Eur. Phys. J. D **11**, 151–157 (2000)

THE EUROPEAN PHYSICAL JOURNAL D

EDP Sciences

Atomic reflection from a magnetic mirror: Beyond the adiabatic approximation

U.V. Poulsen[a] and K. Mølmer

Institute of Physics and Astronomy, University of Aarhus, 8000 Århus C, Denmark

Received 21 October 1999 and Received in final form 18 January 2000

Abstract. We present theoretical calculations for the reflection of atoms from a magnetic surface with a sinusoidal magnetization. A fully quantum mechanical treatment is possible because the problem may be reduced to an effective one-dimensional one. Results of numerical wave-packet calculations are presented and compared with an analytical model in which the atoms separate into different internal state components which follow classical paths in different potentials.

PACS. 03.75.Be Atom and neutron optics – 34.50.-s Scattering of atoms, molecules and ions – 39.20.+q Atom interferometry techniques

1 Introduction

Techniques to cool atoms and to manipulate atomic matter waves have lead to the field of atom optics, where a host of theoretical and experimental results have been obtained in the past few years [1–3]. Atomic interferometers have been applied for measurements of inertial effects and of atomic parameters with unprecedented precision, and optical, electric and magnetic fields have been applied to guide and to hold atoms for several purposes.

Many studies have been carried out both theoretically and experimentally for atomic reflection from evanescent wave laser fields. Some effort has been made to investigate the behaviour of multi-(Zeeman)-level atoms, and the possible coherent transfer of amplitude among such levels has been identified as an effective means to produce coherent superpositions of matter waves with different propagation directions [4,5]. It has been shown that a corrugated prism surface causes non-specular reflection of the atoms, and that this effect, surprisingly, persists even when the turning point for the atomic motion is high above the prism surface [6].

We present here an analysis of the reflection of atoms by the magnetic field above a sinusoidally magnetized surface. This system was proposed and analyzed by Opat *et al.* [7], in the so-called adiabatic limit, where the dipole moment of the atom follows the direction of the magnetic field, and where the reflection potential is thus a simple exponential function of the height above the magnetic surface. Experimentally it is easy to ensure the validity of the adiabatic analysis [8, 9], hence, ideally, the scattering is specular and un-problematic from a theoretical point of view. Within the adiabatic approximation, deviations from the specular reflection due to imperfections in the magnetization of the mirror have been determined and found to agree with experimental observation [10, 11].

Deviation from adiabaticity ruins the simplest picture of the scattering process but, like in the case of scattering by an evanescent field, it provides a number of attractive possibilities for coherent matter wave dynamics. We analyze in this paper the original proposal for the magnetic mirror based on the sinusoidal magnetization of the magnetic material, but we assume parameters for the atomic motion for which the adiabatic approximation is not valid. We show that the full quantum mechanical problem can be reduced by a transformation to an effective one-dimensional reflection problem, which is not more complicated than scattering in the adiabatic potential. Our calculations include the transfer of amplitude among the Zeeman sublevels of the atoms, and a classical model from collision theory is proven to account excellently for the result obtained from a quantum mechanical wave-packet propagation.

The organization of this paper is as follows. In Section 2 we briefly present the basic theory behind magnetic mirrors. In Section 3 we present our reduction of the problem to one dimension and our results for the reflection coefficient obtained by wavepacket simulation. In Section 4 we present our mapping of the problem on a simple level crossing model. The problem of diffraction is treated in Section 5 and we conclude in Section 6.

2 Magnetic mirrors

The basic principle behind magnetic mirrors is the interaction between a magnetic field with some suitable variation in space and the magnetic moments of the atoms.

[a] e-mail: uvp@ifa.au.dk

Several realizations are possible, *e.g.*, the magnetic field above an array of current carrying wires [7,12,13], but in this paper we shall consider the field above a surface with permanent magnetization. This approach has been used in the early experimental work and can be implemented by simply recording a periodic pattern on a commercial storage medium (audiotape or floppy disc). As shown in this section such a simple magnetization leads to a magnetic field which decreases exponentially with the distance to the surface.

2.1 The magnetic field above a surface with periodic magnetization

Let us assume that we are given an infinite, flat and periodically magnetized surface aligned with the xz-plane in our coordinate system. The magnetization is constant along lines of constant x, and in the region above the surface we have no currents. Then the magnetic field is only a function of x and y and it can be derived from a scalar potential [14]:

$$\mathbf{B}(x,y) = -\nabla\Phi(x,y). \tag{1}$$

$\Phi(x,y)$ is determined (up to a constant) by the Laplace equation and the boundary conditions induced *via* $\mathbf{B}(x,y)$.

Let us take Φ at the surface to be a single harmonic,

$$\Phi(x,0) = A\cos(\kappa x). \tag{2}$$

This potential would correspond to, *e.g.*, an (infinitely thick) audio tape with a recorded sine-wave signal where $2\pi/\kappa$ is the wavelength. It then follows from complex function theory that

$$\Phi(x,y) = \mathrm{Re}\left(A\mathrm{e}^{\mathrm{i}\kappa(x+\mathrm{i}y)}\right) = A\cos(\kappa x)\mathrm{e}^{-\kappa y} \tag{3}$$

above the surface, and that

$$\begin{aligned} B_x(x,y) &= A\kappa\sin(\kappa x)\mathrm{e}^{-\kappa y} \\ B_y(x,y) &= A\kappa\cos(\kappa x)\mathrm{e}^{-\kappa y}. \end{aligned} \tag{4}$$

For details, see [7]. Note the simple dependence on x and y: the direction of the field rotates as we move along the surface while the magnitude of the field decreases exponentially as we move away from the surface.

2.2 Motion of a neutral atom

The interaction of the atom with the magnetic field can be described by a potential energy operator of the form

$$\hat{V}(x,y,z) = -\hat{\boldsymbol{\mu}}\cdot\mathbf{B}(x,y,z) \tag{5}$$

where $\hat{\boldsymbol{\mu}}$ is the atomic magnetic moment operator acting on the electronic degrees of freedom. For sufficiently weak fields it takes on the well-known form of the anomalous Zeeman effect:

$$\hat{\boldsymbol{\mu}} = -\frac{g_j\mu_\mathrm{B}}{\hbar}\hat{\mathbf{J}}. \tag{6}$$

The g_j is the Landé factor depending only on the fine structure level of the atom.

The coupling of the magnetic moment of the atom with a spatially dependent magnetic field introduces a coupling between the internal and centre-of-mass degrees of freedom for the atom. The usual resort to the adiabatic theorem assumes that the magnetic moment of the atom retains its projection along the direction of $\mathbf{B}$ as the atom moves. In this picture it is easy to understand qualitatively the motion of an atom. Depending on the sign of the projection of its total angular momentum, $\mathbf{J}$, on the magnetic field it will be either low field seeking or high field seeking, its potential energy increasing or decreasing with field strength. One can then readily design a mirror for low field seekers; it is merely a question of having a sufficient increase in B when the atom approaches the mirror surface. If the reflection is going to be specular it is a further demand that the equipotentials (*i.e.* surfaces of constant $|\mathbf{B}|$) are planes. The field configuration of Section 2.1 satisfies this requirement despite the rotation of the direction of $\mathbf{B}$ as a function of x.

3 Quantum treatment of motion

The adiabatic approximation is both convenient and in most situations well justified [8,9]. It is, however, not too difficult to go further as will be shown in the following sections. In particular, it is quite easy to make a full quantum mechanical analysis, even in case of a non-constant direction of $\mathbf{B}$ along the surface.

3.1 Reduction to 1D problem

The Hamiltonian of an atom moving in a magnetic field will be taken to be

$$\hat{H} = \frac{\hat{p}^2}{2M} - \hat{\boldsymbol{\mu}}\cdot\mathbf{B} \tag{7}$$

where M is the mass of the atom and $\hat{p}$ is the atomic momentum. The problem is effectively two-dimensional as we have assumed only x- and y-dependence of the magnetic field so that the third dimension is separable from the other two. Using the Zeeman form of $\hat{\boldsymbol{\mu}}$ from (6) and the magnetic field of (4) we can write:

$$-\hat{\boldsymbol{\mu}}\cdot\mathbf{B} = V_0\mathrm{e}^{-\kappa y}\left[\hat{J}_x\sin(\kappa x) + \hat{J}_y\cos(\kappa x)\right]. \tag{8}$$

We now realize that the form of $\hat{H}$ only allows certain momentum transfers in the x-motion and only at the expense of an accompanying change in the internal state of the atom. To see this explicitly we rewrite the parenthesis in (8) as

$$\begin{aligned} \hat{J}_x\sin(\kappa x) + \hat{J}_y\cos(\kappa x) = \\ \frac{\hat{J}_+ + \hat{J}_-}{2}\sin(\kappa x) + \frac{\hat{J}_+ - \hat{J}_-}{2\mathrm{i}}\cos(\kappa x) \\ = \frac{1}{2\mathrm{i}}(\hat{J}_+\mathrm{e}^{\mathrm{i}\kappa x} - \hat{J}_-\mathrm{e}^{-\mathrm{i}\kappa x}). \end{aligned} \tag{9}$$

From this we deduce that it is advantageous to expand the centre-of-mass x-dependence and the internal state dependence on the families of basis states of the form

$$\mathrm{e}^{\mathrm{i}(p_x+m\hbar\kappa)x/\hbar}|m\rangle;\ m\in\{-j,\ldots,j\}. \tag{10}$$

This is a mixed notation where the center-of-mass motion is described by a plane wave, while the internal state of the atom is represented as a state vector, $|m\rangle$, $m\hbar$ denoting the $\hat{J}_z$ eigenvalue. p_x labels the families and m labels the $2j+1$ states in each family. Note that all members of a family has different center-of-mass momenta, p_x merely denoting the central value. It is easy to show from (9) that $\hat{\boldsymbol{\mu}}\cdot\mathbf{B}$ does not couple states from different families and that the coupling inside a family is formally analogous to $\hat{J}_y=(1/2\mathrm{i})(\hat{J}_+-\hat{J}_-)$ in a usual angular momentum multiplet.

The family states of (10) are eigenstates of the x component of momentum and they diagonalise the corresponding part of the kinetic energy operator:

$$\int \mathrm{d}x\langle m'|\mathrm{e}^{-\mathrm{i}(p'_x+m'\hbar\kappa)x/\hbar}\frac{\hat{p}_x^2}{2M}\mathrm{e}^{\mathrm{i}(p_x+m\hbar\kappa)x/\hbar}|m\rangle = \frac{(p_x+m\hbar\kappa)^2}{2M}\,2\pi\hbar\,\delta(p_x-p'_x)\delta_{m'm}. \tag{11}$$

Writing the wave-function as

$$\Psi(x,y)=\int\frac{\mathrm{d}p_x}{\sqrt{2\pi\hbar}}\sum_{m=-j}^{j}\phi_{p_x,m}(y)\mathrm{e}^{\mathrm{i}(p_x+m\hbar\kappa)/\hbar}|m\rangle \tag{12}$$

it is thus possible to reduce the problem to a spatially one-dimensional one with p_x entering only as a parameter. For each family, we get the $2j+1$ coupled equations

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\phi_{p_x,m'}(y,t) = \left(-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial y^2}+\frac{(p_x+m\hbar\kappa)^2}{2M}\right)\phi_{p_x,m'}(y,t) + \sum_{m=-j}^{j}V_0\mathrm{e}^{-\kappa y}\langle m'|\hat{J}_y|m\rangle\phi_{p_x,m}(y,t). \tag{13}$$

To summarize we can write equation (13) in the form:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\phi\rangle=\hat{H}_{1\mathrm{D}}|\phi\rangle \tag{14}$$

where $|\phi\rangle$ is the state vector of a spin-j particle moving in one spatial dimension and subject to the Hamiltonian

$$\hat{H}_{1\mathrm{D}}=\frac{\hat{p}_y^2}{2M}+\frac{p_x^2}{2M}+\frac{(\hbar\kappa)^2}{2M}\hat{J}_z^2+\frac{p_x\hbar\kappa}{M}\hat{J}_z+V_0\mathrm{e}^{-\kappa y}\hat{J}_y. \tag{15}$$

Note how the motion along the x-axis is incorporated by means of a constant kinetic energy term ($p_x^2/2M$) and a fictitious magnetic coupling ($p_x\hat{J}_z$, $\hat{J}_z^2$ terms).

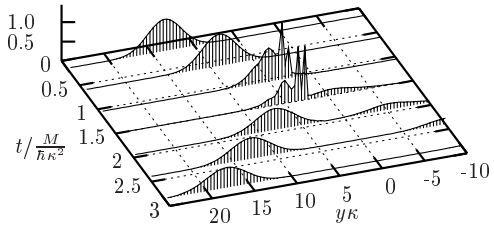

Fig. 1. Wave-packet simulation of a $j=2$ atom interacting with a magnetic mirror. Shown is the squared norm of the wavefunction. The initial wavepacket at $t=0$ is purely $m=+2$ and has a momentum spread of $2\hbar\kappa$ around $p_y=-15\hbar\kappa$. The family momentum is $p_x=3\hbar\kappa$ and the mirror strength is $V_0=800(\hbar\kappa)^2/M$.

3.2 Wave-packet propagation

With the reduction to one spatial dimension it is possible to do a numerical wave packet propagation for small values of j. We have used the split-step technique [15] based on the approximation for the propagator

$$\mathrm{e}^{-\mathrm{i}\frac{\hat{H}_{1\mathrm{D}}}{\hbar}\mathrm{d}t}\cong\mathrm{e}^{-\mathrm{i}\frac{\hat{p}^2}{2M\hbar}\mathrm{d}t}\mathrm{e}^{-\mathrm{i}\frac{\hat{V}}{\hbar}\mathrm{d}t}. \tag{16}$$

The kinetic energy operator can in this way be applied after a FFT to momentum space where it is simple. As for the potential part we are faced with the problem of exponentiating the $\hat{J}_y$-part which is not diagonal in m and is therefore simple neither in direct nor in momentum space. Remember, however, that $\hat{J}_y$ is the generator of rotation about the y-axis. All we have to do is thus to calculate the corresponding Wigner rotation matrix $D^{(j)}_{m'm}$ and apply this to the multiplet $\phi_{p_x,m}$.

A particular concern when doing this wave packet calculation is how to simulate the absorption/incoherent scattering of the parts of the wave that actually reach the surface. Even an imaginary potential will cause some reflection so we have chosen to simply symmetrise the potential allowing the components of the wave moving on attractive potential curves to continue through the mirror. This also allows us to use norm conservation as a check throughout the simulation. We have of course varied the parameters to test independence of our results on the exact details of the potential at and behind the surface.

In Figure 1 is shown a plot of a typical calculation for $j=2$. The wavepacket starts out in the $m=+2$ state. At some point there is a non-adiabatic transfer to other states and soon hereafter reflection takes place. These stages are of course not clearly separable on a wavepacket plot but as we shall see later such a line of events provides surprisingly good analytical predictions for the reflection coefficient.

4 Classical approximation and two-state model

In order to get a more intuitive understanding of the reflection process it is useful to make a classical model. The simplest approximation consist in treating the centre-of-mass motion of the atom classically, *i.e.*, by a trajectory

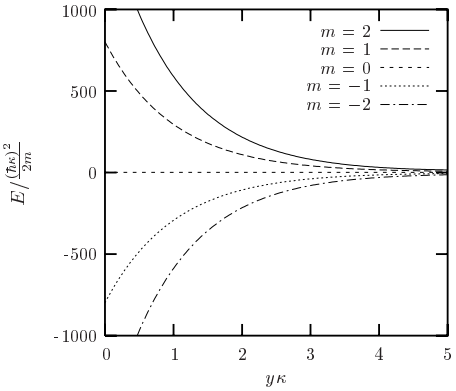

Fig. 2. Adiabatic potential curves for a neutral $j = 2$ atom approaching a magnetic mirror. The family momentum (see Eq. (10)) is $p_x = 5\hbar\kappa$ and $V_0 = 800(\hbar\kappa)^2/M$. The adiabatic potential curves correlate with the $\hat{J}_z$ eigenstates for $y\kappa \gg 1$ and with the $\hat{J}_y$ eigenstates for $y\kappa \ll 1$. In these limits and bases the curves are correctly labelled by the m quantum number in the legend. Note that the transformation $p_x \to -p_x$ reverses the order of the $\hat{J}_z$-eigenstates far from the mirror.

$y(t)$. The internal state of the atom then experiences a time-dependent Hamiltonian and the atom is subject to a mean force and acceleration, determined from the spatial derivative of the coupling to the field. The atom can also be subject to external forces, *e.g.*, gravity or for an ion electrostatic forces, which do not depend on the internal state. This approach is justified when the kinetic energy of the atom dominates any terms in the Hamiltonian depending on the internal state of the atom.

The adiabatic model deals with a somewhat different regime. Here one acknowledges that the internal states have an important effect in determining the potential that the atom experiences. In order for this potential to be well defined it is then necessary to assume that the internal state will follow changes in the Hamiltonian adiabatically. This will be the case if the Hamiltonian changes sufficiently slowly. Note that the adiabatic model does not prevent a fully quantum mechanical treatment of the centre-of-mass motion: it merely translates the coupling of the inner state to a varying field into potential curves for this motion. A plot of the adiabatic potential curves for the problem is shown in Figure 2. Close to the surface the expontial function dominates and the adiabatic states are $\hat{J}_y$ eigenstates. Far from the mirror the adiabatic states are $\hat{J}_z$ eigenstates but their ordering in energy depends on p_x.

We treat the motion classically on these adiabatic potential curves and divide the reflection of an atom into a number of distinct phases:

- free motion treated classically; internal state evolves adiabatically;
- coupling zone with non-adiabatic transfer; all potential curves are relatively flat, and the centre-of-mass motion is treated as classical and free; the internal state experiences a time-dependent Hamiltonian;
- reflection of the components on repulsive energy curves; motion is again adiabatic, but we track different internal state components of the atom along different paths;
- after the reflection a second passage of the coupling region; interference determines the population on outgoing adiabatic states.

The most demanding part is the integration of $2j + 1$ coupled equations in the coupling zone. Fortunately, as we shall see, it is possible to get an excellent analytical prediction for this problem.

4.1 Exponential level crossing model

We treat the centre-of-mass motion classically so the internal part of the Hamiltonian (15) looks like

$$\hat{H}_{\text{internal}} = \frac{(\hbar\kappa)^2}{2M}\hat{J}_z^2 + \frac{p_x\hbar\kappa}{M}\hat{J}_z + V_0 \mathrm{e}^{-\kappa y(t)}\hat{J}_y. \qquad (17)$$

Now if we exclude very small p_x the $\hat{J}_z^2$-term is negligible and the evolution generated by the Hamiltonian is just a rotation of the spin, the well-known spin precession around an applied magnetic field. With this knowledge all we really have to keep track of is the three Euler angles corresponding to this rotation. Direct equations for these angles are quite complicated but an elegant way to get simple substitutes is to note that if we propagate a spin-1/2 subject to (17) (without the $\hat{J}_z^2$-term) it will undergo exactly the same rotation as any other spin-j. From the integration of just two coupled equations for the $m = \pm 1/2$ state amplitudes we therefore gain complete knowledge of the Euler-angles and hence the solution of the original $2j + 1$-equation problem. This approach is described by Kazansky and Ostrovsky in [16] and has roots all the way back to Majorana who analyzed the dynamics of a general angular momentum j in a varying magnetic field in terms of geometric rotation [17]. In [18] an N-level model, equivalent with this problem, is formally solved in terms of Wigner rotation functions with specified rotation angles, and references are given to other models where the N-level dynamics is determined by the solution of a coupled pair of equations, but without the straightforward picture of spin rotation (see also [19]).

Writing down the spin-1/2 two-state problem is only a matter of inserting the Pauli-matrices:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\chi(t) = \begin{bmatrix} \frac{1}{2}\omega_z & -\frac{\mathrm{i}}{2}\omega_y(t) \\ \frac{\mathrm{i}}{2}\omega_y(t) & -\frac{1}{2}\omega_z \end{bmatrix}\chi(t) \qquad (18)$$

where

$$\omega_z \equiv \frac{\kappa p_x}{M},\ \omega_y(t) \equiv V_0 \mathrm{e}^{-\kappa y(t)}. \qquad (19)$$

If $y(t)$ is taken to be a simple motion at constant speed

$$y(t) = y_0 + v_{y0}t \qquad (20)$$

the problem can be recognized as a special case of the *Nikitin* or *exponential level crossing model* [20] describing population transfer among electronic states in atomic collisions.

Letting time run from $-\infty$ to ∞[1] Nikitin provides analytical expressions for both the asymptotic populations on the adiabatic states as well as the dynamic phases accumulated. From these we extract the Euler angles, the most important being the polar angle β:

$$\cos\frac{\beta}{2} = \sqrt{1-\mathrm{P}(\xi)} \quad \sin\frac{\beta}{2} = \sqrt{\mathrm{P}(\xi)}$$
$$\mathrm{P}(\xi) = \frac{1-\mathrm{e}^{-\pi\xi}}{\mathrm{e}^{\pi\xi}-\mathrm{e}^{-\pi\xi}} \tag{21}$$

where

$$\xi = \frac{p_x}{|Mv_{0y}|} = \frac{p_x}{|p_{y0}|}\,. \tag{22}$$

Once we have found the Euler rotation that a particle with magnetic dipole moment experiences when passing the coupling zone it is simple to calculate the reflection coefficient of the surface for a given initial state. We simply apply the appropriate Wigner rotation matrix to the initial state vector and then sum the resulting populations on repulsive potential curves. There is a slight subtlety here: the populations and phases we get from the Nikitin model are referring to adiabatic states, *i.e.*, J_z-eigenstates for $y\kappa \gg 1$ and J_y-eigenstates for $y\kappa \ll 1$. This is convenient as it means that we immediately get the result in the relevant basis and we are able to tell what will be reflected and what will be absorbed.

As an example let us consider a $j = 1$ atom. The Wigner rotation matrix is given by

$$D^{(1)}(\alpha,\beta,\gamma) = \begin{bmatrix} \frac{1+\cos\beta}{2}\mathrm{e}^{-\mathrm{i}(\alpha+\gamma)} & -\frac{\sin\beta}{\sqrt{2}}\mathrm{e}^{-\mathrm{i}\alpha} & \frac{1-\cos\beta}{2}\mathrm{e}^{-\mathrm{i}(\alpha-\gamma)} \\ \frac{\sin\beta}{\sqrt{2}}\mathrm{e}^{-\mathrm{i}\gamma} & \cos\beta & -\frac{\sin\beta}{\sqrt{2}}\mathrm{e}^{\mathrm{i}\gamma} \\ \frac{1-\cos\beta}{2}\mathrm{e}^{\mathrm{i}(\alpha-\gamma)} & \frac{\sin\beta}{\sqrt{2}}\mathrm{e}^{\mathrm{i}\alpha} & \frac{1+\cos\beta}{2}\mathrm{e}^{\mathrm{i}(\alpha+\gamma)} \end{bmatrix}. \tag{23}$$

With an initial state with $m = +1$

$$\chi_{\mathrm{in}} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \tag{24}$$

we get

$$\chi_{\mathrm{out}} = D^{(1)}\chi_{\mathrm{in}} = \begin{bmatrix} \frac{1}{2}(1+\cos\beta)\mathrm{e}^{-\mathrm{i}(\alpha+\gamma)} \\ \frac{1}{\sqrt{2}}\sin\beta\mathrm{e}^{-\mathrm{i}\gamma} \\ \frac{1}{2}(1-\cos\beta)\mathrm{e}^{\mathrm{i}(\alpha-\gamma)} \end{bmatrix}. \tag{25}$$

[1] The level crossing model is analytically solvable for an infinite time interval, but the results apply to our problem as well, because the population transfer in the infinite time model occurs entirely in a narrow coupling region.

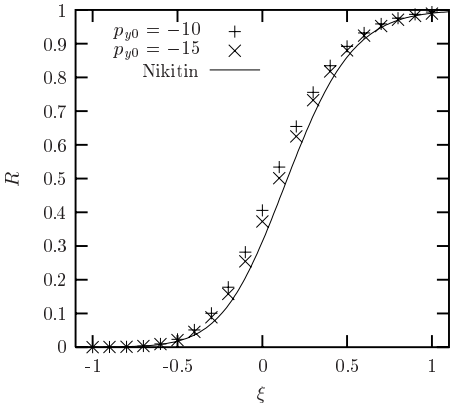

Fig. 3. Nikitin model prediction (line) together with wavepacket results (points) for the reflection coefficient when a $j = 2$ atom initially in $m = +2$ interacts with a magnetic mirror with $V_0 = 800(\hbar\kappa)^2/M$. The Nikitin model predict R to be a function of $\xi = p_x/|p_{y0}|$ only. The discrepancy between the analytical result and the wavepacket calculations at a given ξ is reduced as p_{y0} and p_x are increased. This is expected from the reduced importance of the J_z^2-term.

The amplitudes in (25) are given in the basis of potential eigenstates close to the mirror and the first amplitude refers to the repulsive potential curve. The reflection coefficient of the mirror thus becomes

$$R^{(1)} = \frac{1}{4}(1+\cos\beta)^2 = (1-\mathrm{P}(\xi))^2. \tag{26}$$

For other values of j completely analogous calculations can be made. Wigner rotation matrices for higher j are tabulated or they can be computed by Wigner's formula [21]. For any incident state χ_{in}, it is thus easy to get χ_{out}, the state after the coupling zone. If all repulsive curves exceed the incident energy, the reflection probability equals the sum of the population of states with positive m-values in χ_{out}. If, in particular, the initial state has $m = j$ these populations have the following simple analytical expressions:

$$|\chi_{\mathrm{out},m}|^2 = \binom{2j}{j+m}(1-P(\xi))^{j+m}P(\xi)^{j-m}. \tag{27}$$

Figure 3 shows a plot of the reflected fraction $|\chi_{\mathrm{out},2}|^2 + |\chi_{\mathrm{out},1}|^2$ for $j = 2$ together with results of a number of wavepacket runs with varying p_x. As expected our model is closest to the full calculation when p_x is large. This is the regime where it is well justified to neglect $\hat{J}_z^2$. The reasonable overall agreement leads us to conclude, that the classical treatment of the centre-of-mass degrees of freedom is a good approximation.

As Figure 3 illustrates the adiabatic regime in our 1D problem is the regime of numerically large ξ: an atom initially in a state with positive m and positive p_x approaches the mirror on a repulsive adiabatic potential curve (see Fig. 2 and Eq. (17)) and as expected a large separation of the curves (large p_x) and a slow approach (small p_{y0}) will force it to adiabatically follow this curve

and to be reflected. If we reverse the sign of p_x the order of the adiabatic curves far from the mirror is reversed and the atom is instead on an attractive adiabatic curve. This has the effect that an atom in an extreme $\hat{J}_z$ eigenstate and with sufficient x-momentum is either reflected or absorbed with 100% efficiency depending on the sign of the product $m_z p_x$.

4.2 Mean field inclusion of $\hat{J}_z^2$

As we saw in the previous section it is possible to get reasonable predictions for the reflection by the mirror by treating the external motion classically, neglecting the J_z^2 term in (17) and extracting the evolution as Euler angles from a two state level crossing model. To include the J_z^2 term one would have to solve the set of $2j+1$ equations numerically which would still be a manageable task. Here, however, we want to present an efficient approximate inclusion of this term, retaining the simple two-level treatment and the appealing picture of the evolution as a rotation.

As far as rotations are concerned a spin of length j can always be viewed as made up of $2j$ independent spin-1/2 particles

$$\hat{J}_z = \sum_{i=1}^{2j} \hat{J}_{zi}. \tag{28}$$

Exposed to a magnetic field the spins evolve independently and we only need to follow one spin to solve the full problem. This is another way of stating the method of Section 4.1. We now want to include the $\hat{J}_z^2$ term approximately. We therefore write

$$\hat{J}_z^2 = \sum_i \hat{J}_{zi}^2 + \sum_{\substack{i,k \\ k\neq i}} \hat{J}_{zi}\hat{J}_{zk} \tag{29}$$

and observe that for each spin-1/2, $\hat{J}_{zi}^2$ is proportional to the identity. The effect of the last term, coupling the spins, can be incorporated in a Hartree, or mean field treatment by the approximation

$$\sum_{k\neq 1} \hat{J}_{z1}\hat{J}_{zk} \to (2j-1)\langle \hat{J}_{z1}\rangle \hat{J}_{z1}. \tag{30}$$

where $\langle \hat{J}_{z1}\rangle$ is the mean value, determined in the self-consistent state of the fictitious spin-1/2 system. Note that as the evolution is no longer linear we have to do the integration once for each initial state to be considered. An example of the correction due to this non-linear treatment is shown in Figure 4. It accounts perfectly for the small difference between the exact calculation and the simple Nikitin model.

5 Diffraction

In the previous section we were only interested in how large a fraction of an incoming wavepacket is reflected.

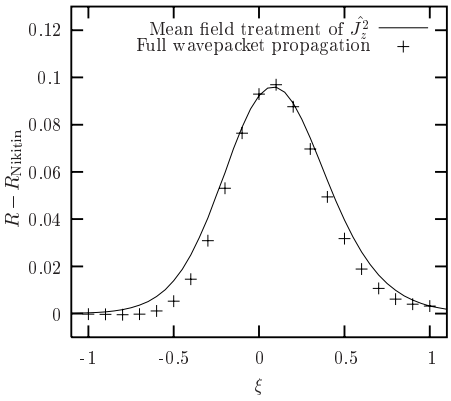

Fig. 4. Effect of mean field inclusion of the $\hat{J}_z{}^2$-term. The physical parameters are: $j = 2$, $p_{y0} = -10\hbar\kappa$ and $V_0 = 800(\hbar\kappa)^2/M$. The deviation of the full wavepacket results from the simple Nikitin model is nicely explained by making the minimum extension: we still make the classical approximation and assume the evolution to be a rotation of the spin, but we approximate the $\hat{J}_z{}^2$ term in the Hamiltonian by the mean field like term (30).

In the adiabatic regime all atoms stay on their initial potential curve and are either absorbed or reflected and leave the mirror in the same internal state as they started in. In the vicinity of $\xi = 0$ nonadiabatic effects are important, and parts of each wavepacket are transfered to other adiabatic potential curves on the way in and on the way out again. Atoms which leave the mirror in different m-states also have different momentum components along the x-axis, *cf.* equation (10). Energy conservation implies that also their momentum along the y-axis is different. This phenomenon is a kind of diffraction (note that the centre-of-mass motion is entangled with the internal state), and the population of different diffraction orders is determined by the population of different internal states.

We write the evolution of the internal atomic state as

$$\chi_{\rm final} = U_{\rm out}\mathsf{R}U_{\rm in}\chi_{\rm in} \tag{31}$$

where $U_{\rm in}$ and $U_{\rm out}$ describe the effect of the coupling zone and R is a matrix describing the accumulated phases on the sufficiently repulsive potential curves and the absorption of the remaining components of the wavefunction. The U matrices for internal state amplitudes are in the adiabatic basis given by the Wigner rotation matrices $D^{(j)}(\alpha,\beta,\gamma)$ of Section 4 (*cf.* comment below Eq. (22)). In this basis, corresponding to $\hat{J}_y$ eigenstates close to the surface, R is diagonal:

$$\mathsf{R}_{m_y m_y'} = \delta_{mm'}\Theta\left(m_y V_0 - \frac{p_{y0}^2}{2M}\right)\mathrm{e}^{\mathrm{i}\phi_{m_y}}. \tag{32}$$

The Heaviside function ensures that the adiabatic potentials only reflect particles if they exceed the incident kinetic energy. In our calculations we always take V_0 large enough to reflect atoms in all states with positive m_y.

As shown in Section 4 the Wigner rotation matrix corresponding to $U_{\rm in}$ can be calculated analytically *via* the

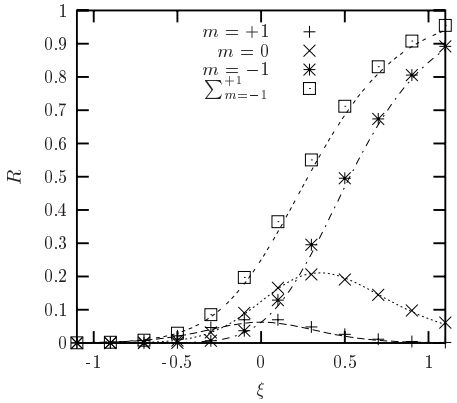

Fig. 5. Population on the three reflected Zeeman components when a $j = 1$ atom interacts with a mirror. The symbols represent the results of the full wavepacket calculation, the curves represent the analytical results (34) from the Nikitin model. Here $p_{y0} = -10\hbar\kappa$ and $V_0 = 800(\hbar\kappa)^2/M$.

Nikitin level crossing model. $U_{\rm out}$ is the result of the same sequence of infinitesimal rotations as $U_{\rm in}$ but in opposite order of appearance. This means that $U_{\rm out}$ in the adiabatic basis is given by:

$$(D(-\alpha,-\beta,-\gamma))^{-1} = D(\gamma,\beta,\alpha). \tag{33}$$

Evaluation of the final state is simple for both spin-1/2 and spin-1. In these cases there is only one repulsive curve and thus no interference can take place and we do not have to keep track of phases. Starting, *e.g.*, from an $m = +1$ state in the $j = 1$ case we get:

$$|\chi_m^{\rm final}|^2 = |d_{m1}^{(1)}|^2 |d_{11}^{(1)}|^2 = \begin{cases} (1-P(\xi))^4 & m=+1 \\ 2\,(1-P(\xi))^3\,P(\xi) & m=0 \\ (1-P(\xi))^2\,P(\xi)^2 & m=-1 \end{cases} \tag{34}$$

$P(\xi)$ is the function introduced in (21). A plot of these curves is shown in Figure 5 together with the corresponding wavepacket results. The agreement is seen to be very satisfactory.

6 Conclusion

We have in this paper developed the theory for scattering of atoms by a sinusoidally magnetized mirror. We have reduced the quantum problem to a one-dimensional wavepacket problem, for which numerical results have been obtained for wide ranges of collision parameters. The quantum treatment was supplemented by a classical description, where internal state amplitudes for the atoms were given analytically by the *Nikitin* model for slow atomic collisions, and where the atomic motion was split according to the distribution on internal states. In this model, the results depend only on the ratio p_x/p_{y0} and on j, and the analytical results of this treatment are in excellent agreement with those of the quantum formulation of the problem. This agreement was verified for $|p_{y0}| = 10\hbar\kappa$ and $15\hbar\kappa$. If the surface magnetization has a period of order of a micrometer, sodium atoms with these momenta have velocities of tens of cm/s, which is experimentally obtainable by dropping the atoms from a MOT above the mirror. The agreement with the quantum calculation should be even better for larger values of the momenta.

Our theory supplements previous works which have concentrated on cases where the internal state follows the direction of the magnetic field adiabatically, and where the problem reduces to a scalar reflection problem. For the construction of perfect mirrors it is not difficult to fulfill the adiabaticity criterion. In practice, one applies a homogeneous magnetic field in the entire region above the surface, which ensures a splitting of the asymptotic potential curves in Figure 2. If such a guiding field is along the z-axis it is easily included in our treatment of the reflection process. Adding $g_J\mu_{\rm B}B_z\hat{J}_z/\hbar$ to the Hamiltonian (17), we find that the results of Section 4.1 still hold but with $\xi = p_x/p_{y0}$ replaced by $\xi = (p_x + g_J\mu_{\rm B}B_zM/\kappa)/p_{y0}$.

Our work, and further work along the lines of the present paper, should contribute to ideas for making more use of the multi-level structure of the atoms, *e.g.*, for diffraction or spatial sorting of atoms according to their internal state.

References

1. C.S. Adams, M. Sigel, J. Mlynek, Phys. Rep. **240**, 143 (1994).
2. H. Wallis, Phys. Rep. **255**, 203 (1995).
3. E.A. Hinds, I.G. Hughes, J. Phys. D: Appl. Phys. **32**, R119 (1999).
4. C. Henkel, K. Mølmer, R. Kaiser, C.I. Westbrook, Phys. Rev. A **56**, R9 (1997).
5. L. Cognet *et al.*, Phys. Rev. Lett. **81**, 5044 (1998).
6. C. Henkel *et al.*, Phys. Rev. A **55**, 1160 (1997).
7. G.I. Opat, S.J. Wark, A. Cimmino, Appl. Phys. B **54**, 396 (1992).
8. T.M. Roach *et al.*, Phys. Rev. Lett. **75**, 629 (1995).
9. A.I. Sidorov *et al.*, Quant. Semiclass. Opt. **8**, 713 (1996).
10. I.G. Hughes *et al.*, J. Phys. B: At. Mol. Opt. Phys. **30**, 647 (1997).
11. I.G. Hughes, P.A. Barton, T.M. Roach, E.A. Hinds, J. Phys. B: At. Mol. Opt. Phys. **30**, 2119 (1997).
12. L. Cognet *et al.*, Europhys. Lett. **47**, 538 (1999).
13. D.C. Lau *et al.*, Eur. Phys. J. D **5**, 193 (1999).
14. J.D. Jackson, *Classical Electrodynamics*, 2nd edn. (John Wiley & Sons, New York, 1975).
15. J.A. Fleck Jr, J.R. Morris, M.D. Feit, Appl. Phys. **10**, 129 (1976).
16. A.K. Kazansky, V.N. Ostrovsky, J. Phys. B: At. Mol. Opt. Phys. **29**, L855 (1996).
17. E. Majorana, Nuovo Cimento **9**, 43 (1932).
18. R.J. Cook, B.W. Shore, Phys. Rev. A **20**, 539 (1979).
19. N.V. Vitanov, K.-A. Suominen, Phys. Rev. A **56**, R4377 (1997).
20. E.E. Nikitin, S.Y. Umanskii, *Theory of Slow Atomic Collisions* (Springer-Verlag, Berlin, 1984).
21. J.J. Sakurai, *Modern Quantum Mechanics*, rev. edn. (Addison-Wesley, Massachusetts, 1994).