INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS B: ATOMIC, MOLECULAR AND OPTICAL PHYSICS

J. Phys. B: At. Mol. Opt. Phys. **37** (2004) 1725–1736 PII: S0953-4075(04)73683-4

Invariants of atom beams

John Lekner

School of Chemical and Physical Sciences, Victoria University of Wellington, PO Box 600, Wellington, New Zealand

Received 17 December 2003
Published 7 April 2004
Online at stacks.iop.org/JPhysB/37/1725 (DOI: 10.1088/0953-4075/37/8/013)

Abstract

Seven invariants are derived for a coherent beam of spinless atoms. The simplest of these arises from the continuity equation and can be interpreted as the momentum content per unit length in the beam. It is an invariant in the sense that it does not change along the length of the beam. Six further invariants arise out of the conservation of momentum and of angular momentum. These are expressed as integrals over planes normal to the beam propagation direction; the integrands are composed of elements of a momentum flux density tensor, analogous to the Maxwell stress tensor in the electrodynamic case.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Seven invariants of electromagnetic beams have recently been derived [1]. Their existence follows from the conservation of energy, momentum and angular momentum. The simplest of them can be interpreted as the momentum content per unit length of the beam, but originates in *energy* conservation. It turns out that the energy content per unit length of the beam is not, in general, an invariant (i.e. constant along the length of the beam): energy conservation is expressed in terms of an energy *flux* density, and this is c^2 times the momentum density.

In this paper we shall derive analogous results for coherent beams of spinless particles, on the assumption that there exists a probability amplitude $\Psi(\mathbf{r}, t)$ for the beam. For such beams we shall write down conservation laws in terms of a momentum density and a momentum flux density, and then deduce the existence of seven beam invariants. The properties of these invariants (and also of non-invariants such as the probability content and angular momentum content per unit length of the beam) will be illustrated with the help of exact beam wavefunctions [2–4].

There are some remarkable recent atom beam experiments. Toennies and collaborators have focused on a ^{4}He atom beam using Fresnel zone plates [5], and diffracted a ^{4}He beam by nanostructure transmission gratings [6]. Atom laser beams based on Bose–Einstein condensates have been optically manipulated [7], their temporal coherence has been measured [8] and a method of continuous detection has been demonstrated [9].

We shall assume in this paper that a probability amplitude $\Psi(\mathbf{r}, t)$ can represent a beam of atoms of mass M, and further that it evolves in time according to $H\Psi = \mathrm{i}\hbar\partial\Psi/\partial t$, where H is an effective Hamiltonian, the same as for an atom of mass M in external potential $V(\mathbf{r})$:

$$H = \frac{-\hbar^2}{2M}\nabla^2 + V(\mathbf{r}). \tag{1}$$

For example, for a stable steady-state Bose–Einstein condensate output, the mean field of the condensate generates an effective potential, so that even if the condensate is in a highly nonlinear regime, the linear description of beam properties is valid [10].

From the time-evolution (Schrödinger) equation, the well-known equation of continuity follows

$$\frac{\partial|\Psi|^2}{\partial t} + \nabla\cdot\left\{\frac{\hbar}{M}\,\mathrm{Im}(\Psi^*\nabla\Psi)\right\} = 0. \tag{2}$$

It may reassure the reader somewhat that the same form of continuity equation holds for the (completely symmetrical) many-body wavefunction and Hamiltonian for N identical bosons:

$$\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N,t), \qquad \frac{-\hbar^2}{2M}\sum_{a=1}^{N}\nabla_a^2 + V(\mathbf{r}_1,\ldots,\mathbf{r}_N). \tag{3}$$

In this case we find

$$\frac{\partial|\Psi|^2}{\partial t} + \sum_{a=1}^{N}\nabla_a\cdot\left\{\frac{\hbar}{M}\,\mathrm{Im}(\Psi^*\nabla_a\Psi)\right\} = 0. \tag{4}$$

If we now define a number density $n(\mathbf{r}, t)$ and a many-body probability flux density $\mathbf{S}(\mathbf{r}, t)$ by

$$n(\mathbf{r}_1,t) = \frac{N\int \mathrm{d}^3r_2\cdots\int \mathrm{d}^3r_N|\Psi|^2}{\int \mathrm{d}^3r_1\cdots\int \mathrm{d}^3r_N|\Psi|^2}, \qquad \mathbf{S}(\mathbf{r}_1,t) = \frac{N\hbar\int \mathrm{d}^3r_2\cdots\int \mathrm{d}^3r_N\,\mathrm{Im}(\Psi^*\nabla_1\Psi)}{M\int \mathrm{d}^3r_1\cdots\int \mathrm{d}^3r_N|\Psi|^2}, \tag{5}$$

we again have a continuity equation, namely

$$\frac{\partial n(\mathbf{r}_1,t)}{\partial t} + \nabla_1\cdot\mathbf{S}(\mathbf{r}_1,t) = 0. \tag{6}$$

Proof. We first note that $\frac{\partial}{\partial t}\int \mathrm{d}^3r_1\cdots\int \mathrm{d}^3r_N|\Psi|^2$ is zero, because from (4) it is equal to a sum of terms each containing an integral of the form $\int \mathrm{d}^3r_a\nabla_a\cdot\mathrm{Im}(\Psi^*\nabla_a\Psi)$, which is zero provided $\mathrm{Im}(\Psi^*\nabla_a\Psi)$ goes to zero suitably fast as r_a tends to infinity. Thus

$$\frac{\partial n(\mathbf{r}_1,t)}{\partial t} = -\nabla_1\cdot\mathbf{S}(\mathbf{r}_1,t) - \frac{\hbar}{M}\frac{\sum_{a=2}^{N}\int \mathrm{d}^3r_2\cdots\int \mathrm{d}^3r_N\nabla_a\cdot\mathrm{Im}(\Psi^*\nabla_a\Psi)}{\int \mathrm{d}^3r_1\cdots\int \mathrm{d}^3r_N|\Psi|^2} \tag{7}$$

and the last term is zero as before. □

We shall henceforth assume that an atom beam can be represented by a probability amplitude $\Psi(\mathbf{r}, t)$ which satisfies the continuity equation (2). In the next section we shall derive a beam invariant from (2), and relate it to the momentum content per unit length of the beam. In sections 3 and 4 we shall deduce the existence of six more beam invariants, three arising from the conservation of momentum, and three from the conservation of angular momentum. Sections 5 and 6 explore these invariants for two members of the set $\psi_{\ell m}$ of exact beam wavefunctions (defined in section 5), and section 7 gives the angular momentum properties of this set.

2. Conservation of probability

Let us define a real momentum density $\mathbf{p}(\mathbf{r}, t)$ for the state $\Psi(\mathbf{r}, t)$ by

$$\mathbf{p}(\mathbf{r}, t) = \tfrac{1}{2}\{\Psi^*\hat{\mathbf{p}}\Psi + \Psi(\hat{\mathbf{p}}\Psi)^*\}, \tag{8}$$

where $\hat{\mathbf{p}}$ is the momentum operator $-\mathrm{i}\hbar\nabla$. We see that

$$\mathbf{p}(\mathbf{r}, t) = \frac{\mathrm{i}\hbar}{2}\{\Psi\nabla\Psi^* - \Psi^*\nabla\Psi\} = \hbar\,\mathrm{Im}(\Psi^*\nabla\Psi) = M\,\mathbf{S}(\mathbf{r}, t), \tag{9}$$

i.e. the momentum density divided by the atomic mass is equal to the probability flux density $\mathbf{S} = \frac{\hbar}{M}\,\mathrm{Im}(\Psi^*\nabla\Psi)$. The continuity equation (2) thus reads

$$\frac{\partial|\Psi|^2}{\partial t} + \frac{1}{M}\nabla\cdot\mathbf{p} = 0. \tag{10}$$

In the case of 'steady' beams, where Ψ is an energy eigenstate and evolves in time according to $\Psi(\mathbf{r}, t) = \mathrm{e}^{-\mathrm{i}Et/\hbar}\psi(\mathbf{r})$, the probability density $|\Psi|^2 = |\psi|^2$ is independent of time, and $\nabla\cdot\mathbf{p} = 0$. (For beams which oscillate in time we can average over an integral number of oscillations, denote such averages by a bar and obtain $\nabla\cdot\bar{\mathbf{p}} = 0$; such extensions will be understood throughout this paper.) The analogous 'steady' electromagnetic beams have energy and momentum densities, and also the elements of the Maxwell stress tensor, all independent of time [4, 11].

The first beam invariant follows from $\nabla\cdot\mathbf{p} = 0$ (or $\nabla\cdot\bar{\mathbf{p}} = 0$): applying $\int \mathrm{d}^2r = \int_{-\infty}^{\infty}\mathrm{d}x\int_{-\infty}^{\infty}\mathrm{d}y = \int_0^{\infty}\mathrm{d}\rho\,\rho\int_0^{2\pi}\mathrm{d}\phi$ to $\partial_x p_x + \partial_y p_y + \partial_z p_z = 0$, we see that the $\partial_x p_x$ and $\partial_y p_y$ terms integrate to zero (we assume throughout this paper that the beam is propagating in the z direction, although of course there has to be convergence or spreading in the lateral directions). For example, $\int \mathrm{d}^2r\,\partial_x p_x = \int_{-\infty}^{\infty}\mathrm{d}y\int_{-\infty}^{\infty}\mathrm{d}x\,\partial_x p_x = 0$, since p_x goes to zero at $x = \pm\infty$. What remains is

$$\partial_z\int \mathrm{d}^2r\,p_z = 0, \quad \text{i.e.} \quad P_z' = \int \mathrm{d}^2r\,p_z = \text{constant}. \tag{11}$$

We use the notation P_z', since $\mathrm{d}P_z = P_z'\,\mathrm{d}z$ is the momentum content in a slice of thickness $\mathrm{d}z$ of the beam, so P_z' may be viewed as $\mathrm{d}P_z/\mathrm{d}z$. Thus the momentum content per unit length of the beam is the same everywhere along the length of the beam, i.e. P_z' is an invariant of the beam. But note that this invariance follows not from momentum conservation but from the continuity equation, and arises because of the proportionality of the probability density flux to the momentum density, equation (9).

One might think that the probability content per unit length,

$$N' = \int \mathrm{d}^2r|\psi(\mathbf{r})|^2, \tag{12}$$

would also be an invariant (independent of z), but it is not. For wide beams of wavenumber k, we do, however, have the approximate equality

$$P_z' \approx \hbar k N' \tag{13}$$

which arises because in a wide beam each atom carries approximately $\hbar k$ of momentum in the beam propagation direction, so $p_z(\mathbf{r}) \approx \hbar k|\psi(\mathbf{r})|^2$. An example of this approximate equality has been given in [4], where the wavefunction (i.e. solution of $(\nabla^2 + k^2)\psi = 0$, which is Schrödinger's equation in free space with energy $\hbar^2k^2/2M$)

$$\psi_{10}(\mathbf{r}) = j_1(kR)P_{10}\left(\frac{z - \mathrm{i}b}{R}\right), \qquad R^2 = \rho^2 + (z - \mathrm{i}b)^2 \tag{14}$$

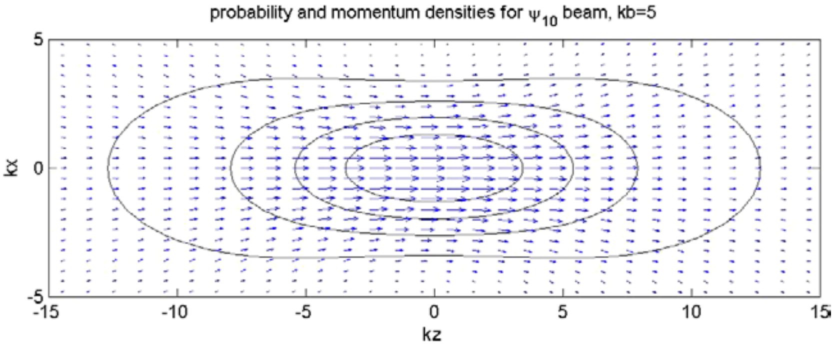

Figure 1. Probability density $|\psi|^2$ and momentum density field-plot for the ψ_{10} beam, plotted for $kb = 5$. The contours are at 0.8, 0.6, 0.4 and 0.2 of the maximum $|\psi|^2$, which occurs at the centre of the focal plane, i.e. at $\rho = 0$, $z = 0$. The arrows show $[p_z, p_x]$. The three-dimensional picture would be obtained by rotating the figure about the z-axis.

was used to evaluate P'_z and N'. Writing β for kb, these are, from equations (51) and (50) of [4],

$$P'_z = \hbar(2\pi b)(8\beta^4)^{-1}\{2\beta^2 \cosh 2\beta - 2\beta \sinh 2\beta + \cosh 2\beta - 1\} \tag{15}$$

$$N' = (2\pi b^2)(8\beta^4)^{-1}\left\{2\beta \sinh 2\beta - \cosh 2\beta + 1 - 2\beta\left(\frac{b}{z}\right)\sin 2kz + \left(\frac{b}{z}\right)^2[1 - \cos 2kz]\right\}. \tag{16}$$

For $\beta = kb \gg 1$, we have, in accord with (13),

$$P'_z/N' = \hbar k\left\{1 - \frac{\beta - 1}{\beta(2\beta - 1)} + O(\mathrm{e}^{-2\beta})\right\}. \tag{17}$$

Figure 1 shows the probability density and momentum density associated with the beam wavefunction given in (14); written out more explicitly, this is

$$\psi_{10}(\mathbf{r}) = \left[\frac{\sin kR}{(kR)^2} - \frac{\cos kR}{kR}\right]\frac{z - \mathrm{i}b}{R}, \qquad R^2 = \rho^2 + (z - \mathrm{i}b)^2. \tag{18}$$

Figure 2 shows $\hbar k N'/P'_z$ for this wavefunction. Note that the deviation of this ratio from unity is greatest for tightly focused beams (small $\beta = kb$), and within the focal region ($|z| < b$).

The energy density $\Psi^* H \Psi$ becomes E times the probability density $|\psi|^2$ for 'steady' beams (for which $\Psi(\mathbf{r}, t) = \mathrm{e}^{-\mathrm{i}Et/\hbar}\psi(\mathbf{r})$ and $H\psi = E\psi$), so the energy content per unit length becomes $E' = EN' = (\hbar^2 k^2/2M)N'$. This is not an invariant: energy conservation for steady beams is expressed in the continuity equation, and thus in the invariance of P'_z.

3. Conservation of momentum

Momentum conservation for the electromagnetic field is written in terms of the Maxwell stress tensor. We wish to write an analogous momentum conservation law for a particle field described by $\Psi(\mathbf{r}, t)$, in the form

$$\frac{\partial p_i}{\partial t} + \sum_j \partial_j \tau_{ij} = f_i, \qquad i = x, y, z, \tag{19}$$

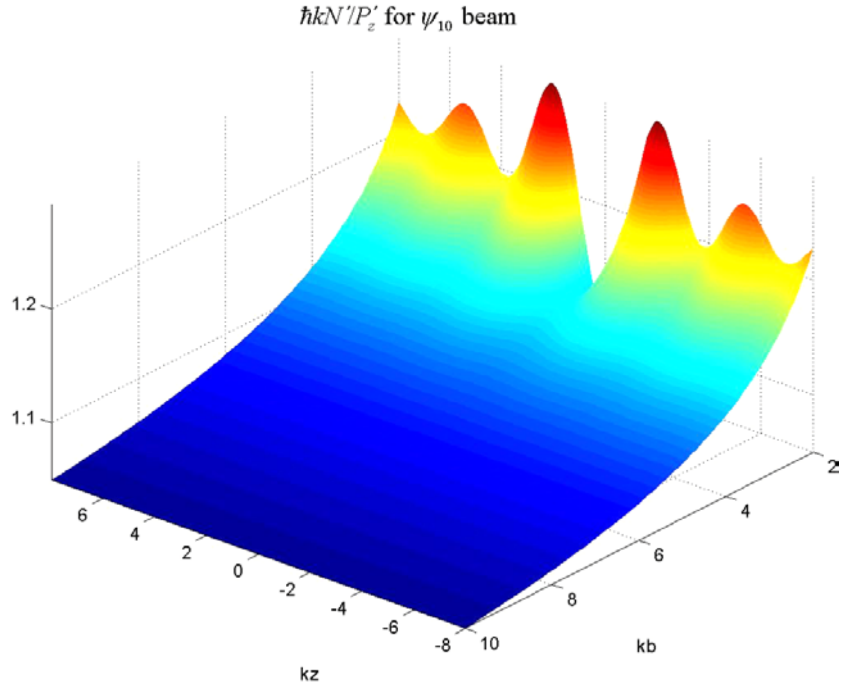

Figure 2. The ratio of the non-invariant $\hbar kN'$ to the invariant P_z' for the ψ_{10} beam, plotted as a function of z and of the parameter $\beta = kb$. The smallest value shown is $\beta = 2$, corresponding to a very tightly focused beam. As β increases (and the beam widens) the ratio $\hbar kN'/P_z'$ tends to unity as $1 + (2\beta)^{-1} + O(\beta^{-2})$, for all z.

where p_i is a component of the momentum density, defined in (8) or (9), τ_{ij} are elements of a momentum flux density tensor, to be derived below, and f_i is a component of force density. From the definition of $\mathbf{p}(\mathbf{r}, t)$ and Schrödinger's time evolution equation $H\Psi = i\hbar\partial\Psi/\partial t$, we find

$$\frac{\partial \mathbf{p}}{\partial t} = \frac{1}{2}\{(H\Psi)\nabla\Psi^* - \Psi\nabla(H\Psi^*) + (H\Psi^*)\nabla\Psi - \Psi^*\nabla(H\Psi)\}. \tag{20}$$

We take H to be given by (1); the right-hand side of (20) splits into potential and kinetic parts. The potential part simplifies to $-\Psi^*\Psi\nabla V$, i.e. a force density $\mathbf{f}(\mathbf{r}, t)$, as expected. The kinetic part is

$$\frac{-\hbar^2}{4M}\{(\nabla^2\Psi)\nabla\Psi^* - \Psi\nabla(\nabla^2\Psi^*) + (\nabla^2\Psi^*)\nabla\Psi - \Psi^*\nabla(\nabla^2\Psi)\}. \tag{21}$$

The ith component of this expression is

$$\frac{-\hbar^2}{4M}\sum_{j=1}^{3}\left\{\left(\partial_j^2\Psi\right)\partial_i\Psi^* - \Psi\partial_i\partial_j^2\Psi^* + \left(\partial_j^2\Psi^*\right)\partial_i\Psi - \Psi^*\partial_i\partial_j^2\Psi\right\}$$

$$= \frac{-\hbar^2}{4M}\sum_{j=1}^{3}\partial_j\{2(\partial_i\Psi^*)\partial_j\Psi + 2(\partial_i\Psi)\partial_j\Psi^* - \partial_i\partial_j(\Psi^*\Psi)\}. \tag{22}$$

Thus a conservation law of the form (19) does indeed hold, with

$$\tau_{ij} = \frac{\hbar^2}{2M}\left\{(\partial_i\Psi^*)\partial_j\Psi + (\partial_i\Psi)\partial_j\Psi^* - \frac{1}{2}\partial_i\partial_j(\Psi^*\Psi)\right\}. \tag{23}$$

This momentum flux density tensor is real and symmetric. Note that it is not the same as the 'stress tensor for the probability fluid' [12, 13], namely

$$T_{ij} = \frac{\hbar^2}{4M}[\partial_i\partial_j(\Psi^*\Psi) - (\Psi^*\Psi)^{-1}\partial_i(\Psi^*\Psi)\partial_j(\Psi^*\Psi)]. \tag{24}$$

We shall now derive three beam invariants associated with momentum conservation by operating with $\int d^2r$ on the steady beam form of (19) (or on the time-averaged (19) in the case of beams which oscillate). In the absence of external forces, equations (19) then become $\sum_j \partial_j\tau_{ij} = 0$, i.e. three equations of the form $\partial_x\tau_{xx} + \partial_y\tau_{xy} + \partial_z\tau_{xz} = 0$. Applying $\int d^2r$ gives zero for the ∂_x and ∂_y terms, e.g. $\int d^2r\, \partial_y\tau_{xy} = \int_{-\infty}^{\infty} dx\, \tau_{xy}\big]_{y=-\infty}^{y=\infty}$, which is zero because ψ is bounded in the transverse (x and y) directions, by assumption. Thus we are left with $\partial_z\int d^2r\, \tau_{xz} = 0$, i.e. the invariant

$$T'_{xz} = \int d^2r\, \tau_{xz} = \frac{\hbar^2}{2M}\int d^2r \left[(\partial_x\psi^*)\partial_z\psi + (\partial_x\psi)\partial_z\psi^* - \frac{1}{2}\partial_x\partial_z(\psi^*\psi)\right]. \tag{25}$$

(When external forces are present, the rate of change of T'_{xz} with z equals $\int d^2r\, f_x$.) The other two invariants, from the other two equations, are

$$\begin{aligned} T'_{yz} &= \int d^2r\, \tau_{yz} = \frac{\hbar^2}{2M}\int d^2r \left[(\partial_y\psi^*)\partial_z\psi + (\partial_y\psi)\partial_z\psi^* - \frac{1}{2}\partial_y\partial_z(\psi^*\psi)\right] \\ T'_{zz} &= \int d^2r\, \tau_{zz} = \frac{\hbar^2}{2M}\int d^2r \left[2(\partial_z\psi^*)\partial_z\psi - \frac{1}{2}\partial_z^2(\psi^*\psi)\right]. \end{aligned} \tag{26}$$

When $\psi(\mathbf{r}) = \psi(\rho, z)$, i.e. ψ is independent of the azimuthal angle ϕ, T'_{xz} and T'_{yz} will be zero. To show this we convert to cylindrical polars ρ, z, ϕ and note that

$$\partial_x = \cos\phi\,\partial_\rho - \rho^{-1}\sin\phi\,\partial_\phi, \qquad \partial_y = \sin\phi\,\partial_\rho + \rho^{-1}\cos\phi\,\partial_\phi. \tag{27}$$

When ψ is independent of ϕ, the integrands of T'_{xz} and T'_{yz} contain the factors $\cos\phi$ and $\sin\phi$, respectively, and thus integrate to zero over ϕ.

4. Conservation of angular momentum

We are considering beams of spinless particles, so the angular momentum density is given by

$$\mathbf{j}(\mathbf{r}, t) = \mathbf{r}\times\mathbf{p}(\mathbf{r}, t), \qquad \text{or} \qquad j_i = \sum_j\sum_k \varepsilon_{ijk} r_j p_k. \tag{28}$$

By analogy with the electromagnetic case [1, 14], we define the angular momentum flux density tensor μ in terms of the momentum flux density tensor τ:

$$\mu_{\ell i} = \sum_j\sum_k \varepsilon_{ijk} r_j \tau_{k\ell}. \tag{29}$$

Then the rate of change of angular momentum density (in the absence of external torques) is given by

$$\frac{\partial j_i}{\partial t} + \sum_\ell \partial_\ell\mu_{\ell i} = 0 \tag{30}$$

For example, $j_z = xp_y - yp_x$ and $\frac{\partial p_i}{\partial t} + \sum_j \partial_j\tau_{ij} = 0$, so

$$\begin{aligned} 0 &= \frac{\partial j_z}{\partial t} + x\sum_j \partial_j\tau_{yj} - y\sum_j \partial_j\tau_{xj} \\ &= \frac{\partial j_z}{\partial t} + \sum_j \partial_j(x\tau_{yj} - y\tau_{xj}) \end{aligned} \tag{31}$$

because $\tau_{yx} = \tau_{xy}$.

Three more beam invariants follow on the application of $\int d^2r$ to the three equations (30), by steps analogous to those used to establish the invariance of T'_{xz}, T'_{yz} and T'_{zz} in section 3. The beam invariants associated with the conservation of angular momentum are

$$\begin{aligned} M'_{zx} &= \int d^2r\, \mu_{zx} = \int d^2r[y\tau_{zz} - z\tau_{yz}] \\ M'_{zy} &= \int d^2r\, \mu_{zy} = \int d^2r[z\tau_{xz} - x\tau_{zz}] \\ M'_{zz} &= \int d^2r\, \mu_{zz} = \int d^2r[x\tau_{yz} - y\tau_{xz}]. \end{aligned} \tag{32}$$

When ψ is independent of the azimuthal angle ϕ, τ_{xz} is proportional to $\cos\phi$, τ_{yz} is proportional to $\sin\phi$ and τ_{zz} is independent of ϕ. Thus the integrands of M'_{zx} and M'_{zy} are proportional to $\sin\phi$ and $\cos\phi$, respectively, and integrate to zero over ϕ. The integrand of M'_{zz} is proportional to $\cos\phi\sin\phi$, and also integrates to zero over ϕ. Thus when the beam wavefunction is independent of the azimuthal angle, only two beam invariants are nonzero: P'_z and T'_{zz}.

The angular momentum content per unit length, $\mathbf{J}'$, has the component along the beam propagation direction $J'_z = \int d^2r\, j_z$,

$$j_z = xp_y - yp_x = \rho p_\phi \tag{33}$$

where $p_\phi = \cos\phi p_y - \sin\phi p_x$ is the azimuthal component of the momentum density. When ψ is independent of the azimuthal angle we have from $\mathbf{p} = \hbar\,\mathrm{Im}(\psi^*\nabla\psi)$ that $p_x = \hbar\cos\phi\,\mathrm{Im}(\psi^*\partial_\rho\psi)$, $p_y = \hbar\sin\phi\,\mathrm{Im}(\psi^*\partial_\rho\psi)$, and so p_ϕ is identically zero. The other two components are not identically zero, but integrate to zero over ϕ when ψ is independent of ϕ, e.g.

$$j_x = yp_z - zp_y \to \hbar\rho\sin\phi\,\mathrm{Im}(\psi^*\partial_z\psi) - \hbar z\sin\phi\,\mathrm{Im}(\psi^*\partial_\rho\psi). \tag{34}$$

We shall see later that $J'_z = \int d^2r\, j_z$ is not an invariant: the angular momentum content per unit length is in general not the same along the length of the beam.

5. Invariants of the ψ_{10} beam

The ψ_{10} beam wavefunction, given in (14) and more explicitly in (18), is the lowest of the set [2–4]

$$\psi_{\ell m} = j_\ell(kR)P_{\ell m}\left(\frac{z - \mathrm{i}b}{R}\right)\mathrm{e}^{\mathrm{i}m\phi} \tag{35}$$

which has a convergent normalization in any slice of the beam, i.e. for which $N' = \int d^2r\,|\psi|^2$ exists. ($\psi_{00} = \sin kR/kR$ has a logarithmically divergent N': see section 2 of [4].) The invariant P'_z and the non-invariant N' were evaluated in [4], and are given above in equations (15) and (16). As we saw in the last section, only two beam invariants are nonzero when the beam wavefunction is independent of the azimuthal angle: P'_z and T'_{zz}. Thus only T'_{zz} (given in (26)) remains to be evaluated.

In performing the differentiations and integrations it is convenient to transform to oblate spheroidal coordinates ξ and η, in which

$$\rho = b\sqrt{(1+\xi^2)(1-\eta^2)}, \qquad z = b\xi\eta, \qquad R = b(\xi - \mathrm{i}\eta). \tag{36}$$

In oblate spheroidal coordinates we have

$$\psi_{10} = j_1[\beta(\xi - \mathrm{i}\eta)]\frac{\xi\eta - \mathrm{i}}{\xi - \mathrm{i}\eta}, \qquad \beta = kb. \tag{37}$$

We shall also make use of (A.7) of [4] to evaluate integrals over a plane of fixed z:

$$\int_0^\infty \mathrm{d}\rho\, \rho p_z = b^2 \int_0^1 \mathrm{d}\eta\, \eta^{-1}\left[\eta^2 + \left(\frac{z}{b\eta}\right)^2\right] p_z. \tag{38}$$

Differentiations with respect to ρ and z are readily transformed to differentiations with respect to ξ and η by means of formulae given in the appendix of [4]. We find, with $\beta = kb$ as before,

$$T'_{zz} = \frac{\hbar^2}{2M}(2\pi)(8\beta^4)^{-1}[(4\beta^3 + 6\beta)\sinh 2\beta - (6\beta^2 + 3)\cosh 2\beta + 3]. \tag{39}$$

Large β corresponds to broad, weakly focused beams: the diffraction length b (also known as the Rayleigh length) gives the length of focal region of the beam, and also determines the beam waist, which is $(2b/k)^{1/2}$. Thus when kb is large, the beam waist $(2\beta)^{1/2}k^{-1} = (2\beta)^{1/2}\lambda/2\pi$ is many wavelengths wide, and the focal region is many wavelengths long. At large β, the ratio of the two nonzero invariants has the limit

$$\frac{T'_{zz}}{P'_z} \to \frac{\hbar k}{M} \tag{40}$$

which is the speed of the atoms in the (wide) beam.

6. Invariants of the ψ_{21} beam

The beam wavefunction

$$\psi_{21} = j_2(kR)P_{21}\left(\frac{z - \mathrm{i}b}{R}\right)\mathrm{e}^{\mathrm{i}\phi}, \qquad R^2 = \rho^2 + (z - \mathrm{i}b)^2, \tag{41}$$

is the next one in the set (35) to have a non-divergent normalization integral $N' = \int \mathrm{d}^2r\, |\psi|^2$. (Those with ℓ–m odd have the necessary convergence [4].) It is also the simplest of the convergent subset to have ϕ-dependence. Replacing $\mathrm{e}^{\mathrm{i}\phi}$ by $\mathrm{e}^{-\mathrm{i}\phi}$ changes the sign of j_z, as expected; see (44).

We shall examine next the properties of beams with wavefunctions which have $\mathrm{e}^{\mathrm{i}m\phi}$ dependence, before evaluating the invariants of the ψ_{21} beam. From (27) we see that

$$\partial_x \to \cos\phi\,\partial_\rho - \mathrm{i}m\rho^{-1}\sin\phi, \qquad \partial_y \to \sin\phi + \mathrm{i}m\rho^{-1}\cos\phi \tag{42}$$

when operating on a wavefunction of the form $f(\rho, z)\,\mathrm{e}^{\mathrm{i}m\phi}$. Thus the x and y components of the momentum density become

$$\begin{aligned} p_x &\to \hbar\cos\phi\,\mathrm{Im}(\psi^*\partial_\rho\psi) - m\hbar\rho^{-1}\sin\phi|\psi|^2 \\ p_y &\to \hbar\sin\phi\,\mathrm{Im}(\psi^*\partial_\rho\psi) + m\hbar\rho^{-1}\cos\phi|\psi|^2. \end{aligned} \tag{43}$$

The longitudinal (z) component of the angular momentum density (33) then simplifies to

$$j_z = xp_y - yp_x = \rho p_\phi \to m\hbar|\psi|^2, \tag{44}$$

i.e. it is just $m\hbar$ times the probability density $|\psi|^2$. Hence the angular momentum component along the beam propagation direction has the content per unit length of beam given by

$$J'_z \equiv \int \mathrm{d}^2r\, j_z \to m\hbar \int \mathrm{d}^2r\, |\psi|^2 = m\hbar N'. \tag{45}$$

We have already established that N' is not an invariant (in general), so J'_z is not an invariant either.

The transverse components of angular momentum density integrate to zero over ϕ: for example,

$$j_x = yp_z - zp_y \to \hbar\rho\sin\phi\,\mathrm{Im}(\psi^*\partial_z\psi) - z\{\hbar\sin\phi\,\mathrm{Im}(\psi^*\partial_\rho\psi) + m\hbar\rho^{-1}\cos\phi|\psi|^2\}. \tag{46}$$

In the evaluation of the momentum and angular momentum invariants T'_{iz} and M'_{zi} we need the elements τ_{xz}, τ_{yz} and τ_{zz} of the momentum flux density tensor. When the beam wavefunction has the form $f(\rho, z)\,\mathrm{e}^{\mathrm{i}m\phi}$, these become

$$\begin{aligned}\frac{2M}{\hbar^2}\tau_{xz} &\to 2\cos\phi\,\mathrm{Re}\{(\partial_\rho\psi^*)(\partial_z\psi)\} - 2m\rho^{-1}\sin\phi\,\mathrm{Im}(\psi^*\partial_z\psi) - \frac{1}{2}\cos\phi\partial_\rho\partial_z|\psi|^2\\ \frac{2M}{\hbar^2}\tau_{yz} &\to 2\sin\phi\,\mathrm{Re}\{(\partial_\rho\psi^*)(\partial_z\psi)\} + 2m\rho^{-1}\cos\phi\,\mathrm{Im}(\psi^*\partial_z\psi) - \frac{1}{2}\sin\phi\partial_\rho\partial_z|\psi|^2.\end{aligned} \tag{47}$$

These integrate to zero over ϕ, so T'_{xz} and T'_{yz} are zero for $\mathrm{e}^{\mathrm{i}m\phi}$ beams. The angular momentum invariants M'_{zx} and M'_{zy} are zero for the same reason. However, M'_{zz} is the section integral of

$$x\tau_{yz} - y\tau_{xz} = \rho[\cos\phi\tau_{yz} - \sin\phi\tau_{xz}] \to 2m(\hbar^2/2M)\,\mathrm{Im}(\psi^*\partial_z\psi), \tag{48}$$

so

$$M'_{zz} \to m\left(\frac{\hbar^2}{M}\right)\int \mathrm{d}^2r\,\mathrm{Im}(\psi^*\partial_z\psi) = \frac{m\hbar P'_z}{M}. \tag{49}$$

The results (45) and (49) are consistent with the picture of each atom carrying (on average) angular momentum $m\hbar$ in orbiting the beam axis, when the wavefunction azimuthal dependence is $\mathrm{e}^{\mathrm{i}m\phi}$.

We therefore have three nonzero invariants P'_z, T'_{zz} and M'_{zz} for beams with $\mathrm{e}^{\mathrm{i}m\phi}$ dependence, of which we need evaluate only the first two, because of (49). For the ψ_{21} beam, with explicit wavefunction

$$\psi_{21} = \left\{\left[\frac{3}{(kR)^3} - \frac{1}{kR}\right]\sin kR - \frac{3}{(kR)^2}\cos kR\right\}\frac{3\rho(z - \mathrm{i}b)}{R^2}\,\mathrm{e}^{\mathrm{i}\phi}. \tag{50}$$

We again transform to oblate spheroidal coordinates to perform the differentiations and integrations. The intermediate expressions are large, but the results are simple:

$$P'_z = (2\pi)(\hbar b)(8\beta^6)^{-1}[(2\beta^3 + 6\beta)\sinh 2\beta - (5\beta^2 + 3)\cosh 2\beta - \beta^2 + 3] \tag{51}$$

$$T'_{zz} = (2\pi)\left(\frac{\hbar^2}{2M}\right)(8\beta^6)^{-1}[(4\beta^4 + 27\beta^2 + 15)\cosh 2\beta - (14\beta^3 + 30\beta)\sinh 2\beta + 3\beta^2 - 15]. \tag{52}$$

The ratio of these invariants has the same wide-beam (large β) limit as we found for the ψ_{10} beam (equation (40)).

We shall also give the two non-invariants: the probability content per unit length, and the angular momentum content per unit length. For the ψ_{21} beam these are functions of z. We use the $\zeta = kz$ in the following:

$$\begin{aligned}N'(z) = \int \mathrm{d}^2r\,|\psi|^2 = (2\pi)b^2(16\beta^6)^{-1}\Bigg\{&(4\beta^2 + 3)\cosh 2\beta - 6\beta\sinh 2\beta + 2\beta^2 - 3\\ &+ \left(\frac{b}{z}\right)^4[(4\zeta^2 - 3)\cos 2\zeta - 6\zeta\sin 2\zeta + 2\zeta^2 + 3]\Bigg\}.\end{aligned} \tag{53}$$

This function is not singular at $z = 0$, where it takes the value

$$N'(0) = 2\pi b^2(16\beta^6)^{-1}\{(4\beta^2 + 3)\cosh 2\beta - 6\beta\sinh 2\beta - 2\beta^4 + 2\beta^2 - 3\}. \tag{54}$$

The angular momentum content for $\mathrm{e}^{\mathrm{i}m\phi}$ beams is (from (45)) $m\hbar$ times the probability content, so $J'_z = \hbar N'$ for the ψ_{21} beam.

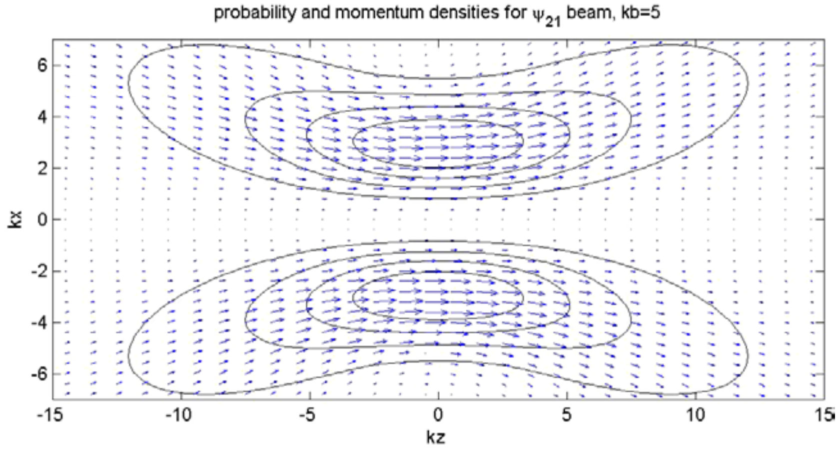

Figure 3. Probability density $|\psi|^2$ and momentum density field-plot for the ψ_{21} beam, plotted for $kb = 5$. The contours are at 80%, 60%, 40% and 20% of the maximum value of $|\psi|^2$. The arrows show $[p_z, p_x]$. Note that the beam is hollow, in probability and in momentum. Rotation about the beam (z) axis gives the three-dimensional picture.

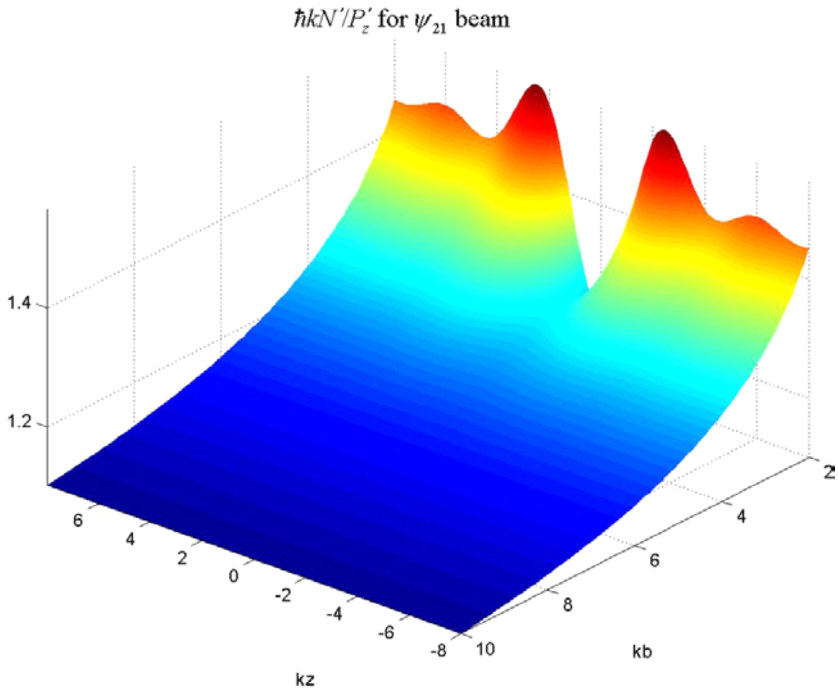

Figure 4. The ratio $\hbar kN'/P_z'$ for the ψ_{21} beam, shown for $kb = 2$ to $kb = 10$ as a function of z. The focal plane is $z = 0$. For large $\beta = kb$, the ratio $\hbar kN'/P_z'$ tends to $1 + \beta^{-1} + O(\beta^{-2})$, for all z. The angular momentum content per unit length J_z' is equal to $\hbar N'$, from (45).

Figure 3 shows the probability density and momentum density of the ψ_{21} beam, while figure 4 shows $\hbar kN'/P_z'$ for this beam. From (51) and (53) we find that this ratio tends to unity for wide beams (large β), as we found to be the case for the ψ_{10} beam in equation (17).

7. Angular momentum properties of the $\psi_{\ell m}$ wavefunctions

When $b \to 0$, the $\psi_{\ell m}$ wavefunctions of equation (35) (with $m = 0$) become the partial waves in the expansion of a plane wave, introduced by Rayleigh in the theory of scattering of sound ([15], section 334):

$$e^{ikz} = \sum_{\ell=0}^{\infty} i^{\ell}(2\ell + 1) j_\ell(kr) P_\ell(\cos\theta). \tag{55}$$

Each term on the right-hand side is an eigenstate of the angular momentum operator $\mathbf{L} = -i\hbar\mathbf{r} \times \nabla$. The eigenvalues of L_z and $\mathbf{L}^2$ are zero and $\ell(\ell + 1)\hbar^2$, respectively. It was noted in [4] that the $\psi_{\ell m}$ wavefunctions (35) are eigenfunctions of the shifted operator

$$\tilde{\mathbf{L}} = -i\hbar(\mathbf{r} - \mathbf{r}_b) \times \nabla, \qquad \mathbf{r}_b = [0, 0, ib]. \tag{56}$$

This shift in the angular momentum operator corresponds to the (imaginary) shift in z, by means of which the $\psi_{\ell m}$ may be obtained from $j_\ell(kr) P_{\ell m}\left(\frac{z}{r}\right) e^{im\phi}$.

We shall give some of the properties of $\tilde{\mathbf{L}}$ and $\tilde{\mathbf{L}}^2$. First we note that $L_z = -i\hbar(x\partial_y - y\partial_x) = -i\hbar\partial_\phi$ is not changed by a translation in the z-coordinate, real or imaginary. Thus $\tilde{L}_z = L_z$ and the $\psi_{\ell m}$ are eigenfunctions of L_z with eigenvalues $m\hbar$. However, L_x and L_y are changed by the imaginary translation:

$$\begin{aligned} L_x &= -i\hbar(y\partial_z - z\partial_y) \to \tilde{L}_x = L_x + \hbar b\partial_y \\ L_y &= -i\hbar(z\partial_x - x\partial_z) \to \tilde{L}_y = L_y - \hbar b\partial_x. \end{aligned} \tag{57}$$

There is a corresponding change in $\mathbf{L}^2 = L_x^2 + L_y^2 + L_z^2$:

$$\begin{aligned} \tilde{\mathbf{L}}^2 &= \mathbf{L}^2 + \hbar^2\left\{(b^2 + 2ibz)\left(\partial_x^2 + \partial_y^2\right) - 2ib(x\partial_x + y\partial_y + 1)\partial_z\right\} \\ &= \mathbf{L}^2 + \hbar^2\left\{(b^2 + 2ibz)\left(\partial_\rho^2 + \rho^{-1}\partial_\rho + \rho^{-2}\partial_\phi^2\right) - 2ib(\rho\partial_\rho + 1)\partial_z\right\}. \end{aligned} \tag{58}$$

The $\tilde{\mathbf{L}}^2$ operator has the expected eigenvalues when operating on the $\psi_{\ell m}$ wavefunctions, namely $\ell(\ell + 1)\hbar^2$.

8. Summary

Seven invariants (quantities which are constant along the beam length) exist for coherent atom beams. These originate from the conservation of particles, the conservation of momentum and the conservation of angular momentum. The simplest invariant can be interpreted as the momentum content per unit length of the beam. The probability content per unit length N' and the angular momentum content per unit length J_z' are not invariants in general, but for wide beams we do have the approximate equalities

$$P_z' \approx \hbar k N', \tag{13}$$

$$J_z' \approx \hbar m N' \tag{45}$$

corresponding to the picture of each atom carrying an average momentum $\hbar k$ in the beam propagation direction and angular momentum $\hbar m$ about the beam direction.

Symmetries reduce the number of nonzero invariants. For beams characterized by wavefunctions which are independent of the azimuthal angle ϕ, only two are nonzero: P_z' and T_{zz}'. For beams which have azimuthal dependence $e^{im\phi}$ there are three nonzero invariants P_z', T_{zz}' and M_{zz}', but the last is determined by P_z'.

The beam invariants, and the non-invariant N', have been calculated for two exact beam wavefunctions. These wavefunctions are part of a set which are all eigenstates of a modified angular momentum operator.

Acknowledgments

The author is grateful to Ashton Bradley and Damien Martin for constructive comments.

References

[1] Lekner J 2004 Invariants of electromagnetic beams *J. Opt. A: Pure Appl. Opt.* **6** 204–9
[2] Sheppard C J R and Saghafi S 1999 Beam modes beyond the paraxial approximation: a scalar treatment *Phys. Rev.* A **57** 2971–9
[3] Ulanowski Z and Ludlow I K 2000 Scalar field of nonparaxial Gaussian beams *Opt. Lett.* **25** 1792–4
[4] Lekner J 2001 TM, TE and 'TEM' beam modes: exact solutions and their problems *J. Opt. A: Pure Appl. Opt.* **3** 407–12
[5] Doak R B, Grisenti R E, Rehbein S, Schmahl G, Toennies J P and Wöll Q 1999 Towards realization of an atomic de Broglie microscope: helium atom focusing using Fresnel zone plates *Phys. Rev. Lett.* **83** 4229–32
[6] Grisenti R E, Schöllkopf W, Toennies J P, Manson J R, Savas T A and Smith H I 2000 He-atom diffraction from nanostructure transmission gratings: the role of imperfections *Phys. Rev.* A **61** 033608
[7] Bloch I, Köhl M, Greiner M, Hänsch T W and Esslinger T 2001 Optics with an atom laser beam *Phys. Rev. Lett.* **87** 030401
[8] Köhl M, Hänsch T W and Esslinger T 2001 Measuring the temporal coherence of an atom laser beam *Phys. Rev. Lett.* **87** 160404
[9] Köhl M, Hänsch T W and Esslinger T 2002 Continuous detection of an atom laser beam *Phys. Rev.* A **65** 021606
[10] Bradley A S, Hope J J and Collett M J 2003 Steady-state quantum statistics of a non-Markovian atom laser II *Phys. Rev.* A **68** 063611
[11] Lekner J 2002 Phase and transport velocities in particle and electromagnetic beams *J. Opt. A: Pure Appl. Opt.* **4** 491–9
[12] Madelung E 1926 Quantentheorie in Hydrodynamischer Form *Z. Phys.* **40** 322–6
[13] Bialynicki-Birula I, Cieplak M and Kaminsky J 1992 *Theory of Quanta* (Oxford: Oxford University Press) p 89
[14] Barnett S M 2002 Optical angular momentum flux *J. Opt. B: Quantum Semiclass. Opt.* **4** S1–S10
[15] Rayleigh J W S 1896/1945 *The Theory of Sound* (New York: Macmillan)