Vortices in the Wake of Rapid Bose-Einstein Condensation

J. R. Anglin[1,2] and W. H. Zurek[2]
[1]*Institut für Theoretische Physik, Universität Innsbruck, Technikerstrasse 25, 6020 Innsbruck, Austria*
[2]*T-6 (Theoretical Astrophysics), MS B288, Los Alamos National Laboratory, Los Alamos, New Mexico 87545*
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A second order phase transition induced by a rapid quench can inject far more topological defects into the ordered phase than would appear in equilibrium. We use quantum kinetic theory to show that this mechanism, originally postulated in the cosmological context, and analyzed so far only on the mean field classical level, should allow spontaneous generation of vortex lines in trapped Bose-Einstein condensates of simple topology, or of winding number in toroidal condensates.

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An as yet unachieved goal of experiments on trapped ultracold alkali gases [1–3] is the exhibition of a persistent vortex. Superfluid vortices persist because there is an energetic barrier between the metastable vortex state and the nonrotating ground state, and so spinning up a condensate is inherently difficult [4]. Here we propose a different approach: cooling so quickly that the system is trapped in the metastable state before reaching the ground state. Our reasoning is based on the *critical slowing down* of the dynamics of the order parameter in the vicinity of a second order phase transition [5]: we consider time-dependent Ginzburg-Landau theory (TDGL) adapted to the Bose-Einstein condensation (BEC) case. The complex order parameter $\psi(\vec{r},t)$ obeys

$$\tau_0\dot{\psi} = \beta[\hbar^2(2M)^{-1}\nabla^2 + \mu - \Lambda|\psi|^2]\psi\,, \qquad (1)$$

where $\beta = (k_BT)^{-1}$, and τ_0 and $\Lambda > 0$ are phenomenological parameters. The thermodynamical variable μ behaves near the critical point, in the case we consider, as

$$\mu = \frac{3}{2}(T_c - T) + \mathcal{O}(T_c - T)^2, \qquad (2)$$

where T_c is the critical temperature. The equilibration time for long wavelengths is $\tau = \tau_0 k_B T/|\mu|$. The system's disordered phase is described by $\mu < 0$, so that $\psi = 0$ is a stable fixed point of (1). The ordered phase has $\mu > 0$, with stable fixed points on the circle $|\psi|^2 = \mu/\Lambda$, and the phase θ of $\psi = |\psi|e^{i\theta}$ a macroscopic variable.

A quench occurs if μ changes with time from negative to positive values. The divergence of the equilibration time τ at the critical point $\mu = 0$ is associated with *critical slowing down*. Because of this critical slowing down, $\dot{\mu}/\mu$ must exceed $1/\tau$ in some neighborhood of the critical point, and so there must be an epoch in which the system is out of equilibrium. What are at the beginning of this epoch mere fluctuations in the disordered phase can thus pass unsuppressed by equilibration into the ordered phase, to seed topologically nontrivial configurations of ψ. One therefore expects persistent currents and vortices to form spontaneously during a rapid quench [5].

The interval within which equilibration fails can be identified as $|t|/\tau < 1$. If we define the quench time scale τ_Q by letting $\beta\mu = t/\tau_Q$ (choosing $t = 0$ as the moment the system crosses the critical point), this implies that the crucial interval is $-\hat{t} < t < \hat{t}$, for $\hat{t} = \sqrt{\tau_Q\tau_0}$ [5]. The correlation length $\hat{\xi}$ for fluctuations at time $t = -\hat{t}$ is then given by $\hbar^2/(2M\hat{\xi}^2) = \mu(-\hat{t})$, which [assuming $T(-\hat{t}) \doteq T_c$] implies that $\hat{\xi} = \lambda_{T_c}(\tau_Q/\tau_0)^{1/4}$, for $\lambda_T = \hbar(2Mk_BT)^{-1/2}$ the thermal de Broglie wavelength. Taking $\hat{\xi}$ as the typical domain size surrounding a defect [6] implies that the vortex line density should scale with $\tau_Q^{-1/2}$ [5]. In a toroidal sample, independent random settings of the order parameter phase, at different points around the torus, can produce a net *winding number*, $W = \frac{1}{2\pi}\oint \vec{d}l\cdot\vec{\nabla}\theta$, proportional to $\tau_Q^{-1/8}$ [5]. This implies a superfluid velocity $\hbar\vec{\nabla}\theta/M$ [7].

Although ingenious experiments have recently been performed to test this theory in liquid helium [8], and numerical studies have supported its scaling predictions [9], analogous results in a weakly interacting system, such as a dilute trapped gas, would be even more instructive. Assuming τ_0 is the scattering time, evaporative cooling techniques yield $(\tau_Q/\tau_0)^{1/4}$ of order one, and so $\hat{\xi}$ is essentially λ_{T_c}. For atoms at several hundred nK, this means $\hat{\xi} \sim 100$ nm, smaller than current condensates. As simulations show [9], this is actually a generously low lower bound on the distance between vortex lines given by TDGL theory, but it does indicate that spontaneous vorticity should be within experimental reach. Considering this intriguing prospect raises an obvious question: is TDGL actually relevant to dilute Bose gases in traps?

To assess TDGL in this new domain, therefore, we consider a trapped dilute Bose gas with the Hamiltonian

$$\hat{H} = \frac{\hbar^2}{2M}\int d^3r\,[|\vec{\nabla}\hat{\psi}|^2 + U(\vec{r})\hat{\psi}^\dagger\hat{\psi} + 4\pi a\hat{\psi}^{\dagger 2}\hat{\psi}^2], \qquad (3)$$

where $\hat{\psi}(\vec{r})$ annihilates a boson at position $\vec{r}$, U gives the trap potential, and a is the s-wave scattering length. As always, $\hat{\psi}(\vec{r}) = \sum_k u_k(\vec{r})\hat{\psi}_k$ defines a decomposition of the system into orthogonal modes described by single-particle wave functions u_k. In the earliest stages of condensation, it is sufficient to take the single-particle energy eigenstates as defining the normal modes of the gas.

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We now construct a quantum kinetic theory (QKT), by treating the lowest energy modes of the trap, up to some energy E_R, as an open quantum system (the "condensate band"), interacting via two-particle s-wave scattering with the higher modes (the "reservoir band"), which are traced over [10]. In the earliest stages of condensation, before nonlinear interactions within the condensate band become important, this leads to a master equation:

$$\dot{\hat{\rho}} = \sum_k \left(\frac{E_k}{i\hbar} [\hat{n}_k, \hat{\rho}] + \Gamma_k e^{\beta\mu} \left[e^{\beta(E_k-\mu)} \hat{a}_k \rho \hat{a}_k^\dagger + \hat{a}_k^\dagger \rho \hat{a}_k - \frac{1 + e^{\beta(E_k-\mu)}}{2} (\hat{n}_k \hat{\rho} + \hat{\rho} \hat{n}_k) - \hat{\rho} \right] \right), \quad (4)$$

where E_k are the energies of the normal modes. The Γ_k are scattering rates, which will generally be of the order of the Boltzmann scattering rate. We actually expect the k dependence of the Γ_k to be weak as long as the temperature is much larger than the trap level spacing, so we will hereafter replace Γ_k with Γ_0, which will play exactly the same role as $1/\tau_0$ did in TDGL. The non-Hamiltonian part of (4) is due to collisions which transfer particles between condensate and reservoir bands.

An ansatz which solves (4) is furnished by

$$\hat{\rho}(t) = \prod_k \frac{1}{\bar{n}_k + 1} \sum_{n_k} \left(\frac{\bar{n}_k}{\bar{n}_k + 1} \right)^{n_k} |n_k\rangle\langle n_k|, \quad (5)$$

where $\bar{n}_k(t) = \mathrm{Tr}(\hat{\rho}\hat{n}_k)$. By (4), the $\bar{n}_k(t)$ evolve under

$$\dot{\bar{n}}_k = \Gamma_0 e^{\beta\mu} [1 + (1 - e^{\beta(E_k-\mu)}) \bar{n}_k]. \quad (6)$$

This equation may be integrated for general $\Gamma_0(t)$, $\beta(t)$, $\mu(t)$. Near the critical point, however, we can impose $\beta(t)[\mu(t) - E_k] = (t - \vartheta_k)/\tau_Q$, defining τ_Q as well as the bias time scales ϑ_k. The $\bar{n}_k(t)$ that result, from the equilibrium initial values $\bar{n}_k(t_i) = (e^{\beta(t_i)[E_k - \mu(t_i)]} - 1)^{-1}$, are incomplete gamma functions; they depart significantly from their equilibrium values after $t - \vartheta_k \simeq -\sqrt{\tau_Q/\Gamma_0} = -\hat{t}$. Past these points, the $\bar{n}_k$ lag below their equilibrium values. This clarifies the effect of the critical slowing down: as Bose enhancement turns on, the rates of scattering into the condensate increase; but the numbers of particles required by equilibrium increase faster still.

Thereafter, we approximate $(1 - e^{\beta(E_k-\mu)}) \doteq (t - \vartheta_k)/\tau_Q$ and match to equilibrium at early times, to get

$$\bar{n}_k(t) \doteq \Gamma_0 e^{(1/2\hat{t}^2)(t-\vartheta_k)^2} \int_{-\infty}^{t-\vartheta_k} dt' \, e^{-(1/2\hat{t}^2)t'^2}. \quad (7)$$

For times after $t - \vartheta_k \simeq \hat{t}$, each $\bar{n}_k$ grows explosively, because the atomic scattering analog of stimulated emission into the kth mode is turning on strongly: $\bar{n}_k$ is becoming large enough that the term proportional to it on the right-hand side of (6) dominates the other term. Bose-enhanced scattering then enables the mode to begin a very rapid "whiplash" to catch up with equilibrium. So the interval $\vartheta_k - \hat{t} < t < \vartheta_k + \hat{t}$ is indeed a transition zone between equilibrium above T_c and the onset of coherent processes below T_c. It is obvious that, for a higher energy mode to have any significant chance of competing successfully for particles with the lowest mode, it cannot afford to begin explosive growth much later than the lowest mode. This implies that $\vartheta_k < \hat{t}$, or $\beta E_k < (\Gamma_0\tau_Q)^{-1/2}$, limits the range of significantly competitive modes. Since in bulk or in a toroidal trap we have $E_k \propto k^2$, this gives

$$\hat{\xi} = \hat{k}^{-1} = \hbar(2Mk_BT_c)^{-1/2}(\Gamma_0\tau_Q)^{1/4}, \quad (8)$$

which is the same conclusion reached by TDGL above.

In the toroidal trap, we can consider the Fourier modes in the coherent state basis $|\{\psi_k\}\rangle$. Density matrices of the form (5) can be taken to describe mixtures of coherent states, with probabilities proportional to $\exp - \sum_k \frac{1}{\bar{n}_k}|\psi_k|^2$. While W is *not* a simple function of ψ_k, there are as many independent random phases as non-negligible $\bar{n}_k(\hat{t})$, so we expect winding numbers of order $(\hat{k}R)^{1/2}$, for R the radius of the torus [5].

Thus far QKT and TDGL agree: for sufficiently rapid quenches the probability of forming a small "seed" of condensate with nonzero vorticity is of order one. But since superfluid currents become metastable only above a threshold density, not all of this vorticity will survive as the condensate grows. Predicting how much of it will be lost requires a quantum kinetic theory of competing protocondensates; no such theory as yet exists. We present here a simple toy model, within which we can compare TDGL and QKT beyond the linear regime.

The toy model replaces the condensate band of low energy modes with a mere two modes, having two different angular momenta. Because the self-Hamiltonian for this two-mode system must conserve both particle number and angular momentum, it must conserve separately the numbers of particles in both modes:

$$\hat{H} = E[\hat{n}_1 + (2N_c)^{-1}(\hat{n}_0^2 + \hat{n}_1^2 + 4\hat{n}_1\hat{n}_0)]. \quad (9)$$

The Bose enhancement of intermode repulsion (the factor of 4 instead of 2 in the $\hat{n}_0\hat{n}_1$ term, the best case value obtained when $|u_0|^2$ and $|u_1|^2$ overlap completely) makes the state with all particles in the 1 mode a local minimum of the energy for fixed $n_0 + n_1 > (N_c + 1)$. For two lowest modes of a typical oblate magneto-optical trap, we have βE of order 10^{-2}; for proposed toroidal traps with perimeter of order 10^{-2} cm, at similar temperatures, βE could be as low as 10^{-5}. (Rotating the gas before condensation could even favor rotating states over the ground state.) The experimental range of N_c is around 100 for compact traps, but as low as 1 for the torus.

We also assume interactions between both condensate modes and the quasicontinuum of reservoir modes, of the form implied by the Hamiltonian (3). Upon tracing over the dilute gas reservoir, we obtain a master equation of more complicated form than (4), which includes saturation effects, as well as scattering of reservoir atoms off the condensate (with no net change in the condensate number). We will need only the equation's diagonal part:

$$\begin{aligned}
\dot{p}_{n_0,n_1} &= -\Gamma(t)[R_{n_0,n_1} - R_{n_0-1,n_1} + S_{n_0,n_1} - S_{n_0,n_1-1}] - \tilde{\Gamma}(t)[T_{n_0+1,n_1} - T_{n_0,n_1+1}],\\
R_{n_0,n_1} &\equiv (n_0 + 1)[e^{\beta\mu} p_{n_0,n_1} - e^{(\beta E/N_c)(n_0+2n_1)} p_{n_0+1,n_1}],\\
S_{n_0,n_1} &\equiv (n_1 + 1)[e^{\beta\mu} p_{n_0,n_1} - e^{(\beta E/N_c)(N_c+2n_0+n_1)} p_{n_0,n_1+1}],\\
T_{n_0,n_1} &\equiv n_0 n_1 e^{-1/2(\beta E/N_c)|N_c+n_0-n_1|}[e^{1/2(\beta E/N_c)(N_c+n_0-n_1)} p_{n_0-1,n_1} - e^{-1/2(\beta E/N_c)(N_c+n_0-n_1)} p_{n_0,n_1-1}],
\end{aligned} \tag{10}$$

where $\Gamma(t)$ and $\tilde{\Gamma}(t)$ are again scattering rates (for scattering into/out of the condensate, and off the condensate, respectively) which may be computed for any specific gas and trap. We will hereafter assume $\tilde{\Gamma} = \beta E \Gamma$, which is accurate for simple trap configurations when the temperature is much larger than the trap level spacing.

Equation (10) provides a complete description of condensation in the toy model, including initial seeding from fluctuations, coherent growth, relaxation into metastable states, and eventual equilibration by thermal barrier crossing. For present purposes we merely extract from it an equation of motion for n_0 and n_1, by taking $n_0 \to Nx$ and $n_1 \to Ny$ for continuous x and y and N of order $(\beta E)^{-1}$. Expanding the finite differences in (10) in powers of derivatives with respect to x and y, one obtains a Fokker-Planck-like equation, the Liouville terms of which describe a flow along deterministic trajectories in (x, y) space. Dropping higher order terms in $1/N$ (since these are significant only at small n_0, n_1, when diffusion dominates systematic evolution but we are able to use the linear analysis described above), these trajectories obey

$$\begin{aligned}
\dot{n}_0 &= \Gamma n_0\left[e^{\beta\mu} - e^{(\beta E/N_c)(n_0+2n_1)} + 2\beta E n_1 e^{-(\beta E/2N_c)|N_c+n_0-n_1|}\sinh\frac{\beta E}{2N_c}(N_c + n_0 - n_1)\right],\\
\dot{n}_1 &= \Gamma n_1\left[e^{\beta\mu} - e^{(\beta E/N_c)(N_c+n_1+2n_0)} - 2\beta E n_0 e^{-(\beta E/2N_c)|N_c+n_0-n_1|}\sinh\frac{\beta E}{2N_c}(N_c + n_0 - n_1)\right].
\end{aligned} \tag{11}$$

While this approximation of the master equation offers the obvious comparison with TDGL, it is of course a bold truncation of the physics, since it ignores diffusion in n_j. Such diffusion can in fact be analyzed by well established methods; if it dominates the systematic evolution described in (11), however, it leads to nucleation of the metastable state by thermal barrier crossing, rather than by the critical slowing down mechanism on which we focus here. We therefore consider the case in which diffusion is only significant during the early epoch before $\hat{t}$, so that the linear analysis described above can be used to generate a distribution of initial data at $\hat{t}$, which will then flow under (11). A fuller investigation of the master equation confirms that this case obtains for fast quenches and small biases: with $\Gamma\tau_Q = 10$ diffusion is weak for $\beta E = 10^{-2}$, and clearly insignificant for $\beta E = 10^{-3}$.

Having established that the systematic evolution of (11) provides a good description, after $\hat{t}$, of a fast quench in the toy model, we can now compare it to the TDGL evolution. When $n_0 + 2n_1$ and $N_c + n_1 + 2n_0$ are both close to $N_c\mu/E$, or for low enough particle numbers, we may replace $n_j \to |\psi_j|^2$ in the first two terms in each equation of (11) to obtain a TDGL equation, in the sense that $\dot{\psi}_j$ is set equal to the variation of a Ginzburg-Landau effective potential with respect to ψ_j^*. But the last term in each equation is not of Ginzburg-Landau form (it does not even involve μ). These non-GL terms conserve $n_0 + n_1$, and describe doubly Bose-enhanced dissipation due to scattering of reservoir particles off the condensate. They turn out to imply that the system equilibrates in energy faster than it equilibrates in particle number.

Representative solutions to (11) are shown in Fig. 1, together with the $|\psi_j|^2$ given by the TDGL theory formed by keeping only the first two terms of each equation in (11) and expanding the exponentials to first order only. It is clear that, for sufficiently fast quenches, the two theories accord quite well, but that for slower quenches TDGL

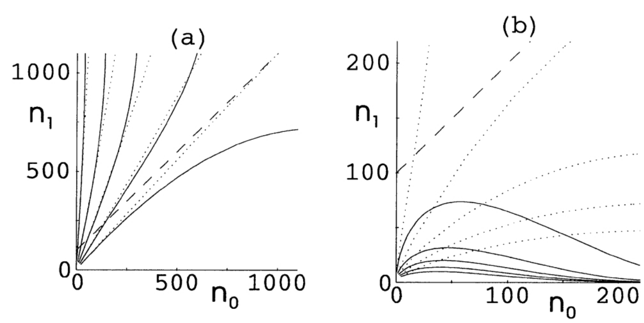

FIG. 1. Trajectories from QKT (solid) and TDGL (dotted); heavy dashed line is threshold for metastability of mode 1. Initial times are $\hat{t}$; quench is $\beta\mu = \tanh(t/\tau_Q)$, $\beta = \beta_c e^{\tanh(t/\tau_Q)}$. Parameters are $N_c = 100$, and (a) $\Gamma\tau_Q = 10$, $\beta_c E = 0.01$; (b) $\Gamma\tau_Q = 100$, $\beta_c E = 0.05$. The two theories agree better for the faster quench, simply because the intermode scattering neglected in TDGL has less time to act before metastability is attained.

significantly overestimates the probability of reaching the metastable state. If our two modes are taken to be different Fourier modes in a toroidal trap, the vorticity of a state is simply the vorticity of the more populated mode, so that the line $n_0 = n_1$ is the border between vorticities; all initial points in Fig. 1 are above this line. So not even TDGL evolution conserves vorticity, but the QKT evolution changes it more easily, especially for slower quenches.

The major addition to TDGL coming from QKT is the doubly Bose-enhanced scattering of particles between modes of the condensate band by reservoir particles. Although phase space factors suppress these processes with a factor of order βE (it is unlikely for a slow particle to remain slow after being hit by a fast particle), they become more important as the condensate grows. Their significance even calls into question our Eq. (4), from which we recovered the TDGL predictions for very young condensates, because it does not include them.

Adding intermode scattering to (4) makes an intractable operator equation; but we can obtain from it a simpler set of equations for $\bar{n}_k(t)$, by setting $\overline{n_j n_k} \rightarrow \bar{n}_j \bar{n}_k$. With the new terms, this is now only an approximation (and one that cannot describe multiple peaks in the probability distribution of the n_k, which is our whole question); but it allows quantitative assessment of the new terms' importance. These equations for the $\bar{n}_k$ have recently been derived by Gardiner *et al.* [11], for a harmonic trap. From them one can see that the relative importance of intermode scattering declines for a smaller condensate band: if $E_R = \eta k_B T (\Gamma \tau_Q)^{-1/2}$, then until times of order $\hat{t}$ the contribution to $\bar{n}_k$ from intermode scattering is a fraction of order η^2 times that given by our (4). This implies that, although one might have to lower the TDGL estimate of $\hat{k}$ by a factor of order unity, (4) indeed describes well the earliest stages of competition for the condensate among eligible modes.

There is, however, a significant consequence of thus lowering E_R: the lower portion of the reservoir will no longer remain in equilibrium as it cools. Nevertheless, numerically solving the equations of Ref. [11], with various E_R up to $k_B T$ and with our time-dependent $\mu(t)$, shows that until times of order $\hat{t}$ all the $\bar{n}_k(t)$ may be reproduced to within a few percent by neglecting intermode scattering, but increasing ("renormalizing") both Γ and τ_Q, by factors ranging between 1.5 and 4. These rescalings reflect the two new phenomena at the bottom of the reservoir: super-Boltzmannian population enhances scattering, and critical slowing down slows the quench. Our Eq. (4) may thus be maintained, but the effective dimensionless quench time $\Gamma_0 \tau_Q$ probably cannot be less than around ten. Whether this effect is ascribed to intermode scattering in the condensate band or to the modified state of the reservoir depends on the (unphysical) choice of E_R.

While the extension of quantum kinetic theory beyond toy models, to realistic descriptions of topological defect formation, will obviously require further study, the prospects for experimental realization of spontaneous defects are very encouraging. Estimates from TDGL suggest vortices may already be forming (not necessarily surviving) in harmonic traps. It would be of great interest to carry out BEC formation experiments such as [12] in traps which are sufficiently anharmonic to retain vortex lines and to allow for their detection. Ideal for these purposes is the torus, in which $W \sim 10$ might be typical, and here diffusive nucleation gives a lower bound of typical $W \sim 1$. With 10^6 atoms, even this has an equilibrium probability of order e^{-10}.

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