Semiclassical Theory of Matter-Wave Detection

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Abstract. We derive a semiclassical theory for the detection of matter-waves. This theory draws on the theories of semiclassical optical detection and of fluid mechanics. We observe that the intrinsically dispersive nature of matter-waves is important in deriving such a theory.

In nature particles exist in either of two forms: those with integer spin and those with half-integer spin. The former of these are known as bosons, and the latter as fermions. At a microscopic level, fermions are guided by the Pauli exclusion principle, which states that no two fermions can occupy the same quantum state. On the other hand, there is no such principle affecting bosons, and thus any number can occupy the same state. This is the basis of Bose-Einstein condensation, which was first proposed theoretically by Bose and Einstein in 1924 [1, 2, 3]. A Bose-Einstein condensate (BEC) is a system in which a macroscopic number of bosons occupy a single quantum state. To achieve this with a dilute gas of atomic bosons requires extremely low temperatures, such that the de-Broglie wavelength of the particles become larger than their mean spacing. Hence no BEC was experimentally realized in these systems until 1995 [4, 5, 6] using bosonic isotopes of Rb, Na and Li.

A BEC is created by cooling the atoms using optical and magnetic forces, and then cooling them again using one of a number of techniques. The BEC is then held in a magnetic trap, which is switched off after a period of time to allow the atoms to expand so that imaging can take place. A recent experiment by Robert *et al* [7] involved the creation of a BEC of metastable triplet He (He*) and highlighted the ability to count single atoms falling from the trap after it was turned off. This allows for the exciting possibility of more detailed investigation of the quantum statistical properties of matter-waves.

As a first step into this field, we must model the detection of matter-waves falling under gravity. We will use a simplistic model of a BEC, not including the effects of interactions which exist between atoms [8, 9]. This will allow the features specific to detection to be more readily illustrated. As we are considering matter-waves, we can draw a direct analogy with the well known theory of the detection of light waves, or photo-detection, which will be outlined here. A more complete description can be found in many texts; e. g. [10].

The classical theory of photo-detection is based on the assumption that the probability of an ionization event occuring in the photo-detector in a time period $\mathrm{d}t$ is proportional to the cycle-averaged intensity $\bar{I}(t)$ of the incoming light:

$$p(t)\mathrm{d}t = \xi \bar{I}(t)\mathrm{d}t, \qquad (1)$$

where ξ is a constant of proportionality which represents the efficiency of the detector, including geometric factors such as its area, and $\mathrm{d}t$ is sufficiently small that the probability of more than one detection event occuring is negligible. In general, the cycle-averaged intensity is taken to be

$$\bar{I}(t) = \frac{1}{2}\epsilon_0 c|E(t)|^2 \equiv cW(t), \tag{2}$$

where $W(t)$ is the energy density. Under assumption (1), if we take a time interval from t to $t+T$, then the probability of m detection events occuring is

$$P_m(T) = \left\langle \frac{\bar{n}^m}{m!}\exp\left[-\bar{n}\right] \right\rangle, \tag{3}$$

where

$$\bar{n} = \xi \int_t^{t+T} \mathrm{d}t' \bar{I}(t') \tag{4}$$

and the angled brackets indicate a statistical average. From (3) we can evaluate the mean number of detection events to be

$$\langle m \rangle = \langle \bar{n} \rangle . \tag{5}$$

We now wish to construct a semiclassical theory of matter-wave detection by analogy with the theory of photo-detection presented above. A natural way to proceed is to replace the electric field $E(\boldsymbol{r},t)$ with the particle wavefunction $\psi(\boldsymbol{r},t)$. Thus the matter-wave analogy to the expression for $\bar{I}(t)$ in (2) will be $|\psi(\boldsymbol{r},t)|^2\,\bar{\boldsymbol{v}}$, where we have included a characteristic velocity $\bar{\boldsymbol{v}}$. This is in direct analogy with the velocity of light c in the photo-detection theory and is of vectorial nature to allow for matter-waves which are not travelling perpendicular to the detector. It is also required so that the equations have the correct dimensionality. In the analysis that follows, $\bar{\boldsymbol{v}}$ will be associated with the mean velocity of the wavepacket. The probability of detection over a time interval from t to $t+T$ would again be given by (3) and the average number of counts $\langle m \rangle$ by (5) where instead of (4), we have

$$\bar{n} = \xi \int_t^{t+T} \mathrm{d}t' \int_A |\psi(\boldsymbol{r},t')|^2\, \bar{\boldsymbol{v}}\cdot \mathrm{d}\boldsymbol{A}. \tag{6}$$

We have now explicitly included the area of the detector A, and $\mathrm{d}\boldsymbol{A}$ is the infinitesimal area element normal to the surface of the detector. If we assume that the particle wavefunction is normalized so that it contains on average N particles, then for all times t

$$\int_{-\infty}^{\infty} \mathrm{d}^3\boldsymbol{r}\, |\psi(\boldsymbol{r},t)|^2 = N. \tag{7}$$

If the detector is of perfect efficiency then we would expect that for a wavepacket falling under gravity, a sufficiently long detection window and large detection area would produce a mean of N detection events. This means that from (5) we might expect that as $T \to \infty$,

$$\xi \int_{-\infty}^{\infty} \mathrm{d}t \int_A |\psi(\boldsymbol{r},t)|^2\, \bar{\boldsymbol{v}}\cdot \mathrm{d}\boldsymbol{A} = N, \tag{8}$$

for the value of ξ corresponding to a perfectly efficient detector.

By drawing analogy with photo-detection of light waves, we have derived (6) which includes the characteristic velocity $\bar{\boldsymbol{v}}$. As a first approximation we might expect that this will be the mean velocity of the wavepacket. This is not an approximation for light in free space because free space is not dispersive; at all frequencies light travels at c. For matter-waves, however, free space *is* dispersive.

In order to take into account matter-wave dispersion we ought to base our theory of detection on the flux-density of particles: the mean rate at which particles cross a unit area of the detector. As particle number is a conserved quantity it must satisfy an equation of continuity [11, 12]

$$\frac{\partial}{\partial t}\left|\psi(\boldsymbol{r},t)\right|^2+\nabla\cdot\boldsymbol{J}(\boldsymbol{r},t)=0, \tag{9}$$

where $\boldsymbol{J}$ is the particle flux-density. This equation is of the same form as the one for local charge conservation in electromagnetic theory or, more relevantly for our purpose, relating particle density ρ and particle flux-density $\boldsymbol{J}=\rho\boldsymbol{v}$ in fluid mechanics [13]. From (9) we obtain a particle flux-density of the form

$$\boldsymbol{J}(\boldsymbol{r},t)=\frac{\hbar}{m}\mathrm{Im}\left\{\psi^*(\boldsymbol{r},t)\nabla\psi(\boldsymbol{r},t)\right\}. \tag{10}$$

As this is analogous to the particle flux-density $\boldsymbol{J}=\rho\boldsymbol{v}$ from fluid mechanics, it seems reasonable that (6) would become

$$\bar{n}=\xi\int_t^{t+T}\mathrm{d}t'\int_A\boldsymbol{J}(\boldsymbol{r},t')\cdot\mathrm{d}\boldsymbol{A}. \tag{11}$$

Indeed, in electromagnetic theory a relation similar to (9) exists between the energy density $W(t)$ and the Poynting vector (which gives the energy flux-density) [14, 15]. Equation (2) is thus an approximation which holds in most experimentally realizable situations. In situations where this approximation is invalid, the cycle-averaged intensity in (2) must be replaced by the magnitude of the Poynting vector.

In order to illustrate fully the difference between the theories given by (6) and (11), it is instructive to evaluate both expressions in the case of the detection of a wavepacket falling in the z-direction under gravity onto a flat, large-area detector aligned parallel to the x-y plane. Such a system closely models the He* experiment mentioned at the beginning of this paper, and it is one in which we would expect all particles to fall onto the detector, which will allow us to check the expression for $\langle m\rangle$.

In evaluating the probability of detection for a wavepacket falling under gravity we will need to calculate the form of the matter-wave. We consider a model BEC, released at time $t=0$, described by a Gaussian wavefunction centred at $\boldsymbol{r}_0$ with width parameter w,

$$\psi(\boldsymbol{r},0)=N^{\frac{1}{2}}(\pi w^2)^{-\frac{3}{4}}\exp\left\{-\frac{|\boldsymbol{r}-\boldsymbol{r}_0|^2}{2w^2}\right\}. \tag{12}$$

The standard solution to the Schrödinger equation takes the form

$$\psi(\boldsymbol{r},t)=\exp\left\{\frac{-\mathrm{i}t\hat{H}}{\hbar}\right\}\psi(\boldsymbol{r},0), \tag{13}$$

where $\hat{H}$ is the Hamiltonian, which in this case has the standard kinetic energy term and a gravitational potential term

$$\hat{H}=\frac{\hat{p}^2}{2m}+mg\hat{z}. \tag{14}$$

We have taken the zero of gravitational potential energy to be at $z = 0$. When written in the position representation, this becomes

$$\hat{H} = \frac{-\hbar^2}{2m}\nabla^2 + mgz, \tag{15}$$

and so the particle wavefunction at a later time t will be

$$\psi(\boldsymbol{r}, t) = N^{\frac{1}{2}}(\pi w^2)^{-\frac{3}{4}} \exp\left\{-\frac{\mathrm{i}t}{\hbar}\left(\frac{-\hbar^2}{2m}\nabla^2 + mgz\right)\right\} \exp\left\{-\frac{|\boldsymbol{r}-\boldsymbol{r}_0|^2}{2w^2}\right\}. \tag{16}$$

Techniques outlined in [16] allow us to evaluate the deriviatives in this expression and obtain a wavefunction for the matter-wave falling under gravity

$$\psi(\boldsymbol{r}, t) = N^{\frac{1}{2}}\pi^{-\frac{3}{4}}\left(\frac{w}{w^2 + \mathrm{i}t\frac{\hbar}{m}}\right)^{\frac{3}{2}} \exp\left\{-\frac{|\boldsymbol{r}-\boldsymbol{R}(t)|^2}{2\left(w^2 + \mathrm{i}t\frac{\hbar}{m}\right)}\right\} \exp\left\{-\frac{\mathrm{i}tmg}{\hbar}\left(z + \frac{1}{6}gt^2\right)\right\}, \tag{17}$$

where we have defined the average "classical" position of the particle $\boldsymbol{R}(t) = \langle \boldsymbol{r}(t)\rangle = \boldsymbol{r}_0 - \frac{1}{2}gt^2\hat{\boldsymbol{k}}$, which gives the position of the centre of the wavepacket. As the wavepacket is accelerating from rest under gravity, the integral in (6) will be given by

$$\int_A |\psi(\boldsymbol{r}, t)|^2\, \bar{\boldsymbol{v}} \cdot \mathrm{d}\boldsymbol{A} = gt \iint |\psi(\boldsymbol{r}, t)|^2\, \mathrm{d}x\mathrm{d}y. \tag{18}$$

It can be seen that the expression in (18) depends on $\exp\{-(z-z_0)^2\}$ and thus depends on the height that the wavepacket starts above the detection screen. With this taken into account, one can see that the integral of (18) over all time cannot give a constant value of N, and so the expression in (8) cannot hold for any ξ which is solely dependent on detector properties. This result can be verified numerically.

If we now use (10) to calculate the flux-density of particles for this system, we obtain an expression for the integral in (11)

$$\int_A \boldsymbol{J}(\boldsymbol{r}, t) \cdot \mathrm{d}\boldsymbol{A} = \left[gt - \frac{z - z_0 + gt^2/2}{t + w^4m^2/(\hbar^2 t)}\right] \iint |\psi(\boldsymbol{r}, t)|^2\, \mathrm{d}x\mathrm{d}y. \tag{19}$$

It is straightforward to show that the integral of this expression over all time gives the average number of particles in the wavepacket N. Thus from (11) we can see that the constant of proportionality ξ is in fact the efficiency of the detector η, which takes values between 0 and 1.

It is clear to see that the expression obtained in (19) is that from (18) plus an additional correction, which is a height-dependent velocity term. This additional velocity term is a direct consequence of the dispersive nature of free space for matter-waves. From (17) it is clear that the wave undergoes dispersion as it falls under gravity. The detection theory based on (18) assumes that this dispersed wavepacket propagates through the detection plane at the mean packet velocity. The detection formula in (19) based on particle flux does not make this assumption and the factor $\hbar/m$ which quantifies the dispersion of the wave in (17) also appears in the detection formula. If this factor is taken to zero either by taking $\hbar \to 0$ or $m \to \infty$, then the dispersion in (17) disappears, as does the additional velocity term in (19). The time variation of the integrals given by the two different theories are plotted in figure 1, where it can be seen that the differences in the expressions are quite pronounced: in a detection theory which takes account of dispersion the majority of particles will arrive earlier than they would in a detection theory in which dispersion is not correctly accounted for.

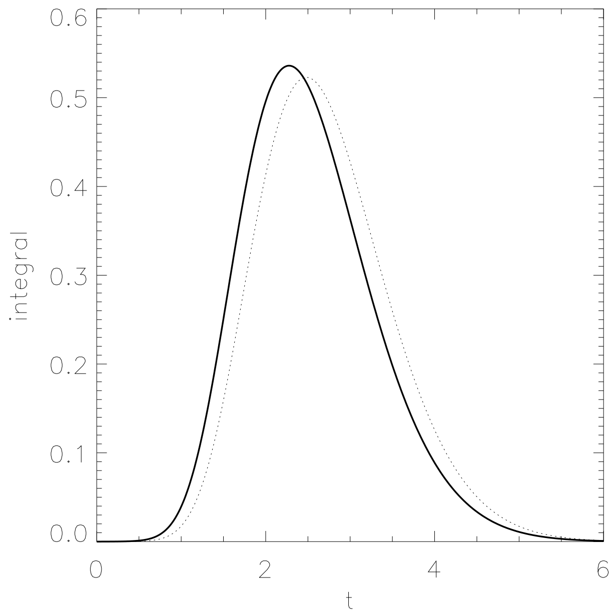

Figure 1. Comparison of integrals in the intensity term for the correct and incorrect detection theories, as a function of time. The units have been chosen in such a way that $g = \hbar/m = 1$, and we have chosen $w = 1$ and $z_0 = 3$. The solid line shows the correct theory (19) and the dotted line shows the incorrect theory (18).

From (17) we can see that if the factor $\hbar t/(mw^2)$ is greater than unity, the wavepacket becomes significantly wider (due to dispersion), and this dispersion ought to be taken account of in detection. As an example of how important dispersion is in the system under consideration, we take values from the He* experiment presented in [7]. The time of flight of atoms here is 0.1s and the mass of a He* atom is 6.68×10^{-27} kg. We thus find that the dispersion factor will be important for any wavepacket with an initial width of less than 0.1mm.

We have described in this paper the construction of a semiclassical theory of matter-wave detection, drawing on the well known theory of photo-detection. It is the intrinsically dispersive nature of matter-waves which prevents the direct analogy from working. We must instead consider the flux-density of particles, which gives an additional velocity term. Indeed if light passes through and is detected in a dispersive medium, the magnitude of the Poynting vector, which represents the flux-density of energy, must be used in place of (2).

An instructive "next step" will be to consider the second quantized version of this theory. We would expect that in doing this, a situation of no detection in the early part of the wavepacket would feed back to modify the later part of the wavepacket. It is also clear that quantities other than particle number - such as energy, momentum and angular momentum - can be conserved. We intend to investigate these conservation laws, fluxes and the deposition of such quantities on a detection screen.

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