using potential (23) for a magnetic grating with the TPGA formula (19, 37, 39). In particular we look at a few examples of regions where we expect the TPGA formula to break down. Specifically these are where conditions (41, 42) are violated.

The potential $U_{\rm a}$ is related to the magnitude of the applied magnetic field $B_{\rm a}$ by

$$U_{\rm a} \approx 277 m_{\rm F} g_{\rm F} Z B_{\rm a} \tag{43}$$

where $m_{\rm F} g_{\rm F}$ is the product of the space quantisation number and the Landé factor and Z is the mass number of the atom. The magnetic field is in Gauss and the potential is in $\mu{\rm m}^{-2}$. In our examples we shall set $m_{\rm F} g_{\rm F} Z = 1$. The results given in our examples are applicable to any paramagnetic atom with mass number Z if our values of the magnetic field are re-scaled by $B_{\rm a} \to B_{\rm a}/Z$. In addition, for simplicity, we shall ignore the quantizing field and set $U_z = 0$.

In the first example we set $\lambda = 0.05$ μm, $a = 1$ μm, $\theta = 0$ and vary the applied magnetic field. From (41, 42) we expect the TPGA formula to be accurate for $B_{\rm a} \ll 4.0$ Gauss. The variation of three diffraction orders, 0, +2 and +4, with the applied field are shown in Figure 1a. The TPGA formula and the RCWA show reasonable agreement that becomes worse as the applied field is increased. Significant differences are becoming apparent for fields greater than about 3 Gauss, consistent with our estimate from (42). The sums of the diffraction efficiencies for these calculations are shown in Figure 1b. It is clear that, unlike the RCWA, the TPGA formula does not satisfy flux conservation since the diffraction efficiencies do not sum to 1, except for very weak fields where there is negligible diffraction. Again the failure to satisfy flux conservation becomes progressively worse as the applied magnetic field is increased.

In the second example we choose a value for the applied field in the region where the TPGA is breaking down and we increase the angle of incidence from normal incidence towards grazing incidence. According to (42) we would expect the value of the applied field for which the TPGA is valid to increase and therefore the agreement between TPGA and RCWA should improve with increasing angle. For example, with $\lambda = 0.05$ μm and $a = 1$ μm, at $\theta = 0$ we require $B_{\rm a} \ll 4.0$ Gauss for the TPGA formula to be valid whereas at $\theta = 40^\circ$ we require $B_{\rm a} \ll 26$ Gauss. The results with $B_{\rm a} = 5$ Gauss are shown in Figure 2a. We observe some improvement between the results of the RCWA and the TPGA with increasing angle but the discrepancies persist for large angles of incidence. Figure 2b shows the flux conservation criterion which suggests that between 30 and 60 degrees the TPGA formula should be reasonably accurate. If we use potentials (26–29) in the RCWA instead of (23) we find that there is a much improved agreement between TPGA and the RCWA (Fig. 2c). This shows that the discrepancies are mainly due to the linearisation of the potential.

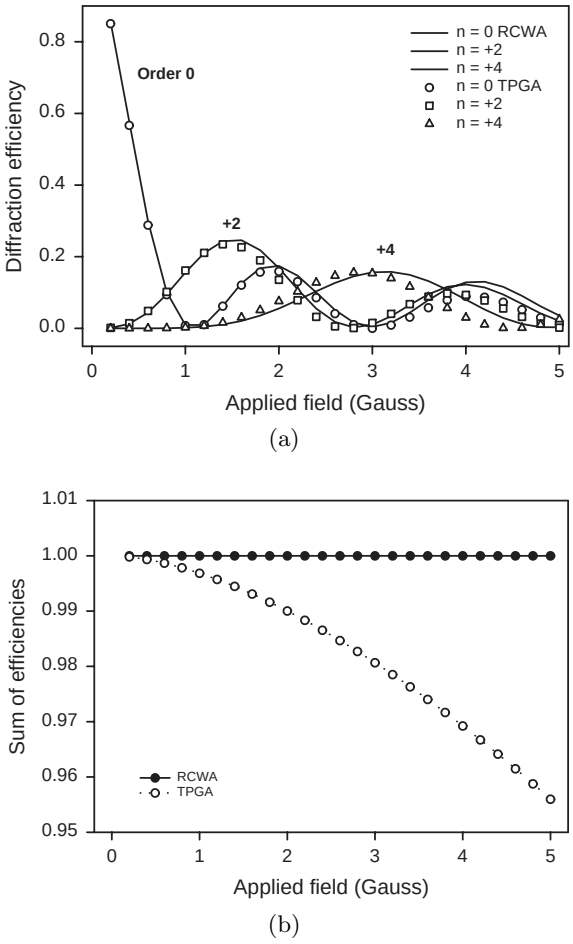
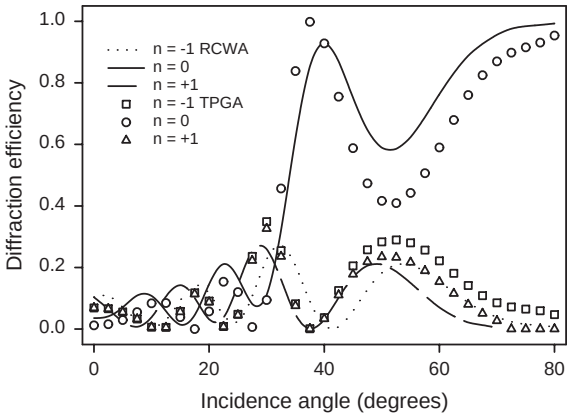


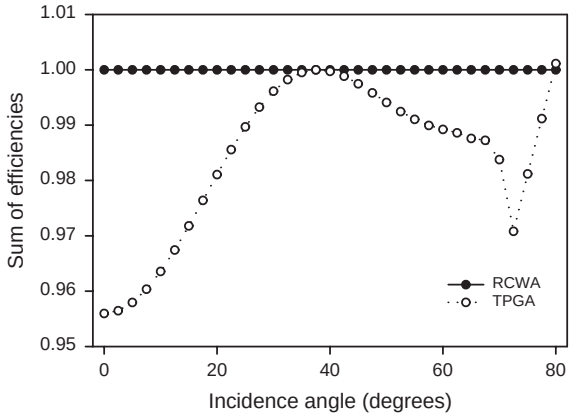
Fig. 1. (a) A comparison between TPGA and RCWA as a function of applied field. The parameters are $\theta = 0^\circ$, $\lambda = 0.05$ μm and $a = 1$ μm. (b) The sum of the diffraction efficiencies associated with (a) including all the diffraction orders not shown.

As a final example, we investigate the diffraction efficiencies as a function of the grating period, particularly as $\lambda/a \to 1$ in violation of (41). The parameters chosen for this example are $\lambda = 0.05$ μm, $\theta = 0$, $B_{\rm a} = 2$ Gauss and we vary the grating period a from 1 μm down to 0.05 μm. The results are shown in Figure 3. Although (41) no longer holds, the TPGA results show good agreement with the RCWA using potential (23). The sums of the diffraction efficiencies for the TPGA formula remain high for all these data, at around 0.99, suggesting that the formula is accurate here.

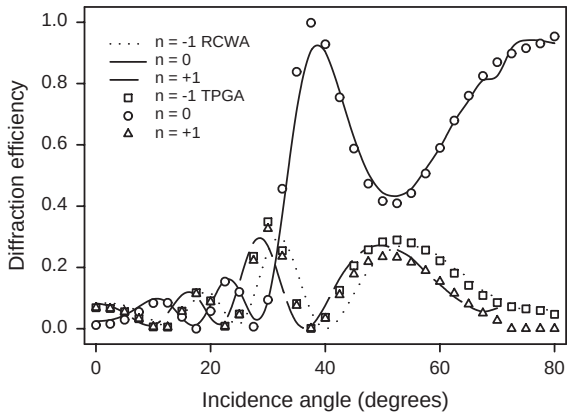
As a general observation, we find that the TPGA formula is accurate when most of the diffraction orders are small compared to the reflected order $n = 0$. In this



(a)



(b)



(c)

Fig. 2. (a) A comparison between TPGA and RCWA for several orders as a function of the angle of incidence. The parameters are $B_{\mathrm{a}} = 5$ Gauss, $\lambda = 0.05$ μm and $a = 1$ μm. (b) The sum of diffraction efficiencies associated with (a) including all the orders not shown. (c) A comparison between TPGA and RCWA both using the linearised potential. The parameters are the same as in (a).

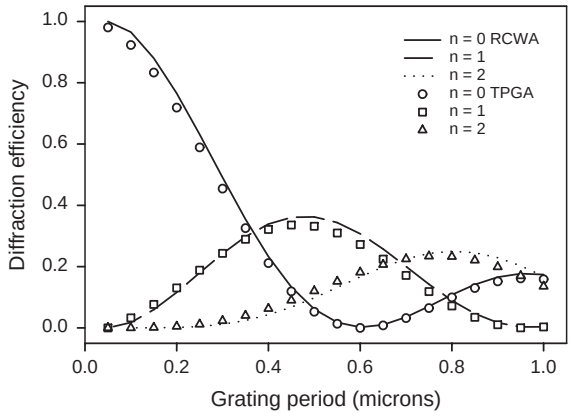


Fig. 3. A comparison between TPGA and RCWA with changes in the grating period. The parameters are $B_{\mathrm{a}} = 2$ Gauss, $\lambda = 0.05$ μm and $\theta = 0^{\circ}$.

situation, the grating appears almost like a mirror, the perturbations leading to diffraction are small and the diffraction efficiencies almost sum to 1. A possible reason for this relates to the semi-classical nature of the method. The TPGA formula is based on the classical trajectory of the atom in the mirror potential. As such, it does not take account of the evanescent waves in the diffraction grating which may give rise to important phase shifts affecting the amplitudes of the diffracting orders. For example, an incident wave at an angle $\theta > 0$ becomes evanescent where the potential energy exceeds the vertical component of the kinetic energy. However, an accompanying diffracted order with $\theta_n < \theta$ will have a greater vertical kinetic energy and may be non-evanescent in this region. The TPGA does not take a proper account of the non-evanescent nature of the diffraction order in this region since it only sums the phase shifts upwards from the classical turning point in the mirror potential. If most of the diffracting orders are small so that the grating is "mirror-like" then the contribution to the diffraction efficiency of the evanescent region is small and the TPGA formula should be more accurate.

Another limitation with the TPGA is that it does not take account of focussing effects. This point is discussed in [22]. It is possible that the waves interacting with the grating can come to a focus within the grating. Such effects arise from large variations in the potential over distances compared to the atom wavelength which clearly violate the TPGA. Focussing effects were noted by Maystre [28] as causing failure in many early theories of optical diffraction gratings and ultimately are associated with numerical instability. The RCWA, by its careful treatment of evanescent orders, avoids these problems

The results of our comparison with the accurate numerical method show that the TPGA formula is accurate in some cases and gives rough estimates of diffraction efficiencies in others. It is apparent that the criteria for estimating the range of parameters for which the TPGA formula is valid are not accurate but act only as a rough guide as to the applicability of the formula. A better indication of the reliability of the TPGA is given by the sum of the diffraction efficiencies which should be close

to 1. In addition, our comparisons demonstrated that the single-harmonic approximations lead to sizeable errors but we have not been able to provide an analytical formula for quantifying them. The subtleties of the diffraction process are best modelled using accurate methods which are usually based on the numerical solution of (2), such as in the RCWA. However, despite these shortcomings, the TPGA formula is useful for estimating the diffraction efficiencies and for determining their dependence on the atom wavelength, the grating period, the applied magnetic fields and the angle of incidence. Such dependence is not always easy to assess from a numerical procedure.

5 Summary

In this paper we have derived a general relation for the reflectance of a diffraction order associated with the interaction of atomic de Broglie waves with a reflecting, periodic potential. The relation has been derived using the thin phase-grating approximation and the range of parameters for which it is valid have been estimated. A formula for the diffraction efficiencies from a potential with a single spatial frequency has been derived and has been applied to the problem of atoms diffracting from a magnetic grating. To obtain an analytical solution, the grating potential is approximated by a single harmonic. This can result in errors that are difficult to quantify. The results from the analytical formula were compared with those from an accurate numerical method. This showed that the analytical formula can provide reasonably accurate results in some cases and gives the general trends in others. The parameters for which the analytical formula is accurate are not always consistent with the estimated range. Based on our comparison with the numerical method, the formula is more accurate when the diffraction efficiencies for all the diffraction orders sum close to 1, which is necessary to conserve atom flux.

Appendix

Here we discuss the mathematical form of the momentum function

$$p_y(y) \equiv -\mathrm{i}(\partial\Psi_\mathrm{m}(\mathbf{r})/\partial y)/\Psi_\mathrm{m}(\mathbf{r}) \tag{A.1}$$

that involves the fractional derivative of the wave function for the atom reflecting from the perfect mirror potential

$$U_\mathrm{m}(y) = (k_y^2 + U_\mathrm{a})\exp(-\kappa y). \tag{A.2}$$

Here $y = 0$ is the classical turning point of the atom's motion. Henkel *et al.* [30] have solved the wave equation for an atom in such a potential in terms of Bessel functions $I_{\mathrm{i}2\nu}(\alpha(y))$. Their solution (Eq. (17) in [30]) contains the interference between downward and upward propagating waves. For our purpose we need only the upward propagating wave proportional to $I_{-\mathrm{i}2\nu}(\alpha(y))$ where, in our notation, $\nu = k_y/\kappa$ and $\alpha(y) = 2\nu\exp(-\kappa y/2)$. The function $I_{-\mathrm{i}2\nu}(\alpha(y))$ can be written as a power series in α

$$I_{-\mathrm{i}2\nu}(\alpha) = \sum_{n=0}^{\infty} \frac{1}{n!\Gamma(n+1-\mathrm{i}2\nu)}\left(\frac{\alpha}{2}\right)^{2n-\mathrm{i}2\nu} \tag{A.3}$$

where Γ here denotes the Euler gamma function. We use this series expansion for $\Psi_\mathrm{m}(y)$ in (A.1), take the derivative and expand the gamma function to $n = 0$ using the relation $\Gamma(n+1-\mathrm{i}2\nu) = (n-\mathrm{i}2\nu)!\Gamma(1-\mathrm{i}2\nu)$. Introducing $\zeta \equiv \exp(-\kappa y)$ gives the result

$$p_y(y) = k_y\left(1 + \frac{\mathrm{i}}{\nu}F(\nu,\zeta(y))\right) \tag{A.4}$$

where

$$F(\nu,\zeta) = \frac{\displaystyle\sum_{n=0}^{\infty}\frac{n\nu^{2n}\zeta^n}{n!(n-\mathrm{i}2\nu)!}}{\displaystyle\sum_{n=0}^{\infty}\frac{\nu^{2n}\zeta^n}{n!(n-\mathrm{i}2\nu)!}}\cdot \tag{A.5}$$

After numerically evaluating this function at the turning point we find that, for $\nu \gg 1$ the magnitude of the momentum can be fitted by a simple function $p_y(0) \approx 0.690\nu^{-0.32}k\cos\theta$.

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