Meanfield treatment of Bragg scattering from a Bose-Einstein condensate.

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A unified semi-classical treatment of Bragg scattering from Bose-Einstein condensates is presented. The formalism is based on Gross-Pitaevskii equations driven by a classical light field, and leads to a single component equation incorporating the effects of meanfield nonlinearity and spatial inhomogeneity. Three dimensional numerical simulations of this equation in cylindrical symmetry are used to investigate Bragg scattering for a number of cases. Scattering from a condensate released from a trap produces characteristic cycling of the atomic momentum, and an analytic description is given using a linear model incorporating spatial nonuniformity. Simple expressions obtained for the momentum packet cycling are shown to accurately describe the full nonlinear behaviour within a well specified validity range and a transition linewidth is derived. For the case of a trapped condensate, a numerical study of momentum spectroscopy is carried out and the shift of the Bragg resonance condition due to meanfield nonlinearity is investigated.

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I. INTRODUCTION

The phenomenon of Bragg scattering, where a wave interacts with an extended periodic structure, was first observed by W. H. and W. L. Bragg \cite{1} in experiments scattering X-rays from crystal planes. In 1988 Martin et al. \cite{2} demonstrated the matter wave equivalent using an atomic beam of neutral atoms interacting with a light grating, and subsequently, Bragg scattering has been widely used in atomic optics and interferometry (e.g see \cite{3}).

Bose condensates, with their extended spatial coherence, offer significantly enhanced scope for the application of this technique, and it has already become an important tool in the investigation and manipulation of this new state of matter. In recent experiments Bragg scattering has been used on condensates to engineer the meanfield wavefunction \cite{4}, to measure coherence and correlations \cite{5,6,7}, and act as a beam-splitter \cite{8,9}. Most of the existing theory of atomic Bragg scattering has concentrated on treating plane-wave single atom states (e.g see \cite{10,11,12}), and while this captures some key behaviour, it does not account for some distinctive properties of condensates, such as nonlinear collisional self interaction and nonuniform spatial distribution. Zhang and Walls \cite{13} have developed a theory of Bragg scattering for cold atom beams which includes some effects of atomic interactions, although the resulting nonlinear interaction term they derive is of an unconventional form. Their accompanying numerical calculation for a beam-splitter process shows that the inclusion of nonlinearity can give rise to qualitatively new effects.

In this paper, we present a unified semi-classical treatment of Bragg scattering from condensates, in which the condensate is described in the meanfield limit, and the applied laser fields are treated as classical fields. Beginning with Gross-Pitaevskii equations we obtain a single component equation describing the interaction of a condensate with a light field grating formed at the intersection of two far detuned laser beams. The lasers may be pulsed or cw, and arbitrary geometries are allowed. This formalism is sufficiently general to include diffraction (where the light grating has rapid transverse spatial variation or the interaction time is short) and channeling (where the lasers have high intensity), but in this paper we concentrate on the regime of Bragg scattering, for which the output state has momentum components only in a single narrow range. Accordingly we consider only those cases for which the transverse spatial laser profiles vary slowly in comparison to the condensate, and the interaction time is long.

In order to characterise the effect of nonlinearity and spatial nonuniformity, we have numerically simulated our single component equation in three dimensions. We consider the case where the light fields are applied immediately after the condensate is released from a trap, and also the case where the condensate remains trapped. Some aspects of the behaviour, notably the shift of the Bragg resonance condition, are due directly to the nonlinearity. However, we also find that over a usefully wide parameter range, much of the behaviour can be understood in terms of a framework provided by the linear results. To facilitate comparison with the linear case, we present a novel treatment of linear Bragg scattering for a released condensate, which conveniently incorporates spatial nonuniformity. This model is based on a partitioned representation of momentum space and under appropriate validity conditions, reduces to a set of two state systems, allowing simple expressions to be found for the dynamical behaviour of momentum wave packets, and the momentum transition linewidth. We determine the validity range over which the linear treatment accurately describes Bragg scattering of nonlinear released condensates, and identify two main mechanisms responsible for the failure of the linear model; meanfield expansion and nonlinear dispersion. We verify our analysis by numerical
simulation of the full nonlinear equations, and also investigate numerically the nonlinear shift of the Bragg resonance in a trapped condensate.

The paper is organised as follows. In section II we begin with Gross-Pitaevskii equations and derive the one component equation that is the basis for the rest of the paper. In section III we present an analytic treatment of linear Bragg scattering from a released condensate, based on a partitioned representation of the momentum wavefunction, and formulate the treatment as a tridiagonal matrix equation. Under well defined approximations, this reduces to a two-state form which is easily solved, and in section IV we examine the properties of the solution and introduce dispersion curve plots to help visualise the implications of our approximations. In section V we consider in detail the effects of nonlinearity on Bragg scattering from released condensates, and finally in section VI, we consider momentum spectroscopy from condensates in harmonic traps.

II. FORMULATION

We consider as our model a coherent system of atoms in a light field grating provided by two crossed laser beams. The laser fields are treated as plane-wave classical fields with wave-vectors and frequencies $k_i$ and $\omega_i$ respectively. For convenience we shall assume the electric fields are of equal intensity, and so the total field is given by

$$ E_T(r, t) = \frac{1}{2} E_0(t) \Lambda(r, t), $$

where

$$ \Lambda(r, t) = [e^{i(k_1 \cdot r - \omega_1 t)} + e^{i(k_2 \cdot r - \omega_2 t)} + c.c]. $$

We have neglected any spatial variation of the slowly varying amplitude $E_0(t)$ (although it would be trivial to include), but include a time dependence to allow for the possibility of pulsed fields. The condensate is treated in the meanfield limit and has two internal states $|g\rangle$ and $|e\rangle$ separated by a Bohr frequency $\omega_{eg}$ and with a dipole matrix element $d$. The coupling of these two states by an electric field is characterised by the Rabi frequency, $\Omega_0(t) = d \cdot E_0(t)/\hbar$. The meanfield equations for the ground and excited state wavefunctions $\psi_g$ and $\psi_e$ are the time dependent Gross-Pitaevskii equations

$$ i\hbar \frac{\partial \psi_g}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi_g + V_Tg(r, t)\psi_g - \frac{1}{2}\hbar \Omega_0(t) \Lambda(r, t) \psi_e + w_{gg}|\psi_g|^2 \psi_g, $$

$$ i\hbar \frac{\partial \psi_e}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi_e + \hbar \omega_{eg} \psi_e + V_Tc(r, t)\psi_e - \frac{1}{2}\hbar \Omega_0^*(t) \Lambda(r, t) \psi_g + w_{eg}|\psi_g|^2 \psi_e + w_{ce}|\psi_e|^2 \psi_{eg}, $$

where $w_{gg}$ and $w_{ee}$ characterise the intra-species collisional interactions, and $w_{eg}$ the interspecies interaction. The functions $V_Tj$ represent the trapping potentials for the respective internal states, and we include time dependence in order that they can be dynamically altered. We assume the laser frequencies $\omega_i$ are sufficiently off resonant from the $|g\rangle \rightarrow |e\rangle$ transition that the laser field undergoes negligible modification in propagating through the condensate, and furthermore that spontaneous emission (and its effect on condensate coherence) can be ignored. In this large detuning limit it is also permissible to adiabatically eliminate the excited state from Eq. (3), leaving only an equation for $\psi_g$. Details of this procedure are given in the Appendix A, where it is shown that the energy $\hbar \Delta$ exceeds all other external energies associated with the excited state, we obtain the one component equation for the ground state wavefunction

$$ i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V_T(r, t)\psi + V(t) \lambda(r, t) \psi + w|\psi|^2 \psi. $$

The wavefunction $\psi = \exp(-i \int_0^t V(s) ds) \psi_g$, is the ground state wavefunction in an interaction picture, and for clarity we have written $w$ for $w_{gg}$ and $V_T(r, t)$ for $V_Tg(r, t)$, and have defined the quantities

$$ V(t) = \frac{|\Omega_0(t)|^2}{2\Delta}, $$

$$ \lambda(r, t) = \cos(\Delta k \cdot r - \delta t), $$

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where $\Delta k = k_1 - k_2$ and $\delta = \omega_1 - \omega_2$. The function $\lambda(\mathbf{r}, t)$ contains the periodic spatial and temporal evolution of the optical potential, and arises by neglecting certain rapidly rotating terms in the adiabatic elimination (see Appendix A for details).

For the coupled system described by Eq. (5) the duration of the grating amplitude $V(t)$ is a key factor in determining the nature of the system response. For Bragg scattering the pulse duration $T_p$ must be of order

$$T_p > \frac{m}{\hbar|\Delta k|^2}. \quad (8)$$

In most of this paper (sections III-V) we will consider the case of Bragg scattering from a condensate released from a harmonic trapping potential (i.e. the trapping potential is set to 0 at $t = 0$). It is also possible to have the trap on during the Bragg pulses, and obtain a result qualitatively similar to scattering from a released condensate, provided the trap does not remain on too long. The time duration should be less than a trap period, (so that the trap itself does not significantly alter momentum components) and less than the characteristic time of momentum spreading of a released condensate (which occurs due to mean field expansion, see section V).

A. Numerical Solutions

Equation (5) is the basic equation for this paper and is familiar in atom optics. In general it is difficult to solve because of the nonlinear term and in order to explore the types of behaviour that can occur, we have obtained numerical solutions for a range of parameters. Our solutions are in three dimensions, but restricted (by computational resources) to the case of cylindrical symmetry, a choice which requires $\Delta k$ to be in the axial direction (i.e. $\Delta k = \Delta k \hat{k}_z$).

We present in Fig. 1 a sequence of images showing the density of a condensate evolving in the presence of a light grating, and illustrating the complexity that can typically occur. The condensate was released from a spherical harmonic trap at time $t = 0$, and the light grating applied immediately after. During this simulation we can see fringes developing in the density profile, which is characteristic of interference between a stationary and a moving wavepacket. As time progresses the spatial distribution extends in the $z$ direction at a much faster rate than spreading occurs in the perpendicular directions, and the density distribution becomes less uniform (see Fig. 1(d)) with distinct regions of high and low density apparent.
FIG. 1. Probability density (in the $x$-$z$ plane) of a condensate evolving in the presence of a light grating. The condensate is initially in the ground state of a spherical harmonic trap, and at time $t = 0$, the trap is switched off and a cw-light grating applied. Parameters are $w = 2500 w_0$, $\Delta k = 14/r_0$ in the $z$-direction, $\delta = 196 \omega_T$ and $V = 20 \omega_T$.

For notational simplicity our numerical solutions are given in dimensionless units. Since the initial states for the simulations we discuss in this paper are related to eigenstates of harmonic traps, we have chosen to use harmonic oscillator units for the problem. The transformation between S.I ($\{t, r, k, \delta, w\}$) and harmonic oscillator units ($\{\tilde{t}, \tilde{r}, \tilde{k}, \tilde{\delta}, \tilde{w}\}$) is

\begin{align}
  t &= \tilde{t}/\omega_T, \quad r = \tilde{r} r_0, \\
  k &= \tilde{k}/r_0, \quad \delta = \tilde{\delta} \omega_T, \\
  w &= \tilde{w} w_0,
\end{align}

where $\omega_T$ is the trap frequency, $r_0 = \sqrt{\hbar/2m \omega_T}$ and $w_0 = \hbar \omega_T r_0^3$. 
III. ANALYTIC TREATMENT OF THE LINEAR CASE

It is evident that the simplified treatment of Bragg scattering of condensates encompassed in Eq. (3) can give rise to quite complex behaviour. Here we derive an analytic treatment of the model that will provide a simple understanding of the behaviour over a wide parameter regime. We begin by transforming the equation into momentum space, where the momentum space wavefunction $\phi(k,t)$ is defined as the spatial Fourier transform

$$\phi(k,t) = \frac{1}{(2\pi)^3} \int \psi(r,t) e^{-ikr} d^3r. \quad (12)$$

Henceforth, for the sake of notational clarity, we will suppress the explicit time dependence of the momentum wavefunction, and simply write $\phi(k)$, for $\phi(k,t)$. Straightforward manipulation of Eq. (3) leads to

$$i\hbar \frac{\partial \phi(k)}{\partial t} = \frac{\hbar^2 |k|^2}{2m} \phi(k) + \hbar V(t) \left[ \frac{i}{2} \phi(k + \Delta k) e^{i\delta t} + \frac{1}{2} \phi(k - \Delta k) e^{-i\delta t} \right] + \frac{w}{(2\pi)^3} \int \int \int \phi(k_1) \phi^*(k_2) \phi(k - k_1 - k_2) d^3k_1 d^3k_2, \quad (13)$$

and we can see that the effect of the light grating is to linearly couple states of momentum $k$ to neighbouring states $k \pm \Delta k$. It is useful to partition momentum space to incorporate this regularity, in an analogous way that Brillouin zones are used in solid state physics to reflect the periodicity of the crystal lattice. Choosing the $\Delta k$ in $k$-space to be along the $z$ direction, we divide the $k_z$ axis into intervals of length $|\Delta k|$, and label them by the integer $n$, such that the centre of the $n_{th}$ interval (along the $k_z$ axis) is at $k_z = n \Delta k$, and $k_z \in [-|\Delta k|/2, |\Delta k|/2]$. The wavefunction $\phi(k)$ can now be re-expressed as a set of wavefunctions $\tilde{\phi}_n(k)$, each defined only within the $n_{th}$ interval of the partitioned $k$-space, i.e.

$$\tilde{\phi}_n(k) \equiv \phi(k) \quad \{ k : (n - \frac{1}{2})|\Delta k| < k_z \leq (n + \frac{1}{2})|\Delta k| \}. \quad (14)$$

Within each interval, the momentum vector is uniquely defined by its offset from the central $k$ value, and thus we finally replace the wavefunction $\phi(k)$ by the set of partitioned wavefunctions

$$\phi_n(q) = \tilde{\phi}_n(k) e^{-in\delta t}, \quad (15)$$

where $q = k - n\Delta k$, i.e. the domain of $\phi_n$ is all values of $q$ which have a $k_z$ component in the range $[-|\Delta k|/2, |\Delta k|/2]$. We have included phases in the definition in Eq. (15), for later convenience. The utility of these new wavefunctions arises because $\phi_n(q)$ and $\phi_{n+1}(q)$ represent the full momentum wavefunction at adjacent positions in $k$-space separated by exactly one momentum kick $\hbar \Delta k$. In terms of this new set of wavefunctions, Eq. (13) can be written as the set of equations

$$i\hbar \frac{\partial \phi_n(q)}{\partial t} = \hbar \omega_n(q) \phi_n(q) + \frac{\hbar}{2} \frac{V(t)}{2} \left[ \phi_{n-1}(q) + \phi_{n+1}(q) \right] + \frac{w}{(2\pi)^3} \int \int \sum_{i,j} \phi_i(q_1) \phi^*_j(q_2) \phi_{n-i-j}(q - q_1 - q_2) d^3q_1 d^3q_2 \quad (16)$$

where

$$\omega_n(q) = \frac{\hbar |q + n\Delta k|^2}{2m} - n\delta. \quad (17)$$

A. Noninteracting Atoms

We derive an analytic solution for Eq. (16) by considering the case where collisional interactions in the BEC are negligible, i.e. $w = 0$. We shall find that this allows us to make a good representation of the full equation for a large regime of interest for condensates. Putting $w = 0$ allows us to write the evolution equation (16) as a linear system:
The matrix in Eq. (18) displays the couplings between the partitioned momentum wavefunctions. For a given momentum \( q \), the effectiveness of the coupling between \( \phi_n(q) \) and \( \phi_{n+1}(q) \), is determined by the size of the coupling \( V \) relative to the momentum detuning,

\[
\Delta_n(q) = \omega_{n+1}(q) - \omega_n(q).
\]

In particular if (for some \( q_r \)), \( \Delta_n(q_r) = 0 \), then the corresponding transition of a particle from momentum state \( |q_r + n\Delta k\rangle \rightarrow |q_r + (n + 1)\Delta k\rangle \) is resonant. Noting that the momentum kick given to the atoms is \( h\Delta k \), (the momentum difference of the photons from the two light fields) and that

\[
\Delta_n(q) = \frac{\hbar}{2m} [(2n + 1)\Delta k + 2q] \cdot \Delta k - \delta,
\]

then the resonance condition \( \Delta_n(q_r) = 0 \) is recognised as a Bragg condition for the process: that is both momentum and energy are conserved.

The typical initial condition for Eq. (18) is a localised momentum wavepacket. If \( |\Delta k| \) is significantly greater than the width of the wavepacket, the initial profile is almost completely contained within a single momentum interval, and thus we can take the initial momentum wavefunction to have only one of the partitioned wavefunctions \( \phi_0(q) \) to be non-zero. It is easy to see from Eq. (20) that if one of the \( \Delta_j(q) \) is very small, then all the others are larger by order \( |\Delta k|^2 \). For example, if \( \Delta_0(q_r) = 0 \) (a first order Bragg resonance), then

\[
\Delta_n(q_r) = \frac{\hbar}{m} [n|\Delta k|^2].
\]

Thus for the case \( \Delta_0(q_r) = 0 \), if the neighbouring detunings are much larger than \( V \) over the entire \( q \)-domain (see also section IV C), we can make the secular approximation [16] that only the coupling \( \phi_0 \rightarrow \phi_1 \) is significant and the evolution equation can be reduced to:

\[
\frac{\partial}{\partial t} \begin{bmatrix} \phi_0(q) \\ \phi_1(q) \end{bmatrix} = \begin{bmatrix} \omega_0(q) + \Delta_0(q) & V(q) \\ \frac{V(q)}{2} & \omega_0(q) \end{bmatrix} \begin{bmatrix} \phi_0(q) \\ \phi_1(q) \end{bmatrix}.
\]

This equation represents a continuous set of two-state Rabi problems, where the members of the set are labelled by the variable \( q \). The solution is easily found in terms of the eigenvectors of the coefficient matrix in Eq. (22) (e.g. see [17]).

1. Separable Wavefunction

The complete Bragg scattering problem in the linear case \( (w = 0) \) is described by Eq. (18), a system of equations in which the momentum argument \( q \) is a three dimensional vector. This three dimensional character remains even when the equations can be reduced to a set of two-state problems, as in the previous section. It is possible, however, to find a solution for the full linear case which simplifies the geometrical character. If we assume the partitioned wavefunction is separable, i.e.

\[
\phi_n(q) = \xi(q_x)\zeta(q_y)\Phi_n(q_z),
\]

and we take the momentum kick to be in the \( z \) direction, then Eq. (18) transforms to a set of independent equations,
\[ i\hbar \frac{\partial \xi(q_x)}{\partial t} = \frac{\hbar^2 q_x^2}{2m} \xi(q_x), \quad (24) \]
\[ i\hbar \frac{\partial \zeta(q_y)}{\partial t} = \frac{\hbar^2 q_y^2}{2m} \zeta(q_y), \quad (25) \]
\[ i\hbar \frac{\partial \Phi_n(q_z)}{\partial t} = \hbar \left[ \frac{\hbar(q_z + n\Delta k)^2}{2m} - n\delta \right] \Phi_n(q_z) + \frac{1}{2} \hbar V(t) \left[ \Phi_{n-1}(q_z) + \Phi_{n+1}(q_z) \right]. \quad (26) \]

The wavefunction \( \Phi_n(q_z) \) obeys an equation identical to Eq. (18), except that the momentum argument is now simply the scalar \( q_z \). The wavefunctions \( \xi(q_x) \) and \( \zeta(q_y) \) describing the \( q_x \) and \( q_y \) momentum behaviour are freely evolving one dimensional wavepackets, and for example with a gaussian initial condition have a well known analytic solution (e.g. [17]). Reduction of the system of equations for \( \Phi_n \) to a two-state system would proceed exactly as in the previous section. We have chosen, in that derivation, to retain the slightly more general form \( \phi_n(q) \), because it also includes the case of non-separable wavefunctions, and we will retain the general form \( \phi_n(q) \) in the remaining sections of this paper for the same reason. We emphasize however that our results can be transformed to the somewhat easier separable case by simply making the transformation \( \phi_n(q) \rightarrow \Phi_n(q_z) \).

IV. RESULTS AND FEATURES OF THE TWO-STATE MODEL

In this section we present the characteristic features of the two state model and compare its behaviour to the numerical solutions of Eq. (3) for the case of \( w = 0 \). We then discuss the parameter regimes for which the two-state model provides a good description of the full \( w = 0 \) behaviour.

A. Rabi Oscillations

The two state system of Eq. (22) will Rabi oscillate between the \( \phi_0 \) and \( \phi_1 \) wavepackets in accordance with previous theory and experiments [2,18]. The frequency at which each momentum state oscillates between the two wavepackets is momentum dependent, and is given by the generalized Rabi frequency, defined as

\[ \Omega'(q) = \sqrt{V^2 + \Delta_0(q)^2}. \quad (27) \]
FIG. 2. Evolution of the momentum distribution for the two-state solution with $\Delta k_z = 14/r_0$, $\delta = 196\omega_T$, and $V = 50\omega_T$. The boundary for the partitioned wavefunctions is indicated by the vertical dotted line. The wavepacket centred about $k_z = 0$ corresponds to $\phi_0$ and has an initial gaussian profile. The wavepacket to the right of the dotted line corresponds to $\phi_1$ (but shifted by $k_z = 14/r_0$). Figures (a)-(c): the analytic two-state solution. Figures (d)-(f): full numerical solution of Eq. (5) for $w = 0$.

This oscillatory behaviour is clearly evident in Fig. 2 (a)-(c), where we present the time evolution of the momentum wavepackets from the two-state model, for a case similar to Fig. 2, but with $w = 0$. As with all examples presented in sections III-IV, the condensate is prepared in an eigenstate of a spherical harmonic trap and at time $t = 0$ the trap is switched off and the light grating is applied. The initial state is thus gaussian (since $w = 0$), and we have also chosen the Bragg detuning at the centre of the $\phi_0$ wavepacket to be zero (i.e. $\Delta_0(0) = 0$ ). In Fig. 2(b), where $t = \pi/\Omega'(0)$, the population has transferred almost entirely to the $\phi_1$ wavepacket. The $q$ dependence of the Rabi cycling becomes evident at later times as the difference in the Rabi periods accumulates, an effect which can be seen in (Fig. 2(c)) where the cycling at the outer edges of the momentum packets now significantly leads the cycling at $q = 0$ giving rise to a pronounced central dip in $\phi_1$. The full numerical solution of Eq. (5) for these parameters is presented in Fig. 2(d)-(f), and clearly confirms the validity of the two-state model in this case.
B. Dispersion curves and resonance-coupling

The two-state model represented by Eq. (22) was obtained by assuming that only one of the couplings in the matrix of Eq. (18) was important. Here we present a simple means of visualising the possible couplings, and determining the validity and manner of breakdown of the two-state approximation.

We first construct a set of dispersion-type curves by plotting the frequencies $\omega_n(q)$ against $q$ for a given choice of $\Delta k$ and $\delta$, as illustrated in Fig. 3(a). The important feature of this graph is the vertical separation of the curves: the coupling between $\phi_n$ and $\phi_{n+1}$ becomes appreciable only when $\Delta_n(q)$ is small, i.e. when the difference between $\omega_n(q)$ and $\omega_{n+1}(q)$ is small. We need only consider $\Delta(q)$ in the case of $q$ in the $z$ direction (the direction of $\Delta k$), because the perpendicular components of $q$ simply offset all the $\omega$ curves by the same amount. We will therefore simply write $q_z$ and $k_z$ for the momentum arguments in the remainder of the paper. On the plots, the first order Bragg resonance condition ($\Delta_n(q_z) = 0$) appears as a crossing of the $\omega_n$ and $\omega_{n+1}$ curves, and we have highlighted this point (for $n = 0$) with a small circle. Appreciable coupling will only occur in the vicinity of this point. In Fig. 3(a) we have chosen the light grating parameters ($\Delta k$ and $\delta$) so that the crossing is at $q_z = 0$, and thus wavepacket momentum components near $q_z = 0$ will undergo Rabi cycling. In Fig. 3(b), the grating parameter choice puts the Bragg resonance at $q_z = -6/r_0$, and the response for a wavepacket centered at $q_z = 0$ depends on the coupling width, which we discuss in the following subsection.

Fig. 3(b) also shows a crossing of the $\omega_0$ and $\omega_2$ curves near $q_z = 0$. This is a second order resonance: $\phi_0$ can link...
to \( \phi_2 \) via the intermediate state \( \phi_1 \), and the overall process of \( \phi_0 \rightarrow \phi_2 \) conserves energy and momentum. However the transition from \( \phi_0 \rightarrow \phi_1 \) (and likewise \( \phi_1 \rightarrow \phi_2 \)) is detuned by the amount \( \Delta_0 = 36\omega_T \) at this point, and thus in order that the transition \( \phi_0 \rightarrow \phi_2 \) may proceed, \( V \) must be sufficiently large for \( \phi_1 \) to be seeded with population and so mediate the resonant second order process. This of course generalises to higher order couplings.

C. Coupling width and breakdown of two-state model

As is well known from the Rabi model, the probability of transition from state 1 to state 2 is given by the expression

\[
P_{12} = \frac{V^2}{V^2 + \Delta_0(q_z)^2}.
\]

As a function of \( q_z \), this is maximum at the first order Bragg resonance \( \Delta_0(q_z) = 0 \) and falls to half its value at \( \Delta_0(q_z) = V \), the power broadened width. Momentum components in \( \phi_0 \) and \( \phi_1 \) (or more generally \( \phi_n \) and \( \phi_{n+1} \)) will be significantly coupled only if the separation of the \( \omega \) curves is less than \( V \). Converting this to the corresponding \( q_z \) width, we find that the momentum width of the transition (i.e. the range of \( q_z \) about the Bragg resonance point for which the probability of momentum transfer exceeds 1/2) is

\[
\sigma_k = \frac{2mV}{\hbar|\Delta k_z|}.
\]

The cycling behaviour of the whole wavepacket depends on the relative size of the momentum width of the initial state, \( \delta k_w \), compared to \( \sigma_k \). If \( \sigma_k > \delta k_w \), the whole packet will cycle, as shown in Fig. 2. In practice this can be achieved using a sufficiently large laser intensity (i.e. large \( V \)) to broaden the transition width \( \sigma_k \). It is then possible to apply a \( \pi \)-pulse so that the initial momentum wavepacket (\( \phi_0 \)) is transferred entirely to the adjacent location in momentum space (\( \phi_1 \)), and then the whole wavepacket receives a quantised momentum change. A \( \pi/2 \) pulse on the other hand acts as a 50/50 beam splitter. For the case of \( \sigma_k \ll \delta k_w \), the Bragg process will couple out only a fraction of the initial state, as we discuss further in Sec. V.

![FIG. 4. Numerical simulation of Bragg scattering for large \( V \), showing probability distribution of z-component of momentum at time \( t = 0.29/\omega_T \). The dotted lines indicate the boundaries between the momentum partitions. Light field parameters are \( V = 100\omega_T \), \( w = 0 \), \( \Delta k = 14/r_0 \) and \( \delta = 196\omega_T \).](image)

From the dispersion curves in Fig. 3 it is apparent that the validity of the two-state model requires that over the momentum width \( \delta k_w \) of the initial wavepacket, only the \( \omega_1 \) curve is within a distance \( V \) of \( \omega_0 \). If on the other hand \( V \) is sufficiently large that \( \omega_{-1} \) and \( \omega_0 \), or \( \omega_2 \) and \( \omega_1 \) are separated by less than (or of order \( V \)), then additional
couplings will occur, and the two-state description will fail. We illustrate this in Fig. 3, where the parameters are the same as in Fig. 2, except that $V$ has been increased, to a value of approximately 25% of the $\omega_1$ to $\omega_2$ separation. By the time $t = 0.29/\omega_T$, as shown in Fig. 4, the additional couplings have resulted in appreciable population transfer to the $\phi_{-1}$ and $\phi_2$ components. Of course coupling to additional $\phi_n$ will occur if $V$ is further increased. In view of this discussion we can formulate a condition that the behaviour of a scattered wavepacket will be two-state in momentum space: the minimum detuning to subsequent dispersion curves over the momentum range of the wavepacket must be much greater than $V$, i.e.

$$\frac{\hbar}{m} \left[ |\Delta k|^2 - \frac{|\Delta k| \delta k_w}{2} \right] \gg V. \quad (30)$$

It is worth emphasizing that for the case of a first order Bragg resonance the accuracy of the two state model improves as $\Delta k$ increases in magnitude.

V. APPLICATION TO NONLINEAR CASE

In this section we compare our analytic results obtained in the linear regime ($w = 0$) to the case of nonzero values of $w$, and characterise the regime where the linear analysis accurately describes the nonlinear case.

A. Numerical Result

We first demonstrate that the main characteristics contained in the two-state analysis still occur in the nonlinear case.
FIG. 5. Spatial and momentum profiles for the numerical solution presented in Fig. 1 at $t = 0.21/\omega_T$. (a) Spatial wavefunction amplitude along the $z$-axis. (b) Momentum wavefunction amplitudes. Solid line corresponds to case in Fig. (a). Dotted line shows the $w = 0$ two-state case, for comparison. (c) Amplitudes of $\psi_0$ (solid) and $\psi_1$ (dotted) spatial wavefunctions corresponding to $\phi_0$ and $\phi_1$ of Fig. (b), respectively.

We consider as an illustration the case presented in Fig. 1, where $w = 2500 w_0$, and we plot in Fig. 5(a) the wavefunction amplitude along the symmetry axis, corresponding to Fig. 1(b). The corresponding momentum wavefunction, obtained by numerical Fourier transform, is shown in Fig. 5(b), and reveals two distinct packets. On the same figure we have drawn for comparison a dashed line representing the momentum wavefunction that would arise from the $w = 0$ two-state case. The agreement is close, and furthermore as time progresses the momentum wavepack-
ets of the \( w = 2500 w_0 \) case oscillate at a frequency approximately equal to the frequency \( V \) predicted by the two state model.

The momentum distribution enables us to understand the fringe structure that developed in Fig. 5(a). We illustrate this by constructing separately the individual spatial wavepackets \( \psi_0 \) and \( \psi_1 \) corresponding to the momentum packets \( \phi_0 \) and \( \phi_1 \) respectively. The wavefunction \( \psi_0 \) (shown as a solid line in Fig. 5(c)), is of course essentially stationary (apart from the effects of expansion), while the wavefunction \( \psi_1 \) (shown as a dotted line) has a mean momentum of \( \hbar k_z = \hbar \Delta k \), and moves to the right at a speed of \( \hbar \Delta k/m \). This packet accordingly has a steep, approximately linear, phase gradient across it, so that superposition of \( \psi_0 \) and \( \psi_1 \) results in the observed interference fringes.

### B. Free Expansion

One of the significant new effects in nonlinear Bragg scattering is that the self repulsion in the free expansion of the condensate causes the momentum wavepackets to expand. In order to clearly demonstrate this effect, it is convenient to isolate the contribution to momentum changes that arise simply from the Bragg kicks. We achieve this by defining a momentum density

\[
\rho_T(q) = \sum_i |\phi_i(q)|^2,
\]

(31)

which gives the total occupation of all momentum states that could be reached from an initial state of momentum \( \hbar q \) by an integral number of momentum kicks \( n\hbar \Delta k \). In the linear case, where Bragg scattering is the only mechanism for changing momentum states, \( \rho_T(q) \) is time independent. In a nonlinear condensate the effect of the ballistic expansion alone can be seen in Fig. 6, where the dashed line shows in successive frames, the momentum expansion of a \( w = 2500 w_0 \) cylindrically symmetric condensate freely evolving after release from a trap. The solid line shows the evolution of the same condensate in the presence of Bragg scattering. One sees that most of the momentum reshaping of \( \rho_T(q) \) is due to the repulsive expansion which occurs on a time scale

\[
\tau_E = \frac{\hbar 7 \sqrt{3}}{\mu 4},
\]

(32)

where \( \mu \) is the chemical potential (see Appendix 3). For times \( t < \tau_E \) (see Table 1), we can neglect the effects of ballistic expansion, and the effects of the condensate nonlinearity are confined to modifications of the resonance conditions, which we consider in the next section.
FIG. 6. Comparison between a purely ballistically expanding condensate (dashed line) and a Bragg scattered, untrapped condensate (solid line). In each case $w = 2500 w_0$. The light field parameters for the Bragg scattered state are $V = 5\omega_T$, $\delta = 36\omega_T$ and $\Delta k = 36/r_0$. 
C. Nonlinear Dispersion Curves

The other significant modification arising from condensate nonlinearity occurs in the Bragg resonance conditions, and the dispersion curve concept provides a useful framework for analysing this effect. In the linear case, the diagonalisation of the Hamiltonian to determine the energy eigenvalues and their momentum dependence is trivial, and leads to the dispersion curves defined by Eq. (17), and illustrated in Fig. 3. In the nonlinear case diagonalisation is rather less straightforward: for small population transfer from the ground state the appropriate dispersion curves are given (for the case of Bragg scattering in a trap) by the Bogoliubov dispersion relation [19], however for large population transfer the dispersion curves have not been investigated. Nevertheless as \( w \) increases from zero we can estimate that the dispersion curves will be shifted by an amount of order \( \mu \), the chemical potential.

In our analysis of the linear case in the previous section, Bragg scattering was shown to occur where the \( \omega_n \) and \( \omega_{n+1} \) curves are separated by less than the power broadened width \( V \) of the laser interaction. Thus if the laser parameters \( \delta \) and \( \Delta k \) are chosen so that \( \omega_0 \) and \( \omega_1 \) cross in the \( w = 0 \) case, we can expect our linear analysis to still apply when \( w \neq 0 \), provided the shift of the dispersion curves, \( \mu \), is less that the transition width. The regime where the results from section IV can be applied in the nonlinear case is therefore

\[
\mu \ll hV, \tag{33}
\]

and we list in Table 1 the values of the \( \mu \) at the instant of release from the trap for a range of condensates. We note that if \( V \) becomes sufficiently large, Bragg scattering will evolve into quantum channeling [20]. A critical test of condition (33) can be made by considering condensate evolution in the spatial picture, and the comparison between the linear and nonlinear cases is facilitated by separating the spatial wavefunctions into their \( \psi_0 \) and \( \psi_1 \) constituents (corresponding respectively to \( \phi_0 \) and \( \phi_1 \)). We have plotted a temporal progression of these wavefunctions in Fig. 7 for the \( w = 0 \) case (Figs. 7(a)-(c)) and for \( w = 2500 w_0 \) (Figs. 7(d)-(f)). For the latter case we have \( \mu = 8.26 \hbar \omega_T \) and \( V = 10 \omega_T \), so that condition (33) is satisfied. It is evident that there is very good agreement between the linear and nonlinear cases in all the qualitative features, with the main difference perhaps being the smoothing of the sharpest features in the nonlinear case.
FIG. 7. Comparison of Bragg scattered spatial wavefunctions in linear and nonlinear condensates. The solid curve represents $\psi_0$ and the dotted curve $\psi_1$. (a)-(c): $w = 0$. (d)-(f): $w = 2500w_0$. Light field parameters are $V = 10\omega_T$, $\delta = 196\omega_T$, $\Delta k_z = 14/r_0$.

Finally we illustrate in Fig. 8 how the linear analysis progressively fails as $\mu$ approaches and then exceeds $\hbar V$. We plot for the range of $w$ values given in Table 1 the time evolution of, $P_0$, the total population in the 0th momentum domain, which is defined according to

$$P_n = \int dk_x \int dk_y \int dq_z |\phi_n(q)|^2.$$  \hspace{1cm} (34)

The linear case is shown as a solid line, and is in close agreement with the $w = 250w_0$ case, and in reasonable agreement with the $w = 2500w_0$ case. However for the $w = 25000w_0$ case, where $\mu$ significantly exceeds $\hbar V$, significant disagreement occurs after the first half cycle. We note that by using $P_0$ rather that $\phi_0(q_z)$ as our basis of comparison, we have minimised the discrepancy that would occur simply from the repulsive expansion.
Fig. 8. Temporal evolution of the population of the 0th momentum domain, for different condensate nonlinearities. \( w = 0 \) solid, \( w = 250 \) dashed, \( w = 2500 \) dash-dot, and \( w = 25000 \) dotted. Light field parameters are as in Fig. (7).

| \( w \) | \( w_0 \) | \( \mu \) | \( \hbar \omega_T \) | \( \tau_E \) | \( 1/\omega_T \) |
|---|---|---|---|---|---|
| 0 | 0 | \( \infty \) |
| 250 | 3.814 | 0.8 |
| 2500 | 8.258 | 0.37 |
| 25000 | 20.42 | 0.15 |

Table: 1 Chemical potentials and expansion time constants for the eigenstates used in section V.C.

VI. MOMENTUM SPECTROSCOPY

The NIST and MIT groups recently reported experiments [4, 6] where Bragg scattering was used to directly measure the momentum composition of condensates. The formalism set out in this paper provides an appropriate framework for the description of those results. Bragg scattering can be used to selectively couple out a portion of the momentum states from a wavepacket, provided the momentum width \( \sigma_k \) of the Bragg transition is less than the momentum width \( \delta k_w \) of the initial wavepacket. The width \( \sigma_k \) is controlled primarily by the laser intensity, and it is easy to see from Eq. (29) that for the purposes of momentum spectroscopy, we require the laser intensity to be chosen such that

\[
V < (\hbar |\Delta k|/4m) \delta k_w.
\]  

We illustrate such a case in Fig. 9 where a low intensity, high momentum coupling causes a narrow fraction of the initial momentum distribution to be out-coupled.
FIG. 9. Momentum spectroscopy. The momentum wavefunction along the symmetry axis of the condensate is shown at \( t = 0.5/\omega_T \). The out coupled state (centred at \( k_z = 20/r_0 \)) is much narrower than the initial packet which is centred at \( k_z = 0 \). Parameters are \( w = 2500 w_0, V = 5\omega_T, \Delta k = 20/r_0 \) and \( \delta = 400\omega_T \).

In the experiments reported by the NIST group, momentum selectivity was obtained by allowing the condensate to ballistically expand before the application of the light grating, so that the self repulsion broadens the momentum distribution to be larger than the Bragg line width \( \sigma_k \). The MIT group achieve precise momentum selectivity by using very low intensity lasers, which allows them to analyse the narrow momentum distribution of a trapped condensate. The MIT group have also been able to measure the shift of the resonant point of the Bragg transition, which was discussed in section [V] and is calculated to be \[ \Delta \delta = \frac{4\mu}{7\hbar} \] in the regime of their experiments.

\[
\Delta \delta = \frac{4\mu}{7\hbar}
\]

Our simulations confirm this expression. Fig. 10 presents the results for the out-coupled population in a sequence of simulations where the detuning \( \delta \) of the two Bragg fields is scanned through a range, while the other field parameters are kept constant. The solid line joins the simulation data points for the linear case \( (w = 0) \), while the dotted line joins the data points for the case \( w = 2500w_0 \). In each case, the Bragg pulse is applied for a time \( T = 0.5/\omega_T \) while the condensate is still in the trap. The two curves have different shapes because the initial momentum wavepackets are different for the two cases, but the offset of the peaks, which represents the nonlinear shift of the Bragg resonance is measured to be \( \sim 5\omega_T \), which is in very good agreement with Eq. (36).
FIG. 10. The total population $P_1$ (as defined in Eq. (34)) coupled into the $\phi_1$ wavepacket as a function of $\delta$ for a $w = 0$ condensate (solid line) and a $w = 2500 w_0$ condensate (dotted) as a function of $\delta$. Parameters of the field are $\Delta k = 6/r_0$, $V = 2\omega T$, and it is applied for a time $T = 0.5/\omega T$, while the harmonic trap still remains on.

VII. CONCLUSION

In this paper, we have presented in detail a meanfield formalism for Bragg scattering in Bose condensates. Starting from the two-component Gross-Pitaevskii equation driven by a far detuned classical light field, we obtained a one-component equation which provides a framework for treating the scattering of trapped or untrapped condensates from an arbitrary light field grating. We have concentrated on the Bragg regime, and solved the one component equation in a number of situations using three dimensional cylindrically symmetric numerical simulations. For the case of Bragg scattering from a condensate released from a trap, the dominating behaviour is the oscillation of the atomic momentum components between an initial value $k_i$ and a shifted value $k_i + \Delta k$. We presented an alternative derivation of linear Bragg scattering based on a partitioned representation of the momentum wavefunction and incorporating spatial nonuniformity, and used this to analyse the full nonlinear system. We showed that this linear model gives an accurate description of the nonlinear system within a well defined validity regime. Dispersion curves in the partitioned momentum representation facilitated visualisation of the possible couplings that may occur, including first and higher order Bragg resonances. We also derived an analytic expressions for the momentum transition linewidth, and used this to define the regime of momentum spectroscopy. Finally, we used numerical simulations to investigate Bragg scattering from a condensate in a trap, and to calculate the nonlinear shift of the Bragg resonance frequency.

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APPENDIX A: ADIABATIC ELIMINATION

Eqs. (3) and (4) detail the EM field coupling, in the dipole approximation, between the meanfields in the internal states $|g\rangle$ and $|e\rangle$ respectively. By defining a new excited meanfield amplitude

$$\tilde{\psi}_e(r, t) = e^{i\omega_1 t} \psi_e(r, t),$$

the evolutions equations are transformed to
\[ i\hbar \frac{\partial \tilde{\psi}_g}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \tilde{\psi}_g + V_{Tg}(\mathbf{r}, t) \tilde{\psi}_g - \frac{1}{2} \hbar \Omega_0(t) \Lambda(\mathbf{r}, t) e^{-i\omega t} \tilde{\psi}_e \] (A2)

\[ + (w_{yg}|\psi_g|^2 + w_{eg}|\tilde{\psi}_e|^2) \tilde{\psi}_g, \]

\[ i\hbar \frac{\partial \tilde{\psi}_e}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \tilde{\psi}_e + V_{Te}(\mathbf{r}, t) \tilde{\psi}_e - \frac{1}{2} \hbar \Omega_0(t) \Lambda(\mathbf{r}, t) e^{i\omega t} \psi_g \] (A3)

\[ -\hbar \Delta \tilde{\psi}_e + (w_{eg}|\psi_g|^2 + w_{ee}|\tilde{\psi}_e|^2) \tilde{\psi}_e, \]

where we have introduced the detuning \( \Delta = \omega_1 - \omega_{eg} \).

For an initial configuration with the ground state fully occupied, we make the approximations that in the region of significant condensate density the magnitude of \( \Delta \tilde{\psi}_e \) greatly exceeds those of \( w_{ee}|\tilde{\psi}_e|^2, \hbar^2 \nabla^2 \tilde{\psi}_e/2m, w_{eg}|\psi_g|^2, \tilde{\psi}_e \) and \( V_{Te}(\mathbf{r}, t) \tilde{\psi}_e \) (which can always be arranged by choosing \( \Delta \) sufficiently large), so that these latter three terms can be dropped from Eq. (A3) allowing the following approximate formal solution

\[ \tilde{\psi}_e(\mathbf{r}, t) \approx +\frac{i}{2} \int_0^t \left\{ e^{i(\Delta t - s)} \Lambda^*(\mathbf{r}, s) e^{i\omega_1 s} \right\} \Omega_0(s) \psi_g(\mathbf{r}, s) \, ds. \] (A4)

The adiabatic elimination of the excited state proceeds by noting that while \( |\Omega_0| \ll |\Delta| \) and \( |\Omega_0'(t)| \ll |\Delta \Omega_0(t)| \), \( \Omega_0(s) \psi_g(\mathbf{r}, s) \) is much more slowly varying in time than the terms in the braces in the integrand of Eq. (A4), which vary at least as fast as \( e^{i\Delta s} \). This means the main contribution to the integral arises near the end point, and so \( \Omega_0(t) \psi_g(\mathbf{r}, t) \) may be taken outside the integral as \( \Omega_0(t) \psi_g(\mathbf{r}, t) \), i.e.

\[ \tilde{\psi}_e(\mathbf{r}, t) \approx \frac{\Omega_0(t)}{2i} \psi_g(\mathbf{r}, t) e^{i\Delta t} \int_0^t e^{-i\Delta s} \left\{ e^{i(k_1 \cdot \mathbf{r} - (\omega_2 - \omega_1) s)} + e^{-i(k_1 \cdot \mathbf{r} - (\omega_2 - \omega_1) s)} e^{-i(k_2 \cdot \mathbf{r} - (\omega_2 + \omega_1) s)} \right\} ds. \] (A5)

The rotating wave approximation (RWA) is now made, in which we neglect the last two rapidly varying terms in Eq. (A5). The resulting approximate solution to Eq. (A4) is

\[ \tilde{\psi}_e(\mathbf{r}, t) \approx -\frac{\Omega_0(t)}{2\Delta} \left( e^{i(k_1 \cdot \mathbf{r} - (\omega_2 - \omega_1) t)} \right) \psi_g(\mathbf{r}, t), \] (A6)

which can be substituted into Eq. (A2) to give

\[ i\hbar \frac{\partial \psi_g}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi_g + \frac{\hbar |\Omega_0(t)|^2}{4\Delta} \left( e^{i(k_1 \cdot \mathbf{r} - \omega t)} + e^{i(k_2 \cdot \mathbf{r} - \omega t)} \right) \Lambda(\mathbf{r}, t) \psi_g \] (A7)

The RWA is again be applied to Eq. (A7), rejecting terms oscillating at optical frequencies. This leads to an optical potential of the form

\[ \frac{\hbar |\Omega_0(t)|^2}{2\Delta} \left[ 1 + \cos(\Delta \mathbf{k} \cdot \mathbf{r} - \delta t) \right]. \] (A8)

Finally the phase choice \( \psi = \exp(-i \int_0^t V(s) ds) \psi_g \), removes the D.C term from this potential and yields Eq. (A6).

**APPENDIX B: MOMENTUM EXPANSION TIME CONSTANT**

Here we derive the approximate expression (Eq. (23)) for the time constant of momentum space expansion of a BEC. To do this we consider the transfer of self energy to kinetic energy for a freely expanding spherically symmetric condensate in the Thomas-Fermi limit. It is convenient to do this calculation in dimensionless units (see section IA).

Writing the full momentum wavefunction as

\[ \phi(k, t) = \varphi(k, t)e^{iS(k, t)}, \] (B1)

where \( \varphi(k, t) \) and \( S(k, t) \) are real, we then approximate the amplitude \( \varphi \) of the momentum space wavefunction as a gaussian,

\[ \phi(k, t) = \varphi(k, t) e^{-\frac{1}{2\Delta} \left( k^2 k^2 \right)} \]

where \( \Delta \) is the width of the wavefunction at half-maximum intensity. The motion of the phase \( t \) is then

\[ \Delta \approx \frac{\hbar^2}{2m} \] (B2)

where \( \hbar \) is the reduced Planck constant.

\[ t \approx \frac{\hbar}{2m} \] (B3)

Finally, the phase \( t \) is

\[ t \approx \frac{\hbar}{2m} \] (B4)

where \( \hbar \) is the reduced Planck constant.
\[ \varphi(k, t) = \left( \frac{3}{2\pi \sigma^2} \right)^{\frac{3}{2}} e^{-\frac{3k^2}{4\sigma^2}}. \]  

(B2)

The time dependence of \( \varphi \) is contained in the function \( \sigma(t) \), the standard deviation of \( \varphi^2 \) (i.e. \( |\varphi|^2 \)). The kinetic energy of \( \phi \) depends only on \( \varphi \), and can be evaluated explicitly to give

\[ \langle KE \rangle = \int_0^\infty 4\pi k^2 k^2 |\varphi(k, t)|^2 dk = 3\sigma(t)^2. \]  

(B3)

We shall use Eq. (B3) to attribute a momentum width to a system whose kinetic energy is known.

During expansion, the total energy, consisting of the self energy and the kinetic energy is conserved, so that the gain in kinetic energy will be equal to the decrease in self energy. We now proceed to calculate the time dependent behaviour of the self energy.

At \( t = 0 \) the harmonic trap is turned off and the initial condensate density profile can be closely approximated by the Thomas-Fermi result

\[ n_{TF}(r) = \frac{\mu - r^2}{w}, \]  

(B4)

where \( 0 < r < 2\sqrt{\mu} \), and

\[ \mu = \left( \frac{15w}{64\pi} \right)^{\frac{2}{3}}. \]  

(B5)

Castin and Dum [22] have shown that in the Thomas-Fermi approximation the spatial profile of a spherically symmetric released BEC behaves as

\[ n(r, t) = b^{-3}(t) n_{TF}(r/b(t)), \]  

(B6)

where

\[ b(t) = \sqrt{1 + t^2}. \]  

(B7)

We use this expression to find the time dependent self energy,

\[ \langle SE \rangle(t) = \int_0^{2b(t)\sqrt{\pi}} 4\pi r^2 \left[ \frac{w}{2} n(r, t)^2 \right] dr, \]  

(B8)

\[ = \frac{1}{14} \left( \frac{15w}{2\pi} \right)^{\frac{2}{3}} \frac{\frac{2}{3}}{(1 + t^2)^{-\frac{1}{3}}}, \]  

(B9)

and from this can from this we can write an expression for the KE as a function of time,

\[ \langle KE \rangle(t) = \langle KE \rangle_i + \langle SE \rangle(0) - \langle SE \rangle(t). \]  

(B10)

An approximation for the initial value of the kinetic energy \( \langle KE \rangle_i \) can be found by calculating the spatial wavefunction corresponding to \( \varphi \) and matching its variance to that of the initial Thomas-Fermi profile of Eq. (B4). This gives us an estimate of \( \sigma(0) \), which from Eq. (B3) yields the initial kinetic energy

\[ \langle KE \rangle_i = \left( \frac{7}{2} \right)^{\frac{3}{2}} \left( \frac{3}{2} \right)^{\frac{2}{3}} \left( \frac{\pi}{5w} \right)^{\frac{2}{3}}. \]  

(B11)

Now using Eq. (B10) and the expression \( \langle KE \rangle = 3\sigma^2(t) \) we obtain the time dependent momentum variance

\[ \sigma^2(t) = \left( \frac{7}{6} \right)^{\frac{3}{2}} \left( \frac{\pi}{5w} \right)^{\frac{2}{3}} \left( \frac{1}{42} \left( \frac{15w}{2\pi} \right)^{\frac{2}{3}} \right) \left( 1 - (1 + t^2)^{-\frac{1}{3}} \right). \]  

(B12)

Defining the time constant, \( \tau_E \), to be the time it takes for the width \( \sigma \) to double, we obtain
\[ \tau_E = \frac{\sqrt{1 - (1 - \alpha)^{3/2}}}{(1 - \alpha)^{3/2}}, \quad (B13) \]

where

\[ \alpha = 147 \left( \frac{3}{2} \right)^{3/4} \left( \frac{\pi}{5w} \right)^{1/4}. \quad (B14) \]

This derivation is only valid when the Thomas-Fermi approximation is valid, in which case \( \alpha \) is a small parameter, and Eq. \((B13)\) can be expanded in inverse powers of \( \mu \) (i.e. \( \alpha^{3/2} \)). To first order in \( \mu^{-1} \) this gives

\[ \tau_E \approx \frac{2\alpha}{3} = \frac{1}{\mu} \left( \frac{7\sqrt{3}}{4} \right). \quad (B15) \]

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