



Time Reversal Techniques for Atomic Waveguides

by William M. Golding

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14. ABSTRACT The modes of an atomic waveguide are analyzed using both the time reversal symmetry of the system and the Frobenius method of series solution to create a general, physically acceptable, solution of the radial differential equations. The general solution is used to obtain precise energies and wavefunctions by imposing various boundary conditions on the radial solution at some distance from the guide center. The use of the time reversal technique to analyze the mode structure allows for a simplified understanding of the transition between the zero Ioffe field case and the moderate Ioffe field case. By understanding the relation between the two time reversed modes, it is expected that a technique based on the time reversal symmetry of the system can be developed to efficiently model decay mechanisms and other dynamics of atomic guides and guided wave magnetic beam splitters used in chip based atom interferometers.					
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1. Introduction

On atom chips, coherent atomic waveguides are important components needed for the construction of certain types of matter wave interferometers that use cold magnetic atoms. Results concerning the use of the time reversal symmetry (Tinkham, 1964) to solve the quantum behavior of a spin one-half particle guided in a type of atom waveguide often used on atom chips are presented here.

The Hamiltonian for the atom guide is symmetric under time inversion, if the reversal of the external magnetic fields is explicitly included in the reversal process. As described in a previous report (Golding, 2010a), the Frobenius power series method can be used to derive a pair of power series solutions that are well behaved at the coordinate origin. These two solutions are related to one another by the time reversal symmetry of the system. Two other solutions that are not finite at the origin are rejected for physical reasons in this waveguide problem.

These series solutions are useful as they allow the basic symmetry properties of the transverse modes of the guided atoms to be studied analytically. In addition, these series can be readily summed for a large range of radial distances using arbitrary precision arithmetic techniques so that the behavior of guided modes can be studied numerically.

In order to form eigenstates and calculate eigenvalues, the pair of physically acceptable solutions derived in this way must be combined to satisfy some type of boundary condition relevant to the problem of interest. Others have essentially used an open boundary condition to describe a quadrupole guide of infinite transverse extent. This leads to an ambiguity in the eigenstates that may be important in understanding the behavior of these guides in practice. In our current work, a hard-wall boundary condition is used, establishing a closed boundary. This forces both components of the spinor solutions to be zero at some fixed radius representing the boundary. When hard-wall boundary conditions are used, a complete system of orthogonal eigenstates is found that satisfies the Sturm-Liouville conditions. Further work is needed to understand the relationship between these two sets of boundary conditions as the limit of a large radius for the hard wall is taken.

Since explicit series solutions are developed, an ordinary differential equation (ODE) solver is not needed to calculate the wavefunctions or eigenvalues. This is extremely useful as the fourth order differential equations involved are stiff and difficult to handle with normal ODE techniques. Both the energy spectra and the wavefunctions can be calculated directly using the series technique for various regimes of magnetic field strength, allowing the direct study of the assumed adiabatic behavior (Sukumar, 1997) as the longitudinal bias field (Ioffe field) is increased from zero to relatively large values.

2. The Atom Guide Model

To study the dynamics of an atom in a magnetic waveguide, the Schrödinger equation describing a single neutral magnetic atom trapped in the magnetic guiding field must be solved. To minimize the initial complexities, the initial model is chosen to be a neutral spin $\frac{1}{2}$ atomic level. Two alkali atoms, ^{40}K and ^6Li , are fermions and have a spin $\frac{1}{2}$ level. The important class of bosonic alkali atoms will be treated by a similar technique in a later work.

3. Hamiltonian for a Magnetic Atom in a Magnetic Waveguide

The quantum description of an atom moving in a spatially dependent magnetic field must include both internal and external degrees of freedom. This means that the momentum, position, and spin degrees of freedom must all be treated as quantum operators. Using m for the mass of the atom and $\vec{M}$ for the magnetic moment, the Hamiltonian is written as the sum of the kinetic energy, $\frac{p^2}{2m}$ and the interaction energy of the magnetic moment and the field $\vec{B}$. The result is

$$H = \frac{p^2}{2m} - \vec{M} \cdot \vec{B}(\vec{r}) \quad (1)$$

The magnetic field $\vec{B}(\vec{r})$ is independent of the z -direction and is taken to be an ideal quadrupole field equation (equation 2) extending to infinity in the x - y plane and uniform along z . An additional uniform bias field B_0 is added in the z -direction to help control possible spin-dependent losses that may occur at the zero field point at the center of the guide. The spatial dependence of the ideal quadrupole field is given by

$$\vec{B}(\vec{r}) = B_1(-x\hat{x} + y\hat{y}) + B_0\hat{z} \quad (2)$$

In the simplified model of the atom described by equation 1, the magnetic moment of the atom is just the magnetic moment of a single outer electron. The atomic model used here can be thought of as an alkali atom with a spin zero nucleus and a total mass m . The magnetic moment is $\vec{M} = \gamma\vec{S}$, where γ is the gyromagnetic ratio of the level considered and $\vec{S}$ is the spin angular momentum of the atom. Since a spin $\frac{1}{2}$ system is being considered, the spin angular momentum is proportional to the Pauli matrices, $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$.

The Schrödinger equation for the guided atom eigenstate $\bar{\Psi}_E$ is

$$-\frac{\hbar^2}{2m}\nabla^2\bar{\Psi}_E(\vec{r})-\gamma\vec{S}\cdot\vec{B}(\vec{r})\bar{\Psi}_E(\vec{r})=E\bar{\Psi}_E(\vec{r}) \quad (3)$$

Equation 3 is made dimensionless by choosing a length scale such that $x \rightarrow \tilde{\lambda}x$, where the new x is dimensionless. Then $\frac{\hbar^2}{2m}\nabla^2\bar{\Psi}_E(\vec{r}) \rightarrow \frac{\hbar^2k^2}{2m}\nabla^2\bar{\Psi}_E(\vec{r})$ and the recoil energy is defined as $E_R = \frac{\hbar^2k^2}{2m}$, where $k = \frac{1}{\tilde{\lambda}}$ is the wavenumber of the optical field used to cool the atom. This is a rather arbitrary choice at this stage, but the recoil energy is a convenient scale for atoms that have been laser cooled. This is done after dividing through by the recoil energy, pulling out the relevant factors, and defining the dimensionless transverse field parameter $b_1 = \gamma \frac{\hbar B_1 \tilde{\lambda}}{2E_R}$, the longitudinal field parameter $b_0 = \gamma \frac{\hbar B_0}{2E_R}$, and the scaled energy $\mathcal{E} = \frac{E}{E_R}$.

4. Time Reversal Symmetry of the Hamiltonian

The Hamiltonian above (equation 1) is invariant to the operation of time reversal if the external field $\vec{B}$ is reversed as well. This is simply because when the spin, $\vec{S}$, reverses sign under time reversal, $\vec{B}$ must reverse sign to leave the Hamiltonian unchanged. The usual time reversal techniques do not act on an external magnetic field. An operator M is defined to explicitly reverse the external magnetic fields in the calculations, thus $M\vec{B}M^{-1} = -\vec{B}$. When the dimensionless field parameters are present in an expression, the field reversal operator simply changes the signs of both b_0 and b_1 . This operator is then combined with the standard time reversal operator, $T \equiv e^{-iS_y\pi/\hbar}K$, where K is the conjugate operator used in scalar time reversal problems, to form a symmetry operation of the system (equation 1). The complete time reversal symmetry of the Hamiltonian is then expressed as

$$(MT)H(MT)^{-1} = H. \quad (4)$$

Using this operator and any given initial state $|\psi\rangle$ an additional state $|\psi'\rangle$ called the time reversed state can be formed as $|\psi'\rangle = MT|\psi\rangle$.

5. Eigenstates Common to H and Λ_z

As described in Golding (2010a), the equations for the radial wave functions of the quadrupole guide are derived by making use of the angular symmetry of the quadrupole magnetic field. This symmetry is expressed as the conservation of the angular momentum, $\Lambda_z \equiv L_z - S_z$ (Hinds, 2000 and 2001; Lesanovsky, 2004; Bergeman, 1989; Golding, 2009). Our approach is to find eigenfunctions that are common to both the Hamiltonian, H and the angular momentum, Λ_z . This approach effectively separates the angular and radial dependence of the problem, leaving only a coupled system of radial equations (equation 6) to solve. These equations are solved exactly using both series techniques and the time reversal symmetry of the Hamiltonian (equation 1) to develop the general solution of the Schrödinger equation. The general solution must then be made to satisfy appropriate boundary conditions so that eigenvalues and eigenfunctions can be calculated.

The component form defining the radial spinor components for a state with angular momentum μ is

$$\bar{\Psi}_\mu(\vec{r}) \equiv e^{i\mu\phi} \begin{pmatrix} R_+(\rho) e^{i\phi/2} \\ R_-(\rho) e^{-i\phi/2} \end{pmatrix}. \quad (5)$$

When the assumed form (equation 5) is used in the Schrödinger equation (equation 3) the angular dependence drops out leaving only the following radial equations to be solved:

$$\begin{aligned} \partial_\rho^2 R_+ + \frac{1}{\rho} \partial_\rho R_+ - \frac{(\mu+1/2)^2}{\rho^2} R_+ + (\varepsilon + b_0) R_+ &= b_1 \rho R_-, \\ \partial_\rho^2 R_- + \frac{1}{\rho} \partial_\rho R_- - \frac{(\mu-1/2)^2}{\rho^2} R_- + (\varepsilon - b_0) R_- &= b_1 \rho R_+. \end{aligned} \quad (6)$$

In the case of a spin half particle with integral orbital angular momentum, the pair of equations must be solved for the allowed half-integral values of the angular momentum $\mu = \pm\frac{1}{2}, \pm\frac{3}{2}, \pm\frac{5}{2}, \dots$.

6. Frobenius Series Approach

When the system of radial equations (equation 6) is uncoupled, a fourth order differential equation results that has a regular singularity at the origin. This equations can be solved using the Frobenius power series technique (Ince, 1956; Bender, 1978). The equation for R_+ is

$$\begin{aligned}
& \rho^4 \frac{d^4}{d\rho^4} R_+ + \\
& \left[2\rho^4 \varepsilon - \left(\frac{5}{2} + 2\mu^2 \right) \rho^2 \right] \frac{d^2}{d\rho^2} R_+ + \\
& \left[-2\rho^3 b_0 + (5 + 4\mu^2 + 6\mu) \rho \right] \frac{d}{d\rho} R_+ + \\
& \left[-b_1^2 \rho^6 + (\varepsilon^2 - b_0^2) \rho^4 + \left(b_0 - 2\mu^2 \varepsilon + 2\mu b_0 + \frac{1}{2} \varepsilon \right) \rho^2 - \frac{19}{2} \mu^2 - 9\mu - \frac{35}{16} + \mu^4 \right] R_+ = 0
\end{aligned} \quad (7)$$

A similar equation for R_- can be found simply by replacing R_+ with R_- and changing the signs of both μ and b_0 . This is readily understood by inspecting the behavior of the coupled radial equations (equation 6) under this transformation and is due to the time reversal symmetry discussed previously.

The Frobenius series technique is applied to equation 7 by assuming a modified power series solution for R_+ of the form

$$R_+ = \sum_{n=0}^{\infty} c_n \rho^{n+\sigma}, \quad (8)$$

where the coefficients c_n and the index σ are unknown except that $c_0 = 1$. This is substituted into equation 7 and the resulting system is solved resulting in the following recurrence relations for c_n ,

$$c_n = \frac{c_{n-6} b_1^2 + c_{n-4} (b_0^2 - \varepsilon^2) - c_{n-2} (\mu + 5/2 - n - \sigma) (2\varepsilon\mu - 2b_0 - 5\varepsilon + 2\varepsilon n + 2\varepsilon\sigma)}{(2\mu + 1 + 2n + 2\sigma)(2\mu - 7 + 2n + 2\sigma)(2\mu + 5 - 2n - 2\sigma)(2\mu + 1 - 2n - 2\sigma)}. \quad (9)$$

For $n = 0$, the denominator of equation 9 is the indicial equation that is used to determine the allowed values of σ in equation 8. The necessary conditions are just that $c_0 = 1$ and $c_n = 0$ for $n < 0$. The corresponding component R_- is found by substituting equation 8 into the first line of equation 6 and solving for R_- producing

$$R_- = \sum_{n=0}^{\infty} c_n \left\{ (n + \sigma)^2 - (\mu + 1/2)^2 \right\} \rho^n + \frac{\varepsilon + b_0}{b_1 \rho} R_+. \quad (10)$$

Since the allowed values of σ differ by integers, the maximal index is the only index that is guaranteed to produce a solution that is finite at the origin (Ince, 1956). This solution is called a type one solution and the solution obtained from this by time reversal is called a type two solution. Type one and type two functions are denoted with a leading superscript such as $^1\psi$ or 2R in the following.

In order to use equation 9 over the full range of angular momenta, μ , the fact that the maximal index σ is a function of μ must be considered. The maximal index σ is defined as a function of μ by

$$\sigma(\mu) = \begin{cases} \mu + 5/2 & \mu > 0 \\ -\mu + 7/2 & \mu < 0 \end{cases}. \quad (11)$$

7. Time Reversal and the Two Solutions

Equations 8 through 11 define a single solution to equation 6 for the specific angular momentum μ that is called the type 1 solution, $^1\psi^\mu$. The type 2 solution, $^2\psi^\mu$, is derived directly from the type 1 solution using the time reversal symmetry of the system. In terms of the radial wavefunctions, the two solutions are defined as

$$\begin{aligned} ^1\psi^\mu &= e^{i\mu\phi} \begin{pmatrix} ^1R_+^\mu(b_0, b_1) e^{i\phi/2} \\ ^1R_-^\mu(b_0, b_1) e^{-i\phi/2} \end{pmatrix} \quad \text{and} \\ ^2\psi^\mu &= e^{i\mu\phi} \begin{pmatrix} ^2R_+^\mu(b_0, b_1) e^{i\phi/2} \\ ^2R_-^\mu(b_0, b_1) e^{-i\phi/2} \end{pmatrix} \end{aligned} \quad (12)$$

The full time reversal symmetry MT acts on $^1\psi^\mu$ to give $^2\psi^{-\mu}$, but the fields and angular momenta have to be properly reversed as in

$$MT ^1\psi^\mu = e^{-i\mu\phi} \begin{pmatrix} -^1R_-^\mu(-b_0, -b_1) e^{i\phi/2} \\ ^1R_+^\mu(-b_0, -b_1) e^{-i\phi/2} \end{pmatrix} = e^{-i\mu\phi} \begin{pmatrix} ^2R_+^{-\mu}(b_0, b_1) e^{i\phi/2} \\ ^2R_-^{-\mu}(b_0, b_1) e^{-i\phi/2} \end{pmatrix} = ^2\psi^{-\mu} \quad (13)$$

where

$$MT = -i\sigma_y MK = M \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} K.$$

Thus, the time reversal operator creates a second spinor solution independent of the first as can be demonstrated by calculating the Wronskian of the solution pair in equation 13. The action of the time reversal operator on the spinors of different type is summarized as

$$\begin{aligned} MT ^1\psi^\mu(b_0, b_1) &= T ^1\psi^\mu(-b_0, -b_1) = ^2\psi^{-\mu}(b_0, b_1) \quad \text{and} \\ MT ^2\psi^\mu(b_0, b_1) &= T ^2\psi^\mu(-b_0, -b_1) = -^1\psi^{-\mu}(b_0, b_1). \end{aligned} \quad (14)$$

By inspection of equation 13 the component radial functions of the two solution types are related by

$$\begin{aligned} ^1R_+^\mu(b_0, b_1) &= ^2R_-^{-\mu}(-b_0, -b_1) \\ ^1R_-^\mu(b_0, b_1) &= -^2R_+^{-\mu}(-b_0, -b_1) \end{aligned} \quad (15)$$

Application of equation 15 to the type one series solutions gives the series solution for the other radial components in terms of the single set of coefficients c_n of equation 9. These series are displayed in equation 16:

$$\begin{aligned}
{}^1R_+^\mu(b_0, b_1) &= \rho^{\sigma(\mu)} \sum_{n=0}^{\infty} c_n(\sigma(\mu), \mu, b_0, b_1) \rho^n \\
{}^1R_-^\mu(b_0, b_1) &= \frac{\rho^{\sigma(\mu)-3}}{b_1} \sum_{n=0}^{\infty} c_n(\sigma(\mu), \mu, b_0, b_1) \left\{ (n + \sigma(\mu))^2 - (\mu + 1/2)^2 \right\} \rho^n + \frac{\varepsilon + b_0}{b_1 \rho} {}^1R_+^\mu(b_0, b_1) \\
{}^2R_-^\mu(b_0, b_1) &= \rho^{\sigma(-\mu)} \sum_{n=0}^{\infty} c_n(\sigma(-\mu), -\mu, -b_0, -b_1) \rho^n \\
{}^2R_+^\mu(b_0, b_1) &= \frac{\rho^{\sigma(-\mu)-3}}{b_1} \sum_{n=0}^{\infty} c_n(\sigma(-\mu), -\mu, -b_0, -b_1) \left\{ (n + \sigma(-\mu))^2 - (\mu - 1/2)^2 \right\} \rho^n + \frac{\varepsilon - b_0}{b_1 \rho} {}^2R_-^\mu(b_0, b_1).
\end{aligned} \tag{16}$$

The series expansions are used in the general form for the spinors (equation 12) to produce a pair of basic solutions to the Schrödinger equation (equation 3).

8. Eigenfunctions and Energies

The coefficients c_n (equation 9) are functions of the energy ε . Some type of boundary condition must be used with the radial functions (equation 16) to determine allowed values of the energy. One possibility is to use a hard-wall boundary condition and force the general spinor to be equal to zero at some radius. Another possibility is to assume there is no hard boundary and to set the general solution equal to the asymptotic solution at some convenient distance from the guide center. Experimental implementations of a quadrupole guide will not extend to infinity and some understanding or model of the physical boundary condition will be needed in order to adequately model the actual guide behavior.

The simplest type of boundary condition is the hard-wall condition. This condition requires setting the general solution equal to zero at the wall. To satisfy this boundary condition, a linear combination of type one and type two solutions is formed and eigenenergies are found such that both the general form for both the plus and minus components of the spinor are simultaneously zero.

The general linear combination of the two types of solution can be formed using a single parameter θ since there will eventually be a normalization requirement on the states. Using this parameter, the general solution is

$$\begin{aligned}
\psi^\mu(\theta) &= \cos(\theta/2)^1 \psi^\mu + \sin(\theta/2)^2 \psi^\mu \\
&= e^{i\mu\varphi} \begin{pmatrix} (\cos(\theta/2)^1 R_+^\mu + \sin(\theta/2)^2 R_+^\mu) e^{i\varphi/2} \\ (\cos(\theta/2)^1 R_-^\mu + \sin(\theta/2)^2 R_-^\mu) e^{-i\varphi/2} \end{pmatrix}.
\end{aligned} \tag{17}$$

Assuming the boundary condition is independent of φ , there are two equations that must be solved simultaneously for a common value of θ and ε . Using ρ_0 as the radius of the hard wall, the equations determining the eigenvalues are

$$\begin{aligned}
\cos(\theta/2)^1 R_+^\mu(\varepsilon, \rho_0) + \sin(\theta/2)^2 R_+^\mu(\varepsilon, \rho_0) &= 0 \\
\cos(\theta/2)^1 R_-^\mu(\varepsilon, \rho_0) + \sin(\theta/2)^2 R_-^\mu(\varepsilon, \rho_0) &= 0
\end{aligned} \tag{18}$$

When these equations (equation 18) are solved a set of orthogonal spinor radial wavefunctions are found that may be used for modeling the behavior of atom guides under hard-wall boundary conditions. To model open boundary conditions of infinite extent, a similar procedure must be performed using the asymptotic solutions of the system (Golding, 2010b).

When the Ioffe field is large and the boundary conditions are open, discrete energy levels may exist but the transverse modes are not well defined. The lack of control or consistency of the transverse mode may lead to difficulties in the construction and operation of beam splitters and other matter wave components needed for guided matter wave interferometry and may be one reason that single mode operation in these guides has not yet been convincingly demonstrated. One solution to this problem would be to develop a new waveguide design that includes both a magnetic quadrupole field and some type of conservative hard-wall boundary defined at fixed distance from the guide center. This may be possible using a combination of optical fields and miniature magnetic quadrupole fields, for example.

9. Conclusions

The multiple solutions found in other atom waveguide work can be easily derived using the time reversal symmetry of a waveguide system. By organizing the series solutions using time reversal, a more complete understanding of guide behavior can be obtained. For example, at large Ioffe fields, the two solutions correspond physically to a bound mode and an unbound mode. The bound mode is a quantum state that is essentially attracted to the center and its time reversed partner is an unbound mode that is repelled from the center. These two modes must be combined to meet prescribed boundary conditions resulting in a specific mixture of bound and unbound modes that can be directly related to the lifetime of waveguide states.

This symmetry will be useful in more complicated devices currently being developed, such as magnetic beam splitters. For example, if one leg of a beam splitter favors the propagation of a

bound state and the other leg favors an unbound state, the splitter will not work as desired. It is also hoped that the time reversal technique presented here will be useful in the analysis of atom guides employing higher spin systems. In such systems, there will be many possible modes involving different spin states. Each state will have a time reversed partner that can easily be obtained, reducing the need to develop many different independent series solutions. Time reversal techniques reduce the analytic and numeric work needed to obtain a general solution as well as enhances the conceptual understanding of atom guide systems.

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