Exact vortex nucleation and cooperative vortex tunneling in dilute Bose-Einstein Condensates

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With the imminent advent of mesoscopic rotating BECs in the lowest Landau level (LLL) regime, we explore LLL vortex nucleation. An exact many-body analysis is presented in a weakly elliptical trap for up to 400 particles. Striking non-mean field effects are exposed at filling factors $\nu \gg 1$. E.g. near the critical rotation frequency pairs of energy levels approach each other with exponential consequences. The elliptical perturbation has the form: $\frac{1}{2}\hbar^2 \nabla^2 + \frac{1}{2} \sum_{n=1}^{N} r_n^2 + \frac{1}{2} \pi \sum_{n \neq m=1}^{N} \delta(r_n - r_m) - \Omega \sum_{n=1}^{N} L_n^z$

Units of length, $a_\perp$, and energy, $\hbar \omega_\perp$, are those provided by the harmonic trap; angular momenta, $L_n^z$, are scaled by $h$. There are two remaining dimensionless parameters. Firstly, $\Omega$, is the angular velocity of the rotating frame divided by the natural frequency of the harmonic trap. Secondly the coupling constant, $\eta = 4\pi a_\perp / a_\perp$. We assume the particles reside in the LLL of this AS trap. The LLL single-particle basis utilises a complex description of the particle positions in the plane, $z = x + iy$, and is defined by the set $\{(z^m / \sqrt{m!}) e^{-|z|^2/2}\}$, where $m = 0, 1, \cdots$.

In the AS case the many-body eigenfunctions, $\psi_L(\{z_k\})$, (labeled by the total angular momentum, $L$) are known analytically for $L \leq N$ [17, 23]. They are $\psi_L(\{z_k\}) \propto \sum_{1 \leq i_1 \leq \cdots \leq i_L \leq N} \left( z_{i_1} - z_c \right) (z_{i_2} - z_c) \cdots (z_{i_L} - z_c)$ where $z_c = 1/N \sum_{j=1}^{N} z_j$ is the centre of mass coordinate. The energies, $E_L$, are also known: for $0 \leq L \leq N(L \neq 1),(L=1$ is special as it corresponds to centre of mass motion and the energy is $E_1 = 1 - \Omega$).

$$E_L = N + L + \frac{1}{2} \eta N (N - \frac{1}{2} L - 1) - \Omega L. \quad (1)$$

At the critical frequency, $\Omega_c(0) = 1 - \frac{\eta N}{4}$, all the eigenstates for $2 \leq L \leq N$, and $L = 0$, are degenerate. The entry is abrupt, but degenerate.

In this Letter we determine how that degeneracy is lifted in a weakly elliptical trap with striking physical consequences. The elliptical perturbation has the form: $\frac{1}{2}\hbar^2 \nabla^2 + \frac{1}{2} \sum_{n=1}^{N} (z_n^2 + z_n^2)$. We will assume that $\epsilon \ll \eta$, to allow a description in terms of the AS states.
To explain the behaviour in the vicinity of vortex nucleation, it is convenient to use equation (4). Then, changing the zero of energy to absorb the term independent of \( \mathcal{L} \), we find the complete rescaled Hamiltonian (choosing \( \epsilon > 0 \) as the unit of energy)

\[
\mathcal{H}_\text{tot} = -\tilde{\Omega}\mathcal{L} + \frac{1}{4}\mathcal{L}_2
\]

where \( \tilde{\Omega} = (\Omega - \epsilon \Omega_c(0))/\epsilon \). This rescaling stretches out the nucleation region where our approximation is valid (\( \epsilon \ll \eta \)) which is convenient numerically. When the energy levels are calculated by exact diagonalisation (ED) for \( N = 400 \), we find the results portrayed in Fig. 1 (the energies are measured relative to the ground-state energy and we scale \( \eta = \eta_0/N \) to provide a sensible thermodynamic limit). We restrict ourselves to even \( N \), as for odd \( N \) there is a trivial residual first order transition (due to the necessary change of parity of the ground state) whose magnitude diminishes as \( N \to \infty \).

To understand the significance of the results, it is useful to consider what the equivalent diagram would have shown in the AS case. There, from equation (11), we should measure the energy from the ground state \( E_g = E_{\mathcal{L}=0} \) for \( \Omega \leq \Omega_c \), and from \( E_g = E_{\mathcal{L}=N} \) for \( \Omega > \Omega_c \), i.e. the appropriate ground states (within the basis set in the latter case at higher \( \Omega \)). Then we find:

\[
E_{\mathcal{L}} - E_g = \begin{cases} 
(\Omega_c - \Omega)L & : \Omega_c - \Omega > 0 \\
(\Omega - \Omega_c)(N - L) & : \Omega - \Omega_c > 0
\end{cases}
\]

This would also give a “V”-shape, however there are substantial differences. Firstly, in the AS case, the apex of the “V” is at \( \Omega - \Omega_c = 0 \), whereas the elliptical case is displaced by roughly \( \epsilon/4 \). Secondly, in the AS case the gradients increase linearly with level index. However in Fig. 1 the energy levels form doublets (which are of opposite parity) as they approach the critical point, and the doublets themselves do not have simply related gradients from doublet to doublet. Of course, the expanded scale of the figure (due to \( \Omega \) being scaled by \( \epsilon \)) emphasises this and at a sufficient distance from the critical point, the AS gradients must be obtained.

Focussing on the minimum (as a function of \( \tilde{\Omega} \)) gap, we have performed a finite size scaling fit of the gap between the ground state and first excited state, in terms of the dependence on the number of particles, \( N \), to

\[
\Delta E = N^\beta e^{-\alpha N}
\]

This form is consistent with a tunneling process (which the doublet structure suggests) occurring prior to the vortex being in the centre of the BEC. Data for \( \Delta E \geq 10^{-14} \) has been kept for a range of \( N \) and a fit found for \( \alpha \), as seen in Fig. 2.

The most significant feature, is a peak in \( \alpha(\tilde{\Omega}) \), whose height appears constant with increasing \( N \). Having found the behaviour of \( \alpha \), we find that the choice of the exponent \( \beta \approx 0.53 \) collapses the data for all \( N \) onto one curve. On the right hand side, there appears to be no single choice for \( \beta \) to collapse the data onto one curve.

The above analysis suggests, via the exponential dependence on \( N \) and the pairs of opposite parity eigenstates, that tunneling is involved in the nature of the states near \( \Omega_c \). By analogy with a particle in a double well, the states linked by tunneling can be exposed by examining the states \( \psi_\pm = \sqrt{2/\alpha} (\psi_0 \pm \psi_\pm) \), which would correspond to states, in the double well case, where the particle is localised in one or the other well. The single particle densities, \( \rho_\pm \), associated with these states, reveal a depression of the density on one side (which is determined by which of the states is being considered) of the semi-major axis. This depression in density moves towards the centre of the trap as \( \Omega \to \Omega_c \). Further analysis of Fig. 1 indicates that gaps between higher pairs of opposite parity levels also vanish asymptotically as \( N \to \infty \).

To establish a physical interpretation of these results, we extend the variational LLL MF Lagrangian \[24\], to the
elliptical case. We work with two vortices, as this is the simplest system with enough parameters to encapsulate the qualitative features of the exact solution. Following [23] we use hydrodynamic variables, \{p_m, \phi_m\}, such that the variational state \(\psi_M(z, z^*) = \sum_{m=1}^{\infty} a_m z^m e^{-|z|^2/2}\) and \(a_m = \sqrt{\pi m!} e^{\beta \phi_m}\). The two-vortex Lagrangian corresponds to maximum angular momentum \(M = 2\). In units of \(\epsilon\), the two vortex Lagrangian becomes (in the first line in unscaled form):

\[
\mathcal{L} = \hbar N \left( \rho_\perp \dot{\phi}_+ + \rho_\perp \dot{\phi}_- \right) - 3\mathcal{H}
\]

\[
\mathcal{H} = \left( \Gamma - \Omega \right) (1 - \rho_-) + \sigma (\rho_+ - \rho_-) \cos(2\phi_-)
\]

\[
+ \Gamma \left( \frac{3}{4} \rho_- + \frac{3}{4} \rho_+ + \frac{3}{4} \rho_-^2 - \frac{3}{4} \rho_+^2 + \frac{1}{4} \rho_+ \rho_+ + \frac{1}{2} \rho_+ \rho_- + \frac{1}{2} \rho_- \rho_- \right) \cos(2\phi_+).
\]  

(3)

where we have: transformed to variables \(\rho_+ = \sqrt{r_0 + p_0}\), \(\phi_+ = (\phi_0 + \phi_2)\), \(\rho_- = (\rho_0 - \rho_2)\) and \(\phi_- = \frac{\pi}{2} (\phi_0 - \phi_2)\); defined \(\sigma (\rho_+ - \rho_-) = (1/2) \left( \frac{\pi}{2} \right) \left( 4 \rho_+^2 - 2 \rho_-^2 \right)^{1/2} \) and \(\Gamma = \eta_0 / 4 \pi E \sqrt{2} \); and used normalisation \(\sum_{i=0}^{\infty} \rho_i = 1\), to eliminate \(\rho_0\). (In the vicinity of vortex nucleation \(\rho_1 \approx 1\) and \(\rho_0\) and \(\rho_2\) are correspondingly small.) We have picked the arbitrary phase such that \(\phi_1 = 0\).

At frequencies, \(\Omega \leq \Omega_c\), consideration of the Lagrangian indicates two degenerate energy minima. By inspection for the phase variables, \(\phi_2\), we see that \(\phi_+ = \pi\) and \(\phi_- = \pm \pi/2\). Minimising the Hamiltonian numerically with respect to the \(\rho_\pm\) gives the equilibrium values \(\hat{\rho}_\pm\) for a given set of interaction and rotation parameters. In the original variables, the minima have associated phase variables \(\phi_0 = 0, \phi_2 = \pi, \phi_0 = \pi, \phi_2 = 0\). This implies that both minima correspond to two vortices on the \(x\)-axis (one either side of the origin, not necessarily at equal distance) and are mirror reflections of each other. Beyond MF one might expect that the vortices tunnel between these configurations if they are not identical.

Noting that the potential involving \(\cos \phi_-\) is the only term not multiplied by the large parameter, \(\Gamma\), we Taylor expand all the other terms to harmonic level around the equilibria. We also evaluate \(\sigma\), at the equilibrium values of \(\rho_\pm\) leading to a potential \(V_{\phi_-} = \sigma (\hat{\rho}_+ - \hat{\rho}_-) \cos \phi_-\).

We follow the standard procedure e.g. Ref. [24] to examine quantum effects beyond MF theory, and re-quantise the Lagrangian, which now only involves the \(\rho_-\) variables, and start from Eqn. (3). The classical conjugate variables to \(\phi_\pm\) are \(p_\pm = N \hbar \hat{p}_\pm\). Thus the commutator for canonically conjugate variables:

\[
[\hat{\phi}_-, \hat{\rho}_-] = [\hat{\phi}_-, N \hbar \hat{p}_-] = i\hbar \Rightarrow [\hat{\phi}_-, \hat{\rho}_-] = iN^{-1}.
\]

Hence the usual quantisation procedure implies: \(\hat{\rho}_- \rightarrow -iN^{-1} \hat{\partial} / \hat{\partial} \hat{\phi}_-\). This is clearly unaltered under the displacement of \(\hat{\rho}_- = \hat{\rho}_- + \delta \hat{\rho}_-\). We note that the quantum effects will vanish in the limit \(N \rightarrow \infty\), i.e. the thermodynamic limit, consistent with the exact results described above.

Making the operator replacements, leads to

\[
- \frac{1}{2M^*} \frac{d^2}{d\phi_-^2} - N^2 (E - \sigma (\hat{\rho}_+ - \hat{\rho}_-) \cos(2\phi_-)) \Psi (\phi_-) = 0
\]

(4)

where we have defined: \(1/M^* = \partial^2 T / \partial \rho^2|_{\rho_\bot = 0}\) and \(E = (E - V_0)/N\), with \(V_0\) being the zeroth order terms from the T expansion. This is a Mathieu equation,

\[
[\partial_{xx} + b - 2q \cos(2x)] y(x) = 0
\]

(5)

and inspection shows that \(b \equiv 2N^2 M^* E \geq 0\) and \(q \equiv N^2 M^* \sigma (\hat{\rho}_+ - \hat{\rho}_-) \geq 0\). In the limiting case of \(q = 0\), the Mathieu functions are simply \(\sin(\sqrt{\sigma} \phi_-)\) and \(\sin(\sqrt{\sigma} \phi_-)\), so the AS result is recovered.

From Eqn. (20.2.31) [23], the level splitting (between the first excited and ground states) of Eqn. (5) is

\[
\Delta \tilde{E} \sim \frac{1}{2} \sqrt{\frac{3}{2} \sqrt{2} \pi^3 e^{-4\sqrt{3}/\pi}} \sim N^{3/2} e^{-\alpha_2 N}
\]

implying that \(\Delta \tilde{E} \sim N^{3/2} e^{-\alpha_2 N}\). The tunnelling coefficient \(\alpha_{2v} \equiv 4 \sqrt{M^*} \sigma (\hat{\rho}_+ - \hat{\rho}_-)\).

Finally reinstating the unscaled \(\eta\) we can estimate the tunnel splitting using say \(N = 10, \epsilon \approx 10^{-3}\) and \(\eta \approx 1\) (i.e. a chip trap). We then find \(E \approx 0.5 \eta \tilde{\omega}_0\), indicating the splitting should be observable under those assumptions.

These results reproduce the exponential suppression of the tunneling splitting of the eigenvalues found in the ED, indicating we have correctly identified the tunneling entities. Qualitatively the behavior of the tunneling coefficient, \(\alpha\), with rotation frequency (shown in Fig. 4) follows that of the exact result, having a maximum in \(\alpha(\bar{\Omega})\). We have scaled the MF frequencies, \(\bar{\Omega}\), by 1/4 to compare the peaks in \(\alpha\). This reflects \(\bar{\Omega}_{\text{exact}} \approx \bar{\Omega}\) as against \(\bar{\Omega}_{\text{MF}} = \epsilon/4\). In addition the exponent of the pre-exponential factor, \(N^3\), has \(\beta_{\text{exact}} = 1/2\) (scaled variables) almost equal to the ED result, \(\beta_{\text{MF}} \approx 0.53\), for \(\bar{\Omega}\) to the left of the peak. We found that adding additional (up to eight) vortices improves the agreement between the approximate calculation and the exact one, at the cost of diminishing the clarity of interpretation (the motivation for the requantised calculation). Finite temperature will blur the peak, but leave it visible under typical experimental conditions.

Working with two vortices the tunneling path may be interpreted in terms of vortex positions. They are:

\[
\xi_{\pm} = -e^{i\phi_2} \sqrt{\frac{p_1}{2p_2}} \left( 1 \pm \left( 1 + \frac{2\sqrt{2}\rho_0 p_2}{p_1} \right)^{1/2} \right)
\]

Varying \(\phi_2\) along \([0, \pi]\) results in both \(\xi_{\pm}\) having semi-circular trajectories, as shown in Fig. 4. Note, that there is always a second anticlockwise trajectory corresponding to \(\phi_2\) from \([\pi, 2\pi]\), and this will result in the major semi-circle being above axis. One might have expected that the tunneling matrix element for a vortex would increase as the initial and final positions of the vortex
approached each other (i.e. the inner circle in Fig. 4). The more surprising aspect is that the vortex at large distances from the centre of the trap does not substantially decrease the matrix element. This is due to the vortex states (labeled by position) becoming increasingly non-orthogonal as the vortices move away from the centre of the trap. The non-orthogonality arises because the Gaussian weight strongly suppresses the region where the states are most different [27]. Hence tunneling is least effective when both vortices are at the same, intermediate, distance from the trap centre. Exploration of experimental observation schemes is underway, including oscillation of the trap along the semi-minor axis and noise spectra which will reveal the density-density correlation function.

In conclusion, we have shown, by exact solution, that mesoscopic rotating BECs will show pronounced deviations from MF theory at low angular velocities. This may be interpreted, using a requantised MF theory, in terms of vortex tunneling in the nucleation process.

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The tunneling parameter from ED (line) and for two-vortex MF theory with $\Gamma = 50, 100, 200$ (triangle, star, square). Our approximations become more valid for increasing $\Gamma$. The MF frequency has been scaled to enable qualitative comparison of the peaks.

Semicircular trajectories of the vortex positions, ensuring the separation between vortices is maintained.

FIG. 3: The tunneling parameter from ED (line) and for two-vortex MF theory with $\Gamma = 50, 100, 200$ (triangle, star, square). Our approximations become more valid for increasing $\Gamma$. The MF frequency has been scaled to enable qualitative comparison of the peaks.

FIG. 4: Semicircular trajectories of the vortex positions, ensuring the separation between vortices is maintained.