Winding up by a quench: vortices in the wake of rapid Bose-Einstein condensation

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A second order phase transition induced by a rapid quench can lock out topological defects with densities far exceeding their equilibrium expectation values. We use quantum kinetic theory to show that this mechanism, originally postulated in the cosmological context, and analysed 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 ultra-cold alkali gases is the exhibition of a persistent vortex. Since the reason that superfluid vortices are persistent is that there is a high energetic barrier between the metastable vortex state and the non-rotating true ground state, spinning up a non-rotating condensate once it is fully grown seems likely to be difficult to accomplish without excessive heating. In this Letter we show that it is possible to generate vortices in a rotating condensate even when the quench time scale is longer than the critical slowing down.

An alternative way of thinking about this is in terms of the time it takes to create a vortex. If we define a quench time scale \( \tau_0 \) by letting \( \beta \psi = \mu \tau_0 \psi \) then the transition to occur within a toroidal vessel, so that independent random settings of the order parameter phase, at different points around the torus, can produce a net vorticity, \( W = \frac{\langle \delta \rangle}{\pi} \oint dl \nabla \theta \). This implies a superflow, with velocity \( \hbar \nabla \theta / M \). In this case one estimates one independently chosen phase within each correlation length \( \xi \); modeling the phase distribution around the torus as a random walk suggests that the net vorticity should be proportional to \( \xi^{-1/2} \), hence to \( \tau_0^{-1/8} \).

Although ingenious experiments have recently been performed to test this theory, in liquid helium, and numerical studies have supported its scaling predictions, it would be even more informative to have analogous results in a weakly interacting system, such as a dilute trapped alkali gas. Assuming \( \tau_0 \) is the scattering time, evaporative cooling techniques yield \( (\tau_Q/\tau_0)^{1/4} \) of order one, and so \( \xi \) is essentially \( \lambda T_c \). For atoms at several hun-
dred nK, this means $\hat{\xi} \sim 100$ nm, smaller than current condensates. As numerical simulations show [9] this is a generously low lower bound on the distance between vortex lines, 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 finite samples of dilute gas, far from equilibrium?

We therefore begin again from first principles, and consider a dilute Bose gas in a trap, with the Hamiltonian

$$\hat{H} = \frac{\hbar^2}{2M} \int d^3r \left( \vec{\nabla} \hat{\psi}^2 + U(\vec{r}) \hat{\psi}^\dagger \hat{\psi}^2 + 4\pi a \hat{\psi}^\dagger \hat{\psi}^2 \right)$$  (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 eigenstates as defining the normal modes of the gas.

We now construct a quantum kinetic theory (QKT), by considering the lowest energy modes of the trap, up to some energy $E_R$, to be an open quantum system (the ‘condensate band’), interacting via two-particle s-wave scattering with the higher modes, treated as a ‘reservoir band’ [8]. We model evaporative cooling by prescribing that the reservoir band is always in equilibrium, but with a time dependent temperature $\beta^{-1}(t)$ and chemical potential $\mu(t)$ (which can become positive as long as it remains below $E_R$). We then form the reduced density operator for the condensate band by tracing out the reservoir. The condensate band will not remain in equilibrium with the reservoir; the time evolution of its reduced density operator is the problem to be solved.

In the earliest stages of condensation, before nonlinear coherent interactions become important, one can derive a simple master equation for the condensate band, strongly reminiscent of that of a multi-mode laser:

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

where $E_k$ are the energies of the normal modes. The $\Gamma_k$ are scattering rates, which may be computed; they will generally be of the order of the Boltzmann scattering rate. We actually expect the $k$-dependence of the $\Gamma_k$ to be weak as long as the temperature is much larger than the trap level spacing, so we will hereafter replace $\Gamma_k$ with $\Gamma_0$, which will play exactly the same role as $\hbar/\tau_0$ did in TDGL. The non-Hermitian part of (4) is due to collisions in which one particle leaves or joins the condensate for or from the reservoir.

An ansatz which solves (4) is furnished by

$$\dot{\hat{n}}_k(t) = \Gamma_0 e^{\beta \mu} \left[ 1 + \frac{1 - e^{\beta(E_k - \mu)}}{2} (\hat{n}_k(t) + \hat{\rho}(t)) - \hat{\rho}(t) \right] ,$$  (5)

where $\hat{n}_k(t) = \text{Tr}(\hat{\rho}(t))$. The equation governing the $\hat{n}_k(t)$ follows simply from (5):

$$\hat{n}_k(t) = \Gamma_0 e^{\beta \mu} [1 + (1 - e^{\beta(E_k - \mu)})] \hat{n}_k(0) .$$  (6)

This equation may be integrated for general $\beta(t), \mu(t)$. But as a simple form valid near the critical point, we impose $\beta(t) \mu(t) - E_k = (t - \vartheta_k)/\tau_Q$, defining $\tau_Q$ as well as the bias time scales $\vartheta_k$. The $\hat{n}_k(t)$ that result, from the equilibrium initial values $\hat{n}_k(t_0) = (e^{\beta(t)}(E_k - \mu))^{-1}$, are incomplete Gamma functions; they only begin to depart significantly from their instantaneous equilibrium values after $t - \vartheta_k \approx -\sqrt{\tau_Q/\Gamma_0} = -\hat{\tau}$. Past these points, the $\hat{n}_k$ 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, and so the ability of scattering to maintain equilibrium rapidly declines.

After these times, we can approximate $(1 - e^{\beta(E_k - \mu)}) \approx (t - \vartheta_k)/\tau_Q$ and match to equilibrium at early times, to see that

$$\hat{n}_k(t) \approx \Gamma_0 e^{\beta \mu} \frac{1}{2\pi} \int_{-\infty}^{t-\vartheta_k} dt' e^{-\frac{1}{2\pi}(t-t')^2} ,$$  (7)

For times after $t - \vartheta_k \approx \hat{\tau}$, each $\hat{n}_k$ grows explosively, because the atomic scattering analogue of stimulated emission into the $k$th mode is turning on strongly: $\hat{n}_k$ is becoming large enough that the term proportional to it on the RHS of (4) 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 $\vartheta_k < \hat{\tau} < t < \vartheta_k + \hat{\tau}$ 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 $\vartheta_k < \hat{\tau}$, 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

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

which is the same conclusion reached by TDGL [8].

For the toroidal problem, the density operator prescribed by the linear quantum kinetic theory is equivalent to a distribution of coherent states with probabilities proportional to $\exp - \sum_k \frac{1}{2} \vert \psi_k \vert^2$, for Fourier modes $k$. While $W$ is not a simple function of $\psi_k$, the idea that there are as many independent random phases as non-negligible $\hat{n}_k(\hat{\tau})$ still seems reasonable, and we expect
typical vonctilities of order \( \sqrt{\kappa L/2\pi} \), for \( L \) the perimeter of the torus. This again coincides with the TDGL prediction.

Our conclusion at this point is that QKT agrees with the phenomenological theory, in predicting that for sufficiently rapid quenching the probability of forming a small ‘seed’ of condensate with non-zero vonctility is of order one. But since superfluid currents only become metastable above a threshold condensate density, not all of this initial vonctility will survive as the condensate grows. To follow the non-equilibrium evolution of a trapped condensate into the non-linear regime, with quantum kinetic theory, is a challenging problem. We therefore restrict our analysis to a simple toy model, which affords some qualitative insight, and allows a comparison between TDGL and QKT.

The toy model replaces the condensate band of many low energy modes by a system with only two modes, representing states with 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. We therefore choose

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

Because we have incorporated the Bose enhancement of inter-mode repulsion (the factor of 4 instead of 2 in front of the \( \hat{n}_1\hat{n}_2 \) term, which is of course the best case value, obtained when \( u_0 \) and \( u_1 \) overlap completely), we make the state with all particles in the 1 mode a local minimum of the energy for \( n_1 + n_2 > (N_c + 1) \). For two lowest modes of a typical oblate magneto-optical trap, we have \( \beta E \) of order \( 10^{-2} \); for proposed toroidal traps with perimeter of order \( 10^{-2} \) cm, at similar temperatures, \( \beta E \) could be as low as \( 10^{-5} \). (Rotating the gas before condensation could also lower the effective energy bias, and even favour 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; this does not take into account the Thomas-Fermi expansion of the condensate wave function, which in fact can make \( N_c \) rise significantly at large particle numbers.

We also assume interactions between both condensate modes and the quasi-continuum 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 \((3)\), which includes saturation effects, as well as scattering of reservoir atoms off the condensate (with no resulting change in the condensate number). For present purposes only the diagonal part of this equation is necessary:

\[
\dot{p}_{n_0,n_1} = -\Gamma(t)[R_{n_0,n_1} - R_{n_0-1,n_1} + S_{n_0,n_1} - S_{n_0,n_1-1}]
-\tilde{\Gamma}(t)[T_{n_0+1,n_1} - T_{n_0,n_1+1}]
\]

\[
R_{n_0,n_1} \equiv (n_0 + 1)[e^{\beta \mu}p_{n_0,n_1} - e^{\frac{\beta E}{2N_c}(n_0+2n_1)}p_{n_0+1,n_1}]
S_{n_0,n_1} \equiv (n_1 + 1)[e^{\beta \mu}p_{n_0,n_1} - e^{\frac{\beta E}{2N_c}(N_c+n_0+n_1)}p_{n_0,n_1+1}]
T_{n_0,n_1} \equiv n_0n_1e^{-\frac{\beta \mu}{2N_c}(N_c+n_0-n_1)}[e^{\frac{\beta E}{2N_c}(N_c+n_0-n_1)}p_{n_0-1,n_1}
\]

\[
- e^{-\frac{\beta E}{2N_c}(N_c+n_0-n_1)}p_{n_0,n_1-1} ,
\]

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 condensate-reservoir coupling. We will hereafter assume \( \Gamma = \beta ET \), which is accurate for simple trap configurations when the temperature is much larger than the trap level spacing. (This \( \beta E \) factor justifies neglecting these bouncing-off processes in the linear regime; it appears because most reservoir particles are so much faster than the condensate particles that they are unlikely to strike them without dislodging them from the condensate band.)

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. While it would be straightforward to solve numerically, we can obtain more understanding of the growth process by extracting from it an equation of motion for \( n_0 \) and \( n_1 \). This may be done, among other ways, by taking \( n_0 \rightarrow N x \) and \( n_1 \rightarrow N y \) 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

\[
\dot{n}_0 = \Gamma_0 e^{\beta \mu} - e^{\frac{\beta E}{2N_c}(n_0+2n_1)}
+ 2\beta En_1 e^{\frac{\beta E}{2N_c}(N_c+n_0-n_1)} \sinh \frac{\beta E}{2N_c}(N_c + n_0 - n_1)
\]

\[
\dot{n}_1 = \Gamma_1 e^{\beta \mu} - e^{\frac{\beta E}{2N_c}(N_c+n_1+2n_0)}
- 2\beta En_0 e^{\frac{\beta E}{2N_c}(N_c+n_0-n_1)} \sinh \frac{\beta E}{2N_c}(N_c + n_0 - n_1).
\]

The first question is, how important is the systematic evolution prescribed by \((11)\) compared to the diffusive evolution also contained in \((10)\)? We can address this question by examining a Gaussian approximation to the Fokker-Planck equation from which \((11)\) came. Fig. 1 shows selected solutions to \((1)\) together with 68% probability contours for Gaussian approximations to \( p(n_0, n_1) \), starting from initial delta functions. Fig. 1(a) shows that for a slow quench, diffusion is in fact very strong; this does not necessarily mean that the metastable state is not reached, but that it may be reached by diffusive nu-
clination rather than via the critical slowing down mechanism we are considering. Even here, though, there are ‘channels’ near the axes in which diffusion is weaker. For fast quenches, as shown in Fig. 1(b), diffusion is clearly a small correction to predominantly systematic evolution. In such cases, therefore, we may obtain accurate estimates of the probability of reaching the metastable state, by using the linear analysis described above to compute the distribution \( p(n_0, n_1) \) at some ‘coherent start time’ \( t_s \approx t \), and then letting the distribution flow under (11).

Having established that the systematic evolution of (11) provides a good description, after \( t \), 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, the first line in each equation of (11) is indeed equivalent to a TDGL equation (as may be seen by replacing \( n_j \rightarrow |\psi_j|^2 \)). But the second line in each equation is not of Ginzburg-Landau form: it does not involve \( \mu \), and the expression it implies for \( \psi_j \) is not a gradient with respect to \( \psi_j^* \). 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.

Some representative solutions to (11) are shown in Fig. 2, together with the \( |\psi_j|^2 \) given by the TDGL equation. It is clear that for sufficiently fast quenches, the two theories accord quite well, but that for slower quenches TDGL 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. 2 are above this line. So not even TDGL evolution conserves vorticity, but the QKT evolution changes vorticity more easily, especially for slower quenches.

Despite the shortcomings of TDGL revealed by our toy model, we would like to emphasize that in fact QKT does show that TDGL is relevant to trapped dilute gases, even very far from equilibrium: what TDGL requires is not outright rejection, but corrections, from diffusion and dissipation. And although these corrections may be substantial, the gross features predicted by TDGL are still recovered, with faster quenches and smaller biases. While the extension of quantum kinetic theory beyond toy models, to realistic descriptions of topological defect formation, will obviously require much further study, we believe that the prospects for experimental realization of spontaneous defects, as predicted by the Ginzburg-Landau theory, are very encouraging.

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