Complex Langevin simulation of quantum vortex nucleation in the Bose-Einstein condensate

Tomoya Hayata\(^1,\)\(^2\) and Arata Yamamoto\(^1,\)\(^2\)

\(^1\)Department of Physics, The University of Tokyo, Tokyo 113-0031, Japan
\(^2\)Theoretical Research Division, Nishina Center, RIKEN, Wako 351-0198, Japan

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The ab-initio simulation of quantum vortex nucleation in the Bose-Einstein condensate is performed by adopting the complex Langevin techniques. We simulate the two-component boson field theory at a finite chemical potential under rotation. In the superfluid phase, vortices are generated above a critical angular velocity and the circulation is clearly quantized even in the presence of quantum fluctuations.

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\section{Introduction}

The Bose-Einstein condensation attracts lots of attention in various areas of physics. The direct observation has been achieved in the experiments of liquid helium \([1]\) and weakly interacting atomic gases \([2, 3]\). In solid state physics, the superconductivity of metals results from the condensation of Cooper pairs, which is a bound state of electrons in momentum space \([4]\). In the core of neutron stars, it is considered that the condensate of the Cooper pairs of nucleons or quarks exists \([5]\). Also, the condensation of Higgs boson results in the dynamical mass generation of gauge bosons in the Standard Model of particle physics \([6]\).

In the presence of external gauge fields, the Bose-Einstein condensate exhibits topological solitons. In type-II superconductors under magnetic fields, the penetrating magnetic flux is quantized and the quanta form the Abrikosov lattice structure \([7, 8]\). As understood from the analogy between magnetism and rotation, the same quantization of vortices has been observed in the rotating Bose-Einstein condensate \([9]\). It has been investigated in detail both from theories and experiments \([10]\).

In dilute and low temperature systems, quantum and thermal fluctuations can be negligible, and thus the mean-field approximation works well. Quantum vortex nucleation in the Bose-Einstein condensate can be described by using the Gross-Pitaevskii equation \([11]\). However, when quantum or thermal fluctuation cannot be negligible, it is highly nontrivial how such topological solitons behave. Around the critical value of temperature, chemical potential, magnetic field, or angular velocity, the fluctuation grows and then the mean-field description breaks down. In fact, effects of quantum fluctuations have been discussed in literatures \([12]\). Since high precision measurements are possible in cold atomic experiments, the deviation from the mean-field approximation can be detectable in experiments. For definite theoretical prediction without uncertainty, the ab-initio simulation of quantum vortex nucleation is necessary.

In this Letter, we will report the first ab-initio lattice simulation of the vortex nucleation in the rotating Bose-Einstein condensate. For this purpose, we adopt the complex Langevin method to nonrelativistic boson field theory. The complex Langevin method has been developed in relativistic field theories to attack complex action problem, such as nonequilibrium system \([13]\) and the phase diagram at finite quark number density \([14]\). We first discuss the superfluid transition without rotation, and then analyze the nucleation of vortices in rotating frames. We show that although the circulation is quantized in the superfluid phase, quantum fluctuations blur the quantized circulation as a chemical potential getting close to its critical value.

\subsection{Bose gas under rotation}

We consider quantum field theory at finite temperature, i.e., in \((1 + 3)\)-dimensional Euclidean spacetime. In Euclidean simulations, although we cannot follow real-time dynamics of vortex nucleation, which can be studied in the real-time Gross-Pitaevskii simulation \([15]\), we can still study the nonperturbative mechanism of it.

The continuum action of a two-component boson field \(\varphi(\tau, \mathbf{x}) = \varphi^1(\tau, \mathbf{x}) + i\varphi^2(\tau, \mathbf{x})\) in a rotating frame is \([16]\)

\begin{equation}
S_{\text{con}}[\varphi^1, \varphi^2] = \int d\tau d^3x \left[ \varphi^* (\partial_\tau - \mu) \varphi + \frac{1}{2m} \left( \mathbf{\nabla} - i m \Omega \times \mathbf{x} \right) |\varphi|^2 \right.
- \frac{1}{2} \left( m \mathbf{x}^2 + q^2 \right) \Omega^2 |\varphi|^2 + \frac{1}{4} \mathbf{A} \cdot \mathbf{A} \left. \right]
\end{equation}

where \(\mu\), \(m\) and \(\mathbf{\nabla}\) denote chemical potential, mass of boson and spatial derivatives, respectively. We consider the rotation around \(z\) axis with angular velocity \(\Omega\), and thus \(\Omega = \Omega \hat{z}\). (\(\hat{z}\) denotes a unit vector in the \(z\) direction.)

We remark here that, except for the centrifugal potential \(-\frac{1}{2}m(x^2 + y^2)\Omega^2 |\varphi|^2\), the action \((1)\) is mathematically equivalent to the spinless charged boson action under a magnetic field. In a rotating frame, particles effectively couple to the “magnetic field” \(q \mathbf{B} = q \mathbf{\nabla} \times \mathbf{A} = 2m\Omega \hat{z}\) with \(\mathbf{A} = \Omega \times \mathbf{x}\). Therefore, our analysis can be applied not only to rotation but also to magnetic fields. In fact, the qualitative behavior of vortex nucleation is the same in the case of magnetic fields. In the following numerical simulations, we only show the results of rotation.

To perform lattice simulations, we discretize the continuum action \((1)\) on the hypercubic lattice. The corresponding lattice
The effective gauge field of rotation is introduced by the same manner as the electromagnetic gauge field [17]

\[ u_i = \exp(-iaqA_i) = \exp(-iam(\Omega \times x)_i). \]  

The chemical potential is introduced on the basis of the standard lattice formulation [18].

In the path integral quantization, the expectation value of operator \( \hat{O} \) is given by

\[ \langle \hat{O} \rangle = \frac{1}{Z} \int d\varphi^1 d\varphi^2 e^{-S_{\text{lat}}[\varphi^1, \varphi^2]} \hat{O}[\varphi^1, \varphi^2], \]  

where \( Z \) is a normalization factor, \( Z = \int d\varphi^1 d\varphi^2 e^{-S_{\text{lat}}[\varphi^1, \varphi^2]} \). In the conventional quantum Monte Carlo simulations based on important sampling techniques, one evaluates this expectation value by means of the ensemble average which is randomly generated by the probability density \( e^{-S_{\text{lat}}}/Z \). However, as discussed in Ref. [19], the lattice action (2) suffers from the notorious sign problem because the temporal hopping term is complex in nonrelativistic systems. The probability interpretation of the weight \( e^{-S_{\text{lat}}}/Z \) breaks down and thus the importance sampling cannot be applied.

To overcome the sign problem and perform nonperturbative evaluation of Eq. (4), we adopt the complex Langevin technique, which is based on the stochastic quantization formalism and does not necessarily require the action to be real.

**Complex Langevin method.** In the stochastic quantization, Eq. (4) is reconstructed by the noise average of the solution of classical equation of motion with random noises [20, 21]. We need to solve the Langevin equation for \( \varphi^a \) (\( a = 1, 2 \)) along the fictitious time direction

\[ \partial_\tau \varphi^a_{\tau, x}(\theta) = -\frac{\partial S_{\text{lat}}[\varphi^1, \varphi^2]}{\partial \varphi^a_{\tau, x}} + \eta^a_{\tau, x}(\theta), \]  

with \( \theta \) being the continuous fictitious time. \( \eta^a_{\tau, x}(\theta) \) is real Gaussian noise. Since the lattice action (2) is complex, the right-hand side of Eq. (5) is complex. Thus, we need to complexify the left-hand side, i.e., the two real fields as \( \varphi^a \rightarrow \varphi^{aC} = \varphi^a + i\varphi^a \). Then, Eq. (5) becomes stochastic differential equations for the two complex fields \( \varphi^{aC} \) (\( a = 1, 2 \)), in which the Gaussian noises are applied only to the real parts [20, 21]. Now, Eq. (5) reads

\[ \partial_\tau \varphi^{aR}_{\tau, x}(\theta) = -\text{Re} \left[ \frac{\partial S_{\text{lat}}[\varphi^{1C}, \varphi^{2C}]}{\partial \varphi^{aC}_{\tau, x}} \right] + \eta^a_{\tau, x}(\theta), \]  

\[ \partial_\tau \varphi^{aI}_{\tau, x}(\theta) = -\text{Im} \left[ \frac{\partial S_{\text{lat}}[\varphi^{1C}, \varphi^{2C}]}{\partial \varphi^{aC}_{\tau, x}} \right]. \]  

The Gaussian noise \( \eta^a_{\tau, x}(\theta) \) satisfies \( \langle \eta^a_{\tau, x}(\theta) \rangle = 0 \) and \( \langle \eta^a_{\tau, x}(\theta) \eta^b_{\tau, x}(\theta') \rangle = 2\delta_{ab}\delta_\tau\delta_{xx}\delta(\theta - \theta') \).

The expectation value (4) is obtained by using the solution of Eqs. (6) and (7) as

\[ \langle \hat{O} \rangle = \lim_{\theta \rightarrow \infty} \langle \hat{O}[\varphi^{1C}(\theta), \varphi^{2C}(\theta)] \rangle, \]  

where the operator is written in terms of the complex field \( \varphi^{aC} \). For example, the number density operator, \( \hat{n}_{\tau, x} = \partial\mathcal{L}/\partial\mu \) with \( \mathcal{L} \) being the lattice Lagrangian density, reads

\[ \hat{n}_{\tau, x} = e^\mu (\delta_{ab} + i\epsilon_{ab}) \varphi^{aC}_{\tau, x} \varphi^{bC}_{\tau, x} \]  

\[ = e^\mu (\delta_{ab} + i\epsilon_{ab}) \left( \varphi^{aR}_{\tau, x} \varphi^{bR}_{\tau, x} - \varphi^{aI}_{\tau, x} \varphi^{bI}_{\tau, x} \right) + i \left( \varphi^{aR}_{\tau, x} \varphi^{bI}_{\tau, x} - \varphi^{aI}_{\tau, x} \varphi^{bR}_{\tau, x} \right), \]  

where \( \epsilon_{ab} \) are completely antisymmetric tensor with \( \epsilon_{01} = 1 \) and the Einstein convention is understood for repeated indices. Other observables are complexified in the same manner and have both real and imaginary parts. We note that the imaginary parts of observables are consistent with zero within error bars. In the following numerical simulation, we assume the ergodicity of stochastic evolution and calculate observables by the long time average over the Langevin trajectories, instead of directly evaluating Eq. (8). We also adopt a higher order algorithm used in Ref. [22] to improve the step size dependence [23].

**Numerical simulation.** We have numerically solved Eqs. (6) and (7) by adopting the higher order algorithm with the fictitious time step \( \epsilon = 2.0 \times 10^{-4}a \). The total number of lattice sites is \( V = N_x N_y \times N_z N_x = 11^2 \times 10^2 \), and \( x \) and \( y \) are ranged to \([-5a, 5a]\), and the position of rotational axis is set to \((x, y) = (0, 0)\). We take the Dirichlet boundary conditions in \( x \) and \( y \) directions, and take periodic boundary conditions in \( z \) and \( \tau \) directions. We set \( ma = \lambda/a^2 = 1.0 \). Errors were estimated by using the jackknife method.

First, we analyze the superfluid transition without rotation, i.e., \( \Omega = 0 \). The two-point correlation function

\[ G(|x - y|) = \langle (\delta_{ab} + i\epsilon_{ab}) \varphi^{aC}_{\tau, x} \varphi^{bC}_{\tau, y} \rangle \]  

at \( \mu a = 0.1, 0.3, \) and 0.5 is shown in Fig. 1. We see the signature of the off-diagonal long-range order at \( \mu a = 0.5 \). In Fig. 2, we show the condensate fraction

\[ R = \frac{\text{Re}[G(aN_x/2)]}{\text{Re}[G(0)]}, \]  

and the number density \( n = \sum_{\tau, x} \langle \hat{n}_{\tau, x} \rangle \), as functions of chemical potential. The transition from the U(1) symmetric
phase to the U(1) broken phase is clearly seen in Fig. 2, which is accompanied by brow up of number density. Below the critical value \( \mu_\text{c} a = 0.2 - 0.3 \), physical observables should be completely independent of \( \mu \) (at strictly zero temperature), even though it is explicitly introduced in the density matrix as 

\[
\rho = \exp(-\beta(H - \mu N))
\]

with the inverse temperature \( \beta = 1/T \). This is because the chemical potential cannot excite any particles until it exceeds the gap of lowest excitations. This exact cancellation is known as the “Silver Blaze” problem [24] and correctly reproduced in our simulation.

Next, we analyze quantum vortex nucleation by rotation. The direct evidence of a quantum vortex is the quantized circulation. The circulation of a vortex is defined as the phase integral around it. On the hypercubic lattice, the circulation is given by integrating the phase difference along the square loop. We calculated the circulation of the O(2) angle (U(1) phase) of \( \varphi^1 R \) and \( \varphi^{2R} \):

\[
\hat{\Gamma}(l) = \frac{1}{2\pi} \int_{l \times l} dx \left[ \tan^{-1}\left( \frac{\varphi^{2R} R}{\varphi^{1R} R} \right)|_\tau x + j \right] - \tan^{-1}\left( \frac{\varphi^{2R} R}{\varphi^{1R} R} \right)|_\tau x, \tag{12}
\]

where \( j \) is unit vector along the loop. The size of the loop is \( l \times l \) (2 \( \leq l \leq 10 \) in our simulation) and the center of the loop is placed at \((x, y) = (0, 0)\). In each configuration of the ensemble, \( \hat{\Gamma}(l) \) is integer because of single-valuedness of wave functions, but is not necessarily the same in different configurations. Therefore, the ensemble average \( \langle \hat{\Gamma}(l) \rangle \) becomes non-integer if the number of vortices strongly fluctuates. The mean-field approximation, where the circulation takes an exact integer value, works well when the fluctuation is negligible.

In Fig. 3, we show the circulation as a function of angular velocity \( \Omega \) in the superfluid phase slightly above \((\mu a = 0.3)\) and far above \((\mu a = 0.5)\) the critical chemical potential. The circulation is clearly quantized at \( \mu a = 0.5 \). On the other hand, it is not quantized at \( \mu a = 0.3 \), which indicates the breakdown of the mean-field approximation as the chemical potential getting close to its critical value. To see the fluctuation of vortices, we show the profile of circulation \( \hat{\Gamma} \) obtained from each configuration at \( \mu a = 0.5 \) in Fig. 4. At a small angular velocity, the profile shows broad Gaussian distribution. As \( \Omega \) increases, the profile becomes sharper and finally becomes a single peak, where the fluctuation can be negligible and the mean-field approximation works well.

The spatial positions of vortices can be estimated from the \( l \)-dependence of \( \Gamma(l) \) shown in Fig. 5. At \( a\Omega = 0.06 \) (circle), \( \Gamma(l) = 1 \) and it is almost independent of \( l \) in \( l \geq 2 \). Thus, one vortex exists inside the \( 2 \times 2 \) loop, i.e., in \( |x| \leq a \) and \( |y| \leq a \). At \( a\Omega = 0.14 \) (triangle), \( \Gamma(l) \) increases at \( l = 4 \), and thus two vortices exist in \( a \leq |x| \leq 2a \) and \( a \leq |y| \leq 2a \) at \( a\Omega = 0.20 \) (diamond), two vortices exist in \( a \leq |x| \leq 2a \) and \( a \leq |y| \leq 2a \) and one vortex exists \( 2a \leq |x| \leq 3a \) and \( 2a \leq |y| \leq 3a \). By calculating two-point or three-point correlation functions of loops, we can obtain more detailed information, such as intervortex distance or the Abrikosov lattice structure, although we must use finer lattice than the present one.

**Concluding remarks.** We have performed the first lattice simulation of quantum vortex nucleation in the Bose-Einstein...
condensate. We have adopted the complex Langevin method instead of the conventional quantum Monte Carlo method, which suffers from the sign problem because of the complex action (2). In this ab-initio simulation, all quantum fluctuations are exactly taken into account.

We have numerically showed the superfluid transition at a finite chemical potential by the off-diagonal long-range order analysis. The complex Langevin simulation reproduces a sharp transition and resolves the Silver Blaze problem. We have successfully simulated vortices in the rotating Bose-Einstein condensate. While the quantization of the average circulation is clearly seen, the quantum fluctuation of vortex number is also seen. At first glance, these two facts seem contradicting or counterintuitive. However, our simulation has clarified that the fluctuation behaves as Gaussian and, as a result of cancellation, the average circulation is integer.

There are several future applications: We can apply anisotropic harmonic trapping potential, which corresponds to the time-dependent rotating potential in cold atomic experiments [9]. By tuning the trapping potential and angular velocity, we can study the quantum Hall effect expected in the rotating Bose-Einstein condensate [25]. Another application is relativistic field theory under rotation, where the sign problem exists [26]. Nonperturbative study of relativistic vortex nucleation is helpful to understand the physics of, e.g., vortices inside neutron stars [5] and cosmic strings in the early universe [27].

The complex Langevin method is powerful not only for the rotating Bose-Einstein condensate but also for other condensed matter systems. First, nonperturbative simulations at finite temperatures are interesting. We can estimate the critical temperature of Bose-Einstein condensation with including all orders of density corrections [28]. We can also study the effect of thermal fluctuations to the condensate and discuss the break down of the Gross-Pitaevskii equation. Furthermore, our approach is applicable to the Bose-Hubbard model, which is a model of Bose gases on optical lattices and is known to suffer from the sign problem.

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