Modelling the diffraction of laser-cooled atoms from magnetic gratings

T.J. Davis[a]

CSIRO, Manufacturing Science & Technology, Private Bag 33, Clayton South, Victoria 3169, Australia

Abstract. The diffraction of laser-cooled atoms from a spatially-periodic potential is modelled using rigorous coupled-wave analysis. This numerical technique, normally applied to light-diffraction, is adapted for use with atomic de Broglie waves incident on a reflecting diffraction grating. The technique approximates the potential by a large number of constant layers and successively solves the complex eigenvalue problem in each layer, propagating the solution up to the surface of the grating. The method enables the diffraction efficiencies to be calculated for any periodic potential. The results from the numerical model are compared with the thin phase-grating approximation formulae for evanescent light-wave diffraction gratings and idealised magnetic diffraction gratings. The model is applied to the problem of diffracting Rb atoms from a grating made from an array of permanent magnets.

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1 Introduction

The development of laser-cooling techniques for creating clouds of ultra-cold atoms has renewed interest in performing wave-optical experiments on matter waves. One such experiment is to observe the diffraction of atoms from a periodic potential. The diffraction of atoms from the standing wave pattern produced by an evanescent light field has been observed by a number of groups [1–3]. Another method for producing reflecting diffraction gratings for atoms has been proposed based on fine arrays of permanent magnets or current-carrying wires [4]. These structures can be used to form mirrors that reflect [5–15] or deflect paramagnetic atoms [16,17] (also see the review [18]). A periodic variation in the strength of the magnetic field is obtained when a uniform field is applied. The aim is to diffract atoms from this spatially periodic potential.

The potential associated with a periodic array of magnets may have a complicated spatial dependence, making exact analytical formulations difficult. For this reason we develop a numerical method for calculating the intensity of the diffracting orders of atom de Broglie waves from any periodic potential. This provides a tool for simulating atom diffraction experiments, limited only by the accuracy of the model for the potential. The starting point for the model is the time-independent Schrödinger equation for the atoms in a periodic potential. This can be written as a scalar wave equation which is the same as that

for light in a dispersive optical medium. This allows us to draw upon the extensive optics literature on the modelling of optical diffraction gratings.

The problem of calculating the diffraction of waves from a reflecting diffraction grating at first seems straightforward. However, unless great care is taken in formulating the problem the calculations are prone to numerical instabilities [19]. There are now many different techniques developed by the optics community that solve this problem. The method that we choose for modelling the diffraction of atoms, known as rigorous coupled-wave analysis (RCWA), is described by Moharam *et al.* [20,21]. This implementation is specifically formulated to be numerically stable for dielectric gratings that have arbitrary refractive index profiles, including arbitrary surface relief. As shown below, this is equivalent to a periodic but otherwise arbitrary potential that will reflect atoms. The theory of the diffraction of atoms from evanescent light waves has been investigated by a number of authors [22–26] (also see the review [27]). The multi-slice method employed by Murphy [25], originally formulated for electron diffraction calculations, is quite similar to the RCWA method that we review below.

In the following sections we first review the method of RCWA. We then compare results using this method with the thin phase-grating approximation formulae for both evanescent wave and magnetic potentials. Finally we consider a grating made from an array of permanent magnets with square cross-sections to be used as a beam splitter and give an example calculation to optimise the splitting.

[a] e-mail: tim.davis@cmst.csiro.au

2 Rigorous coupled-wave analysis for atoms

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

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

where E is the total energy of the atom of mass m, V is the potential energy with $\hbar$ Planck's constant divided by 2π. We express the total energy in terms of the kinetic energy of the atom at a point where the potential is zero, $E = \hbar^2 k_\mathrm{I}^2/2m$, where k_I is the wave number of the incident atom, and rescale the potential $U(\mathbf{r}) \equiv \left(2m/\hbar^2\right)V(\mathbf{r})$, which enables us to write (1) in the form

$$\nabla^2\Psi(\mathbf{r}) + (k_\mathrm{I}^2 - U(\mathbf{r}))\Psi(\mathbf{r}) = 0. \qquad (2)$$

This has the same form as the scalar wave equation for light in an inhomogeneous, dispersive, dielectric medium with a refractive index $n = \sqrt{1 - U(\mathbf{r})/k_\mathrm{I}^2}$.

The potential U is responsible for reflecting and diffracting the atoms. For simplicity we lie the diffraction grating in the x–z-plane so that the potential is independent of z, periodic in x and decreases with height y, $U(x,y)$. Let k_z be the component of the incident wave vector parallel to the z-axis, write $\Psi(\mathbf{r}) = \Psi(x,y)\exp(ik_z z)$ and define $k_i = \sqrt{k_\mathrm{I}^2 - k_z^2}$, then (2) can be written as

$$\frac{\partial^2\Psi(x,y)}{\partial x^2} + \frac{\partial^2\Psi(x,y)}{\partial y^2} + \left(k_i^2 - U(x,y)\right)\Psi(x,y) = 0. \qquad (3)$$

This is a scalar wave equation in two dimensions. It is the same wave equation satisfied by the electric field of an electromagnetic wave when the vector characteristic of the field can be ignored, such as for planar diffraction with TE polarization. This enables us to use techniques developed for optical diffraction problems from non-uniform dielectrics and apply them to the problem of atom diffraction. Specifically we shall use rigorous coupled-wave analysis (RCWA) that we briefly review.

In this analysis, the grating potential U plays the role of a dielectric medium and we assume that it is appreciable only in some region of space about $y = y_0$. The points above and below y_0 where U becomes negligible are identified respectively with the top and the bottom of the grating. These points are separated by a distance d. For a totally reflecting grating we choose the "bottom" of the grating at some point deep in the grating where the potential energy is much greater than the atom kinetic energy. Following Moharam *et al.* [21], the wave in a region above the grating is the sum of the incident wave (of unit amplitude) and a series of diffracted waves

$$\Psi_+(x,y) = \exp\left(ik_x x - ik_y y\right)$$
$$+ \sum_{n=-\infty}^{\infty} R_n \exp(ik_n x + ik_n' y) \qquad (4)$$

where $k_y = \sqrt{k_i^2 - k_x^2}$ is the magnitude of the component of the wave number in the y-direction and where R_n is the reflectance of the grating for diffraction order n. The x-component of the diffracted wave number is

$$k_n = k_x + n\kappa \qquad (5)$$

where $\kappa = 2\pi/a$ with a the period of the grating, and the y-component is

$$k_n' = \sqrt{k_i^2 - k_n^2}, \quad k_i > k_n,$$
$$k_n' = i\sqrt{k_n^2 - k_i^2}, \quad k_i < k_n. \qquad (6)$$

Note that this becomes imaginary if k_n becomes greater than the incident wave number. It is this term that leads to exponentially increasing amplitudes that can result in numerical instability. In (6) we take the positive square-root so that these evanescent orders decay as $y \to \infty$. Note also that we have assumed that the potential is zero above the grating. If instead the potential has some value U_0 in the region where k_i is defined, then k_i^2 represents the energy of the atom in this potential, that is $k_i^2 = k_\mathrm{I}^2 - k_z^2 - U_0$.

For a thin grating we must also take account of waves that are transmitted through it. The wave below a grating of thickness d is written as

$$\Psi_-(x,y) = \sum_{n=-\infty}^{\infty} T_n \exp\left(ik_n x - ik_n'(y - d)\right) \qquad (7)$$

where T_n is the transmittance of the grating for order n. The thickness of the grating d is included in (7) to explicitly take account of evanescent waves. Thus when k_n' is imaginary we have the solution explicitly decaying exponentially with distance d.

The wave within the grating is given by the expansion

$$\Psi(x,y) = \sum_n \phi_n(y)\exp(ik_x x + in\kappa x) \qquad (8)$$

and likewise the potential is represented by a Fourier series

$$U(x,y) = \sum_n U_n(y)\exp(in\kappa x). \qquad (9)$$

These two expansions, together with (3) give the equation

$$d^2\phi_n/d\widetilde{y}^2 + \left(1 - \widetilde{k}_n^2\right)\phi_n = \sum_m \widetilde{U}_{n-m}\phi_m \qquad (10)$$

where we have introduced the reduced co-ordinates $\widetilde{y} = k_i y$, $\widetilde{k}_n^2 = k_n^2/k_i^2$, and $\widetilde{U}_{n-m}(y) = U_{n-m}(y)/k_i^2$. For convenience we have not shown explicitly the dependence on y (or $\widetilde{y}$).

We wish to solve (10) with boundary conditions (4, 7). The set of coupled-wave equations (10) has the form of a matrix problem. This is solved by dividing the potential into a large number of layers indexed by a layer number l. The top of the lth layer is located at $\widetilde{y}_l$. Within each layer, located between $\widetilde{y}_{l-1} < \widetilde{y} \le \widetilde{y}_l$, the potential $\widetilde{U}_{n-m}$ is taken to be constant, perhaps given by its average value in the layer. This reduces the problem to finding the eigenvalues and eigenvectors of the matrix

$$M_{nm}^l = \left(\widetilde{k}_n^2 - 1\right)\delta_{nm} + \widetilde{U}_{n-m} \qquad (11)$$

allowing us to diagonalise (10) within the layer, yielding a coupled plane-wave solution

$$\phi_n^l = \sum_m S_{nm}^l \left(A_m^l \exp\left(q_m^l(\widetilde{y} - \widetilde{y}_l)\right)\right.$$
$$\left. + B_m^l \exp\left(-q_m^l(\widetilde{y} - \widetilde{y}_{l-1})\right)\right). \quad (12)$$

The q_m^l are vectors equal to the square-roots of the eigenvalues for each layer. The sign of the root is chosen so that the real part of q^l is positive. S_{nm}^l is the mth eigenvector with components indexed by n. The coefficients A_m^l and B_m^l are vector constants for each layer and have values that are determined by matching boundary conditions between layers. If the lth layer has a thickness $d_l = y_l - y_{l-1}$, with $\widetilde{d}_l = k_i d_l$, then matching wave amplitudes and gradients between layers l and $l+1$ gives

$$\begin{bmatrix} S^l & S^l X^l \\ V^l & -V^l X^l \end{bmatrix}\begin{bmatrix} A^l \\ B^l \end{bmatrix} = \begin{bmatrix} S^{l+1} X^{l+1} & S^{l+1} \\ V^{l+1} X^{l+1} & -V^{l+1} \end{bmatrix}\begin{bmatrix} A^{l+1} \\ B^{l+1} \end{bmatrix} \quad (13)$$

where

$$V_{nm}^l \equiv S_{nm}^l q_m^l \quad (14)$$

and

$$X_{nm}^l \equiv \delta_{nm} \exp\left(-q_m^l \widetilde{d}_l\right). \quad (15)$$

Note that each element of the matrices in (13) is also a matrix. The problem has been cast into this form for mathematical convenience.

The problem with a reflecting diffraction grating is that the boundary conditions are specified only at the top of the grating. Moharam *et al.* [21] devise a method that gives the reflectance at the top of the grating without requiring any knowledge of the values of the wave at the lower boundary, or at any point within it. We start by assuming that there is some matrix a^l linking vector coefficients A^l and B^l

$$B^l = a^l A^l. \quad (16)$$

Then the left side of (13) can be written in the form

$$\begin{bmatrix} S^l & S^l X^l \\ V^l & -V^l X^l \end{bmatrix}\begin{bmatrix} A^l \\ B^l \end{bmatrix} = \begin{bmatrix} S^l & S^l X^l a^l \\ V^l & -V^l X^l a^l \end{bmatrix}\begin{bmatrix} A^l \\ A^l \end{bmatrix} = \begin{bmatrix} f^l \\ g^l \end{bmatrix} A^l \quad (17)$$

where

$$\begin{bmatrix} f^l \\ g^l \end{bmatrix} = \begin{bmatrix} S^l(I + X^l a^l) \\ V^l(I - X^l a^l) \end{bmatrix}. \quad (18)$$

After rearranging (13) we find that

$$\begin{bmatrix} -S^{l+1} & f^l \\ V^{l+1} & g^l \end{bmatrix}\begin{bmatrix} B^{l+1} \\ A^l \end{bmatrix} = \begin{bmatrix} S^{l+1} X^{l+1} \\ V^{l+1} X^{l+1} \end{bmatrix} A^{l+1} \quad (19)$$

which relates B^{l+1} to A^{l+1} by an equation of the form (16). Specifically, after relabelling indices we have

$$\begin{bmatrix} a^l \\ b^l \end{bmatrix} = \begin{bmatrix} -S^l & f^{l-1} \\ V^l & g^{l-1} \end{bmatrix}^{-1}\begin{bmatrix} S^l X^l \\ V^l X^l \end{bmatrix} \quad (20)$$

where the matrix b^l is obtained numerically as a part of the matrix calculation but we never use it. Now, given f^0 and g^0 at the lower boundary of the grating, we can use (20) to get a^1 at the next layer and (18) to calculate f^1 and g^1. By repeating these calculations, the solution can be propagated to the top of the grating. Note that these equations do not require the coefficients A^l or B^l to be specified at the lower boundary.

The starting values f^0 and g^0 are found by matching amplitudes and gradients of the solution (12) at layer $l = 1$ to the wave (7). After rearranging the result to have the same form as (18) we find that $f^0 = I$ and $g^0 = -iK$ where

$$K_{nm} = \delta_{nm} \widetilde{k}_n' \quad (21)$$

and I is the identity matrix.

Finally, we need to relate these matrices to the boundary conditions at the top layer. Let the top of the uppermost layer be located at $\widetilde{y} = \widetilde{y}_L$. Following the form of (4) we write the wave beyond the top of the grating as

$$\Psi_+(x,y) = \sum_{n=-\infty}^{\infty} \left[\delta_{n0} \exp\left(-i\widetilde{k}_i'(\widetilde{y} - \widetilde{y}_L)\right)\right.$$
$$\left. + R_n \exp\left(i\widetilde{k}_n'(\widetilde{y} - \widetilde{y}_L)\right)\right] \exp(ik_n x). \quad (22)$$

On matching amplitudes and gradients with (12) at $\widetilde{y} = \widetilde{y}_L$ then

$$\begin{bmatrix} R + \Delta \\ iK(R - \Delta) \end{bmatrix} = \begin{bmatrix} S^L & S^L X^L \\ V^L & -V^L X^L \end{bmatrix}\begin{bmatrix} A^L \\ B^L \end{bmatrix} \quad (23)$$

where we have introduced the column vector $\Delta_n = \delta_{n0}$. Equation (23) has the same form as (13). As before we can write B^L in terms of A^L and then we solve for R by eliminating A^L. Thus we obtain the reflectance of the grating in the form of a matrix equation

$$R = -\left(g^L\left(f^L\right)^{-1} - iK\right)^{-1}\left(g^L\left(f^L\right)^{-1} + iK\right)\Delta. \quad (24)$$

In summary, we solve the diffraction problem numerically by dividing the potential into a number of layers, determine a^l, f^l and g^l at each layer, and propagate these to the top of the grating. These matrices depend on S^l, V^l, X^l and q^l which are obtained from the eigenvectors and the eigenvalues of the matrix (11) in each layer.

As a check on our diffraction calculation, there are two physical conditions that must be obeyed. Firstly, for a reflecting grating where there is no transmission, the sum of the diffraction efficiencies must be unity

$$\sum_n e_n = 1 \quad (25)$$

with

$$e_n = R_n^* R_n \mathrm{Re}\,(k_n'/k_y) \qquad (26)$$

where Re( ) means the real-part. This follows from energy conservation in the case of light or flux conservation for atoms. Taking the real part in (26) means that we only sum over the non-evanescent orders. In general, the RCWA satisfies condition (25) to at least one part in 10^{10}, as discussed in [21]. The second condition is known as reciprocity [19] which is also a consequence of energy conservation. The reciprocity theorem states that the diffraction efficiency e_n in the nth order at angle θ_n from a wave incident at angle θ is equal to the diffraction efficiency in the nth order at angle $-\theta$ from a wave incident at angle $-\theta_n$. All angles are measured with respect to the grating surface normal. Again we find that the RCWA satisfies this condition in all cases we have tested.

The start position for a calculation defines the lower boundary of the grating, below which we assume that the waves are transmitted (see Eq. (7)). The start position is chosen some distance beyond the classical turning point which is where the initial downwards kinetic energy of the atom equals the potential energy. If the sum of the diffraction efficiencies (25) is not unity then some of the waves are leaking from below the grating which implies that the start position is not deep enough in the potential. The stop position defines the upper boundary of the grating and is taken where the potential becomes negligible compared with the atom energy. The width of each layer is chosen by trial and error until the diffraction efficiencies do not change. Usually the layer width is a small fraction of the potential decay length.

The total number of terms in the expansion (8) depends on the highest diffracted order required of the wave (including evanescent orders). This, in turn, depends on the grating period and depth, the wavelength of the atom and its angle of incidence. In practise we increase the number of orders until the results of the calculation do not change significantly.

The above methods have been combined in a computer program for calculating the diffraction patterns of atoms from gratings based on any periodic potential, such as from evanescent waves or arrays of magnets. The code was tested by comparing results for a perfectly reflecting sinusoidal diffraction grating with those from a rigorous integral theory of Maystre [19]. The code was also tested in the regime of very small wavelength to period ratio where the sinusoidal reflector should behave classically. In the next section we compare the results of the RCWA implementation with the TPGA formula of Henkel *et al.* [26] for evanescent wave gratings and that of Davis [28] for magnetic gratings.

3 Comparison with TPGA theories

In this section we compare the results from RCWA calculations with two approximate analytical formulae based on the thin phase grating approximation (TPGA). The TPGA formulae are derived from a semi-classical method for estimating the wavefunction of the diffracting wave. In essence, the diffraction problem for a reflecting grating is separated into two parts, that of reflection and that of diffraction. The trajectory of the atom in the reflecting potential is solved classically and the atom wavefunction is found by integrating the phase shift arising from the diffracting (periodic) part of the potential along the classical trajectory.

We consider two types of diffraction gratings: one made from an evanescent wave and one from a periodic array of magnets.

3.1 Evanescent light grating

A periodic potential can be formed from a standing evanescent light wave [22]. This acts as a reflecting diffraction grating for atoms. Following Henkel *et al.* [26] we write the potential for the evanescent wave grating in the form

$$U(x, y) = U_0 \exp(-\kappa y)(1 + \varepsilon \cos \kappa x) \qquad (27)$$

where $\kappa = 2\pi/a$ with a the period of the grating and ε is the normalised grating potential, also known as the interference contrast [3]. This contains a mirror term that reflects the atoms and a diffraction term with a strength controlled by ε. Henkel *et al.* [26] derive an analytical expression for the diffraction probabilities using the thin phase-grating approximation. In terms of diffraction efficiencies this takes the form

$$e_n^{\mathrm{TPGA}} = (\cos \theta_n / \cos \theta) J_n^2 (2 \cos \theta \beta(\theta) \varepsilon k_i / \kappa) \qquad (28)$$

where J_n is a Bessel function, θ the incidence angle, θ_n the angle of diffraction and

$$\beta(\theta) = \pi \tan \theta / \sinh(\pi \tan \theta). \qquad (29)$$

This formula is valid provided that the atom wavelength is small compared to the grating period, $\lambda \ll a$ and that the contrast is small, $\varepsilon \ll 1$. Note that θ_n is obtained from the grating equation

$$\sin \theta_n = \sin \theta + n\lambda/a \qquad (30)$$

which is a consequence of (5).

To compare the RCWA method with the approximate formula (28) we consider the case of normal incidence $\theta = 0$ and vary the contrast ε. To ensure $\lambda \ll a$ we set $\lambda/a = 0.1$. Figure 1a compares the diffraction efficiencies for the first three orders calculated using the RCWA method and (28). The two methods show good agreement for small contrast but the results diverge as the contrast gets larger. This is because the assumption of small contrast in the TPGA formula is failing. The sum of the diffraction efficiencies, shown in Figure 1b, should obey the energy conservation criterion (25). Note that the TPGA formula gets progressively worse at satisfying this relation and that this also follows the divergence between
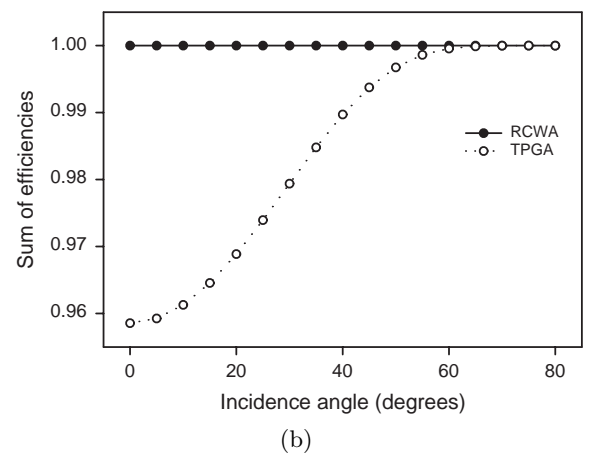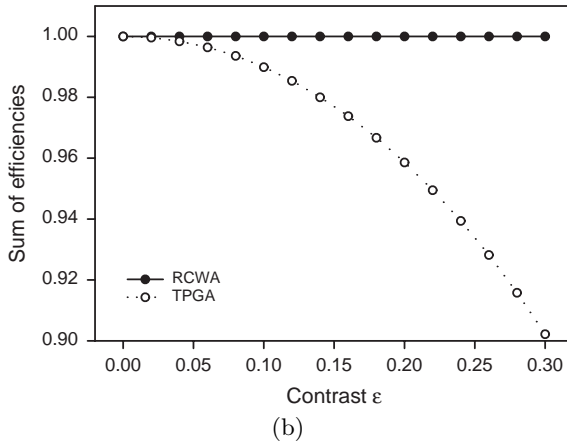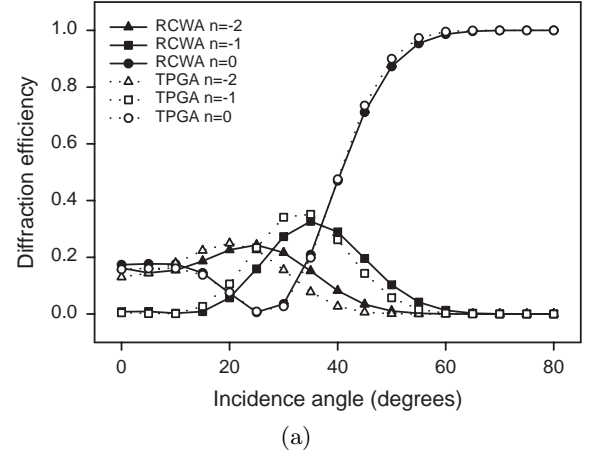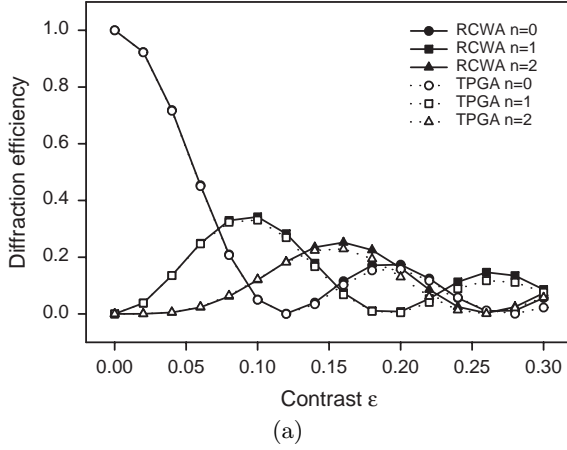
Fig. 1. (a) The results of RCWA and TPGA for an evanescent wave grating as a function of the contrast. The parameters are: $\theta = 0, \lambda/a = 0.1$. (b) Sums of diffraction efficiencies associated with (a).

Fig. 2. (a) The results of RCWA and TPGA for an evanescent wave grating as a function of incidence angle. The parameters are: $\varepsilon = 0.2, \lambda/a = 0.1$. (b) Sums of diffraction efficiencies associated with (a).

results in Figure 1a. This suggests that we might use condition (25) as a qualitative measure of the reliability of the TPGA calculation.

As another example, we compare the RCWA with the TPGA for a range of incidence angles. Here we set $\varepsilon = 0.2$ and $\lambda/a = 0.1$. The results are shown in Figure 2. Again the TPGA formula gives acceptable results. As $\theta \to 90°$ the TPGA formula becomes more accurate as the higher orders decay.

3.2 Magnetic gratings

Our motivation for developing the RCWA for atoms is to model the diffraction from magnetic diffraction gratings. These can be formed using a periodic array of permanent magnets or current carrying wires and applying an appropriate uniform magnetic field [4]. In the adiabatic approximation a paramagnetic atom experiences a potential proportional to the magnitude of the magnetic field B, which, depending on the source of the field, may have a complicated spatial dependence. This makes it difficult to solve the diffraction problem analytically, forcing us to use numerical techniques such as RCWA. In this section, however, we consider an ideal case. Following Opat *et al.* [29] we approximate our potential U by

$$U(x,y) = \sqrt{U_{\mathrm{a}}^2 + 2U_{\mathrm{a}}U_{\mathrm{m}} \cos \kappa x \exp(-\kappa y) + U_{\mathrm{m}}^2 \exp(-2\kappa y)}. \quad (31)$$

This approximation is reasonable provided the atom does not approach too close to the source of the field. Here U_{m} is the potential associated with the magnet array, U_{a} the potential arising from the magnetic field applied perpendicular to the mirror surface and $\kappa = 2\pi/a$ with a the period of the grating. The potential is related to the magnitude of the magnetic field B by

$$U(x,y) = \left(2m/\hbar^2\right) \mu_{\mathrm{B}} m_{\mathrm{F}} g_{\mathrm{F}} B(x,y) \quad (32)$$

where μ_{B} is the Bohr magneton and g_{F} the Landé factor. This assumes the atom is paramagnetic and adiabatically follows the variations in the field direction, *i.e.* the space quantisation number m_{F} is constant.

The grating described by the potential (31) has a large number of spatial harmonics as a consequence of its nonlinear character. If we approximate this by linear terms

$$U(x,y) \approx U_{\rm m} \exp(-\kappa y) + U_{\rm a} \cos \kappa x \qquad (33)$$

when $U_{\rm m} \exp(-\kappa y) \geq U_{\rm a}$ and by

$$U(x,y) \approx U_{\rm a} + U_{\rm m} \exp(-\kappa y) \cos \kappa x \qquad (34)$$

when $U_{\rm m} \exp(-\kappa y) \leq U_{\rm a}$ then the potential is amenable to analysis by the semi-classical method. The result is a TPGA formula for magnetic gratings [28]

$$e_n^{\rm TPGA} = (\cos \theta_n / \cos \theta) J_n^2(\alpha U_{\rm a}/k_i \kappa) \qquad (35)$$

where

$$\alpha = \cos(\gamma + \theta) + \sin \gamma / \sin \theta \qquad (36)$$

and

$$\gamma = \frac{k_i \sin \theta}{\sqrt{k_i^2 \cos^2 \theta + U_{\rm a}}} \ln \left(\frac{\sqrt{k_i^2 \cos^2 \theta + U_{\rm a}} + k_i \cos \theta}{\sqrt{k_i^2 \cos^2 \theta + U_{\rm a}} - k_i \cos \theta} \right). \qquad (37)$$

In these formulae, the value of the incident wavenumber k_i is that of the atom in the constant potential $U_{\rm a}$ (see discussion in Sect. 2). The TPGA formula (35) with (36, 37) is valid provided that $\lambda \ll a$ and that $U_{\rm a} \ll k_{\rm T}^2$ where $k_{\rm T}$ is the atom wave number at the classical turning point. This can be estimated from $k_{\rm T} \sim 0.69(\lambda/a \cos \theta)^{0.32} k_i$ [28].

As with the evanescent wave grating, we compare the RCWA method using potential (31) with the approximate formula (35) as a function of the applied magnetic field $B_{\rm a}$ for the case of normal incidence $\theta = 0$ with $\lambda = 0.1$ μm and $a = 1$ μm. Here we set $Z m_{\rm F} g_{\rm F} = 1$ where Z is the atom mass number. Figure 3a compares the diffraction efficiencies for the first three orders calculated using the RCWA method and TPGA (35) while Figure 3b shows the sum of the diffraction efficiencies. As before, the TPGA formula gives reasonable values but becomes progressively worse as the diffraction efficiency sum deviates from 1. We observe that the errors become significant for applied fields greater than about 1 Gauss. This is consistent with the requirement that $B_{\rm a} \ll 1.5$ Gauss to satisfy $U_{\rm a} \ll k_{\rm T}^2$. Figures 4a and 4b compare the RCWA with the TPGA for a range of incidence angles. Here we set $B_{\rm a} = 1$ Gauss, $\lambda = 0.1$ μm, $a = 1$ μm and $Z m_{\rm F} g_{\rm F} = 1$. The results are similar to those in Figure 2 where the result improves with increasing incidence angle.

3.3 Discussion

The TPGA formulae are obtained by ignoring higher-order terms in the wave equation [28]. This requires that the potential vary slowly with position compared to the atom wavelength and that the potential be weak. Since the atom wavelength becomes quite large near the classical turning point these conditions may well be violated, leading to errors.
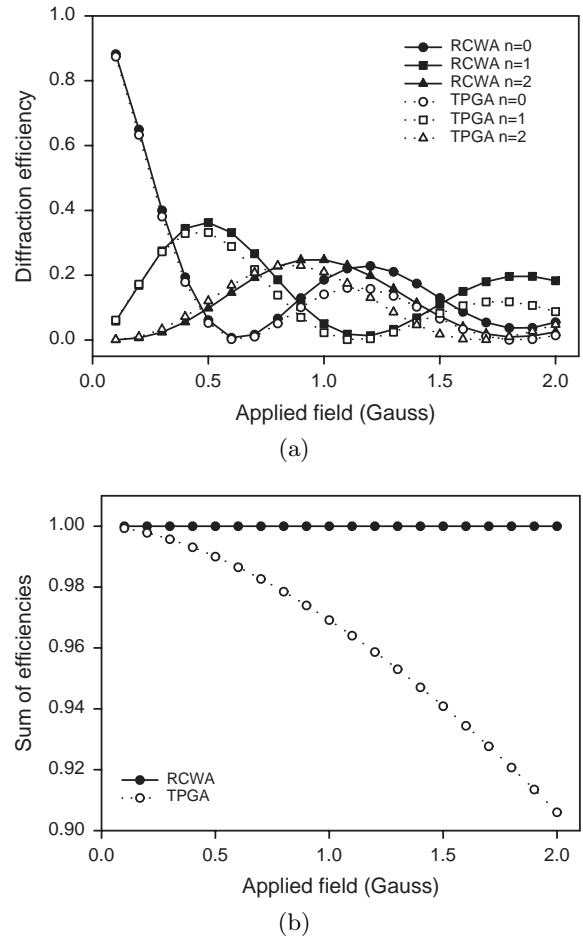

(a)

(b)

Fig. 3. (a) The results of RCWA and TPGA for a magnetic grating as a function of the applied magnetic field. The parameters are: $\theta = 0$, $\lambda = 1$ μm, $a = 1$ μm and $Z m_{\rm F} g_{\rm F} = 1$. (b) Sums of diffraction efficiencies associated with (a).

The TPGA formula are based on the classical trajectory of the atom in the mirror potential. As such, these formulae do not take account of the evanescent waves in the diffraction grating. These waves may be important in some circumstances. For example, an incident wave at an angle $\theta \gg 0$ 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. Coupling between the evanescent incident wave and the non-evanescent diffracting order can take place, altering the overall diffraction efficiencies. Such coupling would be important for reflecting potentials that vary slowly in the region of the classical turning point for this would extend the region of the evanescent coupling. Furthermore, evanescent wave effects are important for gratings with large amplitudes (e.g. large ε) because the waves can be evanescent in one region, such as where $\varepsilon \cos \kappa x > 0$ and non-evanescent in an adjacent region, where $\varepsilon \cos \kappa x < 0$. The RCWA takes
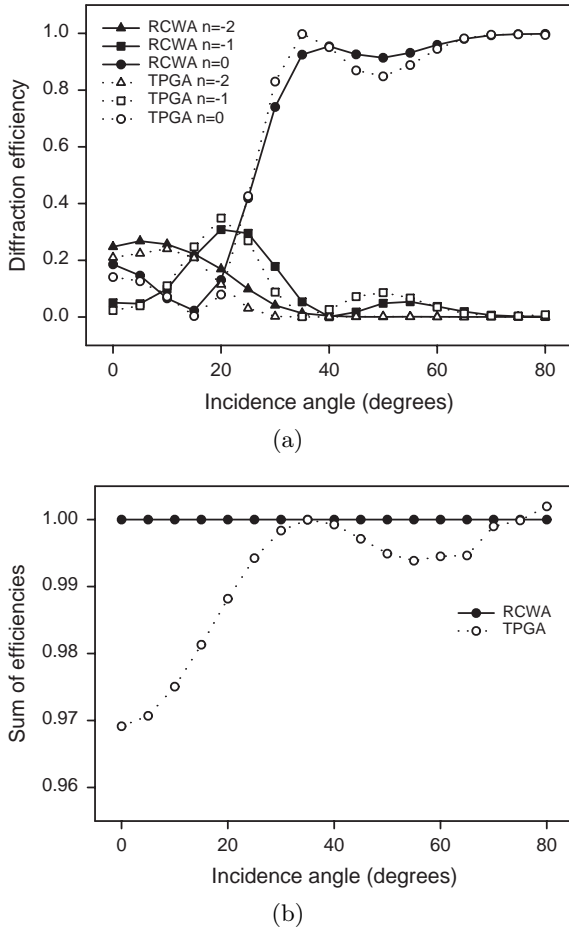
(a)

(b)

Fig. 4. (a) The results of RCWA and TPGA for a magnetic grating as a function of incidence angle. The parameters are: $B_a = 1$ Gauss, $\lambda = 1$ μm, $a = 1$ μm and $Zm_F g_F = 1$. (b) Sums of diffraction efficiencies associated with (a).

account of such coupling and this may explain some of the discrepancies.

Another limitation with the TPGA is that it does not take account of focussing effects. This point is discussed in [26]. 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 [19] 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.

4 Diffraction from an array of magnets

One method for creating a diffraction grating is to sputter a thin magnetic film onto a surface with a "square wave" profile. Mirrors have been made and tested using this technique and these can be formed into diffraction gratings by applying an appropriate uniform magnetic field. These
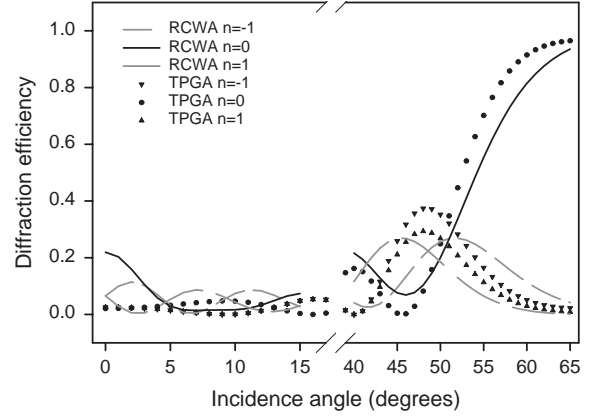

Fig. 5. The diffraction efficiencies in the orders -1, 0 and $+1$ calculated using RCWA for 50 nm wavelength ^{85}Rb atoms incident on an array of permanent magnets. The magnets have width and height 500 nm and the array has a period of 700 nm. The TPGA results are also shown.

diffraction gratings may be used as beam splitters in an interferometer. Our interest is to determine the optimum angle for beam splitting given a grating and a specified atom wave length. As an example calculation, we consider ^{85}Rb with $\lambda = 50$ nm and a grating with a period $a = 700$ nm. We ignore any effects due to gravity.

The magnet array is taken to consist of magnets of height h and width w of 500 nm with a magnetic field at the centre top of 100 Gauss. The magnetic field from an array of these magnets is given by

$$\mathbf{B}(x,y) = \frac{\mu_0 M}{4\pi} \sum_n \left(B_x(x+na,y)\hat{\mathbf{x}} + B_y(x+na,y)\hat{\mathbf{y}} \right)$$

(38)

where

$$B_x(x,y) = \ln\left(\frac{\left(y^2 + (x-\frac{w}{2})^2\right)\left((y-h)^2 + (x+\frac{w}{2})^2\right)}{\left(y^2 + (x+\frac{w}{2})^2\right)\left((y-h)^2 + (x-\frac{w}{2})^2\right)} \right)$$

(39)

and

$$B_y(x,y) =$$
$$2\arctan\left[\frac{hw\left(y(y-h) - x^2 + \frac{w^2}{4}\right)}{\left(x^2 + y(y-h) + \frac{w^2}{4}\right)^2 + h^2\left(x^2 - \frac{w^2}{4}\right) - x^2 w^2} \right].$$

(40)

The sum in (38) is over the magnets in the array. The diffraction efficiencies for the orders -1, 0 and $+1$ with an applied field of 0.2 Gauss are shown in Figure 5. For comparison we have included the TPGA results based on (35). For normal incidence the TPGA formula gives a poor result. For the parameters given it is only valid for $B_a \ll 0.2$ Gauss. Following the trends seen in Figure 4a we might expect the TPGA formula to become more accurate with increasing incidence angle. While there is a

qualitative improvement, there are still significant differences. This highlights the value of an accurate method for determining diffraction efficiencies.

For a beam splitter we usually require efficient splitting into two beams. With the grating in this example and the given atom wavelength, this is not possible since many high orders exist in the diffraction pattern. This grating would make a poor beam splitter. The best that can be done is about 22% efficiency into two orders -1 and $+1$ at $\theta = 49$ degrees with about 12% into order 0, or about 18% into two orders, 0 and $+1$, at $\theta = 41$ degrees. Uneven splitting can be achieved at angles greater than 50 degrees, but whether or not this is of use depends on the application.

5 Conclusion

The method of rigorous coupled-wave analysis is a useful numerical tool for calculating the diffraction of laser-cooled atoms from periodic potentials, such as formed by arrays of magnets, where approximate theories are not applicable. We have reviewed the theory behind the method and have outlined the procedures required for its implementation. Results of the RCWA applied to some example diffraction problems have been compared with formulae based on the thin phase-grating approximation. An indication of the quality of the predictions of a diffraction theory is the deviation from 1 of the sum of the diffraction efficiencies. The RCWA method satisfies this to better than 1 part in 10^{10}. The sum gives an indication of the regimes under which the TPGA formulae fail. We have also presented an example calculation of the diffraction efficiencies for grating made from an array of permanent magnets in the regime where the TPGA formula is not applicable. The results of the RCWA has highlighted the weakness as a beam splitter of the grating design used in the example.

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