# Vortex formation in a two-dimensional Bose gas



2010 J. Phys. B: At. Mol. Opt. Phys. 43 095004

(http://iopscience.iop.org/0953-4075/43/9/095004)

IOP Publishing Journal of Physics B: Atomic, Molecular and Optical Physics
J. Phys. B: At. Mol. Opt. Phys. **43** (2010) 095004 (8pp) doi:10.1088/0953-4075/43/9/095004

# Vortex formation in a two-dimensional Bose gas

**Esteban Calzetta[1], Kwan-yuet Ho[2] and B L Hu[3]**

[1] IFIBA (CONICET) and Departamento de Fisica, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires-Ciudad Universitaria, 1428 Buenos Aires, Argentina
[2] Institute of Physical Sciences and Technology and Department of Physics, University of Maryland, College Park, MD 20742-4111, USA
[3] Joint Quantum Institute and Maryland Center for Fundamental Physics, University of Maryland, College Park, MD 20742-4111, USA

E-mail: blhu@umd.edu

Received 10 November 2009, in final form 19 March 2010
Published 15 April 2010
Online at stacks.iop.org/JPhysB/43/095004

**Abstract**
We discuss the stability of a homogeneous two-dimensional Bose gas at finite temperature against the formation of isolated vortices. We consider a patch of several healing lengths in size and compute its free energy using the Euclidean formalism. Since we deal with an open system, which is able to exchange particles and angular momentum with the rest of the condensate, we use the symmetry-breaking (as opposed to the particle number conserving) formalism, and include configurations with all values of angular momenta in the partition function. At finite temperature, there appear sphaleron configurations associated with isolated vortices. The contribution from these configurations to the free energy is computed in the dilute gas approximation. We show that the Euclidean action of linearized perturbations of a vortex is not positive definite. As a consequence the free energy of the 2D Bose gas acquires an imaginary part. This signals the instability of the gas. This instability may be identified with the Berezinskii–Kosterlitz–Thouless transition.

## 1. Introduction

Below a certain temperature in a three-dimensional bosonic system, a long-range order is established in an ordered phase called the Bose–Einstein condensate (BEC). In the two-dimensional (2D) Bose gas, there does not exist an ordered state since its existence means that the correlation of its fluctuations is logarithmically divergent, as proven by Mermin, Wagner [1], Hohenberg [2] and Coleman [3]. However, it has been shown by Berezinskii [4] and Kosterlitz and Thouless [5] (BKT) that there exists a superfluid phase with a quasi-long-range order below a certain temperature. The superfluid phase has only the bounded vortex pairs but above the BKT temperature single vortices proliferate as this is the more stable configuration [5].

Many theoretical studies on the BKT transition in the 2D Bose gas, including the original theory of BKT, are based on equilibrium thermodynamics of many-body systems [6–10]. There have been studies of 2D vortex dynamics, viewed as massive charged particles in relativistic two-dimensional electrodynamical systems [11, 12]. This analogy has been applied to the study of vortex dynamics of 2D superfluid via a Fokker–Planck equation [13] and using field theoretical approaches [14–16]. There were also numerical studies based on the Gross–Pitaevskii equation [17, 18] on the lifetime of spontaneous decay of a pancake-shaped condensate with a vortex [19]. There were also studies around the critical region of the BKT transition with Monte Carlo simulations [20, 21] with the local density approximation. With the use of the projected Gross–Pitaevskii equation (PGPE) [22], the thermal activation of vortex pairs in the presence of a harmonic trap [23–25] and its emergence of superfluidity [26] were studied, and the various consequences of the improved mean-field Holzmann–Chevalier–Krauth (HCK) theory [27] of the 2D Bose gas [28–31] were presented. The non-equilibrium response of a 2D Bose gas is less understood. One encounters such a situation when the trap is suddenly turned off, as was done in recent experiments [32–34] described below.

Recently, a 2D quantum Bose gas has been experimentally realized by the Dalibard group [32, 33] by slicing a 3D BEC into pieces of 'pancakes' with 1D optical lattices, and by the Phillips group [34] through trapping the atoms in a 3D harmonic potential with a very large frequency in one of the directions. In both experiments, measurements on the gas are performed some time after the confining potential is abruptly turned off. Dalibard group's experiment showed that there are more isolated vortices formed at higher temperatures. The Phillips group measured the density profile after 10 ms time of flight, and identified different states of the gas. In one regime the gas develops a bimodal distribution with only thermal and quasi-condensate components without long-range order, as different from a superfluid. For a sufficiently long time of flight, they observe a trimodal distribution with thermal, quasi-condensate and superfluid components indicative of a BKT transition.

In this paper, we compute the free energy of a 2D Bose gas by means of thermal field theory. We consider the action in the Madelung representation (in terms of density and phase), and convert it to a Euclidean action by a Wick rotation in time and in phase. The system that we study is a patch of a size of several healing lengths within the larger 2D gas. Because we are dealing with the homogeneous configuration, we put no confining potential, i.e. $V(\mathbf{x}) = 0$. Since the vortices form at the centre of the gas patch [28] at the beginning where the density of the gas is effectively homogeneous, and the vortex core structure is very small compared to the size of the gas patch, we expect to reduce the physically more relevant inhomogeneous situation to the homogeneous situation discussed here through a local density approximation. Since particle number and angular momentum are not conserved for this system, we do not constrain the former (unlike in the particle number conserving formalism, see e.g. [35]) and consider configurations with all values of angular momentum. In particular, we consider configurations with different numbers of vortices and the fluctuations around them. Although these configurations are time independent, they have finite Euclidean action as a consequence of the compactification of the Euclidean time axis, namely Euclidean time is periodic with periodicity $\hbar\beta$. These time-independent configurations with nonzero angular momentum play in our problem the same role as the usual sphaleron configurations in electroweak symmetry breaking [36]. The contribution from these configurations to the free energy is computed within the dilute gas approximation.

We find that the Euclidean action for fluctuations around an isolated vortex is not positive definite. In real time, this means an instability of the isolated vortex, and we characterize the direction of greatest instability in configuration space. In imaginary time the fact that the Euclidean action is not positive definite means that the partition function must be defined by an analytic continuation, whereby the free energy becomes complex. We calculate the imaginary part of the free energy due to this instability. This is similar to the argument of Langer who considered the decay of a metastable state due to classical fluctuations [37, 38], that of Coleman who considered the quantum fluctuations around the spatially separated instantons [39–41] and that of Affleck who considered the decay of a quantum-statistical metastable state using instantons [42, 43]. We find that the canonical 2D Bose gas is indeed unstable at finite temperature, and the decay rate, which is also the rate of vortex nucleation, increases with temperature. For $T > T_{\mathrm{BKT}}$, the gas evolves to a state of isolated vortices.

The paper is organized as follows. In section 2 we introduce the Gross–Pitaevskii treatment and write it in the Madelung representation. In section 3 we obtain the Euclidean action by a Wick rotation and model the density profile of the gas with a vortex at the origin. In section 4 we introduce the linear perturbation about the configuration for each $q$. In section 5 we outline the formalism of computing the lifetime of the gas and obtain the BKT transition temperature. In section 6 we use Bohr–Sommerfeld quantization to show that the effective energy is complex, indicating the instability of the 2D Bose gas. We end with conclusions in section 7.

## 2. The model

The dynamics of a two-dimensional (2D) bosonic atomic system with a $\delta$-potential inter-atomic interaction is described by the action [17, 18]

$$S = \int \mathrm{d}t\, \mathrm{d}^2\mathbf{x} \left\{ \mathrm{i}\hbar\Psi^\dagger \frac{\partial\Psi}{\partial t} - H \right\}, \tag{2.1}$$

where $\Psi(\mathbf{x})$ and $\Psi^\dagger(\mathbf{x})$ are respectively the annihilation and creation operators of an atom at point $\mathbf{x}$. The Hamiltonian is

$$H = \frac{\hbar^2}{2m}\nabla\Psi^\dagger\nabla\Psi + F[\Psi^\dagger\Psi], \tag{2.2}$$

and

$$F[\rho] = (V(\mathbf{x}) - \mu)\rho + \tfrac{1}{2}g\rho^2, \tag{2.3}$$

where $g$ is the coupling constant due to the $\delta$-potential between the atoms. In the Madelung representation

$$\Psi = \sqrt{\rho}\,\mathrm{e}^{\mathrm{i}\theta}, \tag{2.4}$$

the density of atoms in the lowest macroscopically occupied state $\rho$ and the phase $\theta$ are canonical to each other, obeying the commutation relation [44, 45]

$$[\rho(\mathbf{x}), \varphi(\mathbf{x}')] = -\mathrm{i}\delta(\mathbf{x} - \mathbf{x}'). \tag{2.5}$$

With (2.4), action (2.1) is written as

$$S = \int \mathrm{d}t\, \mathrm{d}^2\mathbf{x} \left\{ \hbar\theta\frac{\partial\rho}{\partial t} - H \right\}, \tag{2.6}$$

where

$$H = \frac{\rho}{2m}(\nabla\hbar\theta)^2 + F_q[\rho], \tag{2.7}$$

and

$$F_q[\rho] = F[\rho] + \frac{\hbar^2}{8m\rho}(\nabla\rho)^2. \tag{2.8}$$

The length scale that characterizes the local alteration of the gas density healing back to the mean-field density is given by the healing length, which is

$$\xi^2 = \frac{\hbar^2}{4m\mu}. \tag{2.9}$$

Experimentally there is a harmonic trap to prepare the initial patch of the Bose gas in two dimensions. At the time when the trap is turned off, the Bose gas is still highly inhomogeneous. However, in recent experiments, the vortex core structure is very small compared to the patch of the quasi-two-dimensional Bose gas. Take Phillips group's experiment for example. The sodium atom is used and therefore $m \sim 3.8 \times 10^{-26}$ kg. And $\omega_\perp = 20$ Hz and $\omega_z = 1$ kHz [34]. It is known that $\mu = g\rho_0$, where $\rho_0 = \frac{4}{\lambda^2}$ [20], $\lambda = \sqrt{\frac{2\pi\hbar^2}{mk_BT}}$ being the thermal de Broglie wavelength. Near the transition point, $T \sim 100\,\mathrm{nK}$ [33, 34], $\rho_0 \sim 3\times 10^{12}\ \mathrm{m}^{-2}$. By $g = \frac{\hbar^2}{m}\frac{a}{L_z}$ (where $a$ is the scattering length and $L_z$ is the thickness of the gas) and the fact that for most current experiments $\frac{a}{L_z} \sim \frac{1}{30}$ [46], $g \sim 9.7 \times 10^{-45}$ J m$^2$. Then $\mu \sim 2.9 \times 10^{-32}$ J. Then from (2.9), $\xi^2 \sim 2.5 \times 10^{-12}$ m$^2$. The area of the gas is given by the circle of the TF radius, $A \sim \pi R_\perp^2 \sim \frac{2\pi\mu}{m\omega_\perp^2} \sim 1.20 \times 10^{-8}$ m$^2$. Hence $A \gg \xi^2$, which means that the vortex structure is very small compared to the size of the gas. Hence, the experimental situation can be recovered from our subsequent analysis through local density approximation [21] that locally the gas is effectively homogeneous at the centre of the trap [28], which is best described by $V(\mathbf{x}) = 0$.

## 3. Euclidean action

To compute the partition function of such a system, we perform a Wick rotation by writing $t = -\mathrm{i}\tau$. To preserve the same canonical relation between the density and the phase (2.5) and to keep the density real, the phase has to be rotated accordingly by

$$\chi = -\mathrm{i}\hbar\theta. \tag{3.1}$$

whence $\exp\left(\mathrm{i}\frac{S}{\hbar}\right)$ becomes $\exp\left(-\frac{S}{\hbar}\right)$. The action in this Euclidean space is given by

$$\mathcal{S} = \int \mathrm{d}\tau\, \mathrm{d}^2\mathbf{x} \left\{\chi\frac{\partial\rho}{\partial\tau} + \mathcal{H}\right\}, \tag{3.2}$$

where the Hamiltonian density is

$$\mathcal{H} = -\frac{\rho}{2m}(\nabla\chi)^2 + F_q[\rho]. \tag{3.3}$$

Let us introduce the following dimensionless variables:

$$\tau = \frac{\hbar}{\mu}s, \qquad \mathbf{r} = \xi\mathbf{y}, \qquad \rho = \frac{\mu}{g}n, \tag{3.4}$$

and the Euclidean phase

$$\chi = \hbar\zeta. \tag{3.5}$$

With these new variables the Euclidean action (3.2) becomes

$$\mathcal{S} = \frac{\hbar\mu\xi^2}{g}\int \mathrm{d}s\, \mathrm{d}^2\mathbf{y}\left\{\zeta\frac{\partial n}{\partial s} - 2n(\nabla_y\zeta)^2 - n + \frac{n^2}{2} + \frac{(\nabla_y n)^2}{2n}\right\}. \tag{3.6}$$

Because $\Psi$ is a single-valued function its value is unchanged upon having the phase $\mathrm{i}\xi$ added by $2\pi q$, for any integer $q$, so it does not change the value of the field. As a result, for any integer $q$,

$$\oint \mathrm{d}\mathbf{l}\cdot\nabla_y\zeta = -2\pi\mathrm{i}q, \tag{3.7}$$

where the line integral goes around a loop about a point. If the vorticity $q$ is positive (negative) while the loop is small enough, there is a vortex (an antivortex) at that point whereas $q = 0$ indicates there is no vortex at that point. But if the loop of the line integral is larger, $q$ is the sum of the vorticities of all vortices inside the loop, while vortex and antivortex cancel each other in the integration. The phase may have a curl-free part even if there is a vortex. The simplest configuration representing a single vortex at the origin has $\zeta = -\mathrm{i}q\varphi$. The Euclidean angular momentum density of the system is given by

$$l = \rho\frac{\partial\chi}{\partial\varphi} = -\mathrm{i}\hbar q\rho, \tag{3.8}$$

which is proportional to $q$. The fact that the angular momentum commutes with the Hamiltonian and is conserved implies the conservation of vorticity in the whole system.

Assuming there is a vortex at the origin with the density profile $n_q(y)$, presumed to be rotationally invariant,the equation of motion is obtained by putting $\zeta = -\mathrm{i}q\varphi$ into (3.6):

$$\frac{1}{y}\frac{\mathrm{d}}{\mathrm{d}y}\left(y\frac{\mathrm{d}n_q}{\mathrm{d}y}\right) - \frac{1}{2n_q}\left(\frac{\mathrm{d}n_q}{\mathrm{d}y}\right)^2 + \left(1 - \frac{2q^2}{y^2}\right)n_q - n_q^2 = 0. \tag{3.9}$$

For $q = 0$, $n_q = 1$ exactly. In the general case, it is convenient to introduce a 'Euclidean wavefunction of the condensate' by writing $n_q = \psi_q^2$ [18, 47]. It then becomes

$$\frac{1}{y}\frac{\mathrm{d}}{\mathrm{d}y}\left(y\frac{\mathrm{d}\psi_q}{\mathrm{d}y}\right) + \frac{1}{2}\left(1 - \frac{2q^2}{y^2}\right)\psi_q - \frac{1}{2}\psi_q^3 = 0. \tag{3.10}$$

The vortex solution interpolates between the no-vortex profile $\psi_q = 1$ for $y \mapsto \infty$ and the trivial solution $\psi_q = 0$ for $y \mapsto 0$. Equation (3.10) may be solved numerically (see [18, 47]). For large $y$, we may expand $\psi_q$ in inverse powers of $y^2$:

$$\psi_q = 1 - \frac{q^2}{y^2} - \frac{[8q^2 + q^4]}{2y^4} + O\left(\frac{1}{y^6}\right). \tag{3.11}$$

Likewise for the density

$$n_q = 1 - \frac{2q^2}{y^2} - \frac{8q^2}{y^4} + O\left(\frac{1}{y^6}\right). \tag{3.12}$$

For $y \ll 1$, the cubic term in (3.10) can be neglected, and $\psi_q$ becomes a Bessel function [48]. For our purposes, it is enough to keep only the first (linear) term in the Taylor expansion of $\psi_q$. The density profile is then quadratic:

$$n_1 = 0.08\, y^2. \tag{3.13}$$

We shall adopt approximation (3.12) for $y > 2.7$ and (3.13) otherwise. The matching point and the constant in (3.13) are chosen so that the approximated density profile is smooth (see figure 1).

## 4. Linear perturbation

Consider linear perturbations around a configuration of the 2D Bose gas with a vortex at the origin:

$$n = n_q(1 + \delta), \qquad \zeta = -\mathrm{i}q\varphi + \zeta_1, \tag{4.1}$$

where $\delta = \delta(y, \varphi, s)$ and $\zeta_1 = \zeta_1(y, \varphi, s)$ are the functions of the radial and azimuthal coordinates $y$ and $\varphi$. Define the

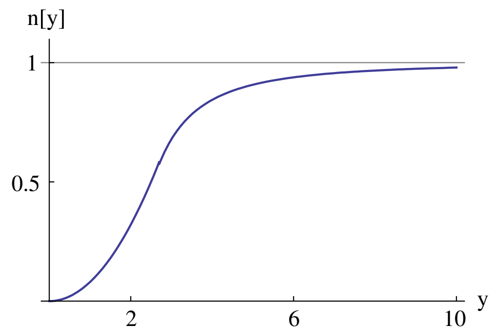


**Figure 1.** The density profile for an isolated vortex at the origin, as given by (3.13) for $y < 2.7$ and (3.11) for $y > 2.7$.

operator

$$\tilde{\nabla}_y^2 = \frac{1}{yn_q}\frac{\partial}{\partial y}\left(yn_q\frac{\partial}{\partial y}\right) + \frac{1}{y^2}\frac{\partial^2}{\partial\varphi^2}. \tag{4.2}$$

Note that for $q = 0$ (i.e. $n_q = 1$), $\tilde{\nabla}_y^2 = \nabla_y^2$. Putting perturbation (4.1) in action (3.6), it becomes

$$\begin{aligned}\mathcal{S}(q) \approx \mathcal{F}_0(q) &+ \frac{\hbar\mu\xi^2}{g}\int_0^{\mu\beta} \mathrm{d}s \int \mathrm{d}^2y \cdot n_q\delta\left(\frac{n_q}{2} - \frac{1}{2}\tilde{\nabla}_y^2\right)\delta \\ &+ \frac{\hbar\mu\xi^2}{g}\int_0^{\mu\beta} \mathrm{d}s \int \mathrm{d}^2y \cdot \zeta_1\left(2n_q\tilde{\nabla}_y^2\right)\zeta_1 \\ &+ \frac{\hbar\mu\xi^2}{g}\int_0^{\mu\beta} \mathrm{d}s \int \mathrm{d}^2y \cdot n_q\zeta_1\left(\frac{\partial}{\partial s} - \frac{4\mathrm{i}q}{y^2}\frac{\partial}{\partial\varphi}\right)\delta,\end{aligned} \tag{4.3}$$

where

$$\begin{aligned}\mathcal{F}_0(q) &= \frac{\hbar\mu\xi^2}{g}\int_0^{\mu\beta} \mathrm{d}s \int \mathrm{d}^2y \\ &\quad\cdot\left[\frac{2n_q q^2}{y^2} - n_q + \frac{n_q^2}{2} + \frac{1}{2n_q}\left(\frac{\mathrm{d}n_q}{\mathrm{d}y}\right)^2\right] \\ &= -\frac{\pi\hbar\xi^2\mu^2\beta}{g}\int \mathrm{d}y \cdot yn_q^2,\end{aligned} \tag{4.4}$$

which is the equilibrium free energy, with the second equality owing to (3.9). Then the equations of motion are given by

$$\frac{\partial\zeta_1}{\partial s} = n_q\delta + \frac{4\mathrm{i}q}{y^2}\frac{\partial\zeta_1}{\partial\varphi} - \tilde{\nabla}_y^2\delta, \tag{4.5}$$

$$\frac{\partial\delta}{\partial s} = \frac{4\mathrm{i}q}{y^2}\frac{\partial\delta}{\partial\varphi} - 4\tilde{\nabla}_y^2\zeta_1. \tag{4.6}$$

The Fourier transform of the fluctuations can be defined as

$$\delta(y,\varphi,s) = \sum_{j=-\infty}^{\infty}\delta_j(y,s)\,\mathrm{e}^{\mathrm{i}j\varphi}, \tag{4.7}$$

$$\zeta_1(y,\varphi,s) = \sum_{j=-\infty}^{\infty}\zeta_{1j}(y,s)\,\mathrm{e}^{\mathrm{i}j\varphi}. \tag{4.8}$$

If $\delta$ and $\zeta_1$ are real, then

$$\delta_j^* = \delta_{-j}, \qquad \zeta_{1j}^* = \zeta_{1-j}. \tag{4.9}$$

Representation (4.8) assumes that

$$\oint \mathrm{d}\mathbf{l}\cdot\nabla\zeta_1 = 0, \tag{4.10}$$

which means that the fluctuation does not change the total vorticity. The counterpart of $-\tilde{\nabla}_y^2$ in the Fourier representation is

$$L_{jq} = -\frac{1}{yn_q}\frac{\partial}{\partial y}\left(yn_q\frac{\partial}{\partial y}\right) + \frac{j^2}{y^2}. \tag{4.11}$$

Action (4.3) becomes

$$\begin{aligned}\mathcal{S}(q) \approx \mathcal{F}_0(q) &+ \frac{\hbar\mu\xi^2}{g}\int_0^{\mu\beta} \mathrm{d}s \int \mathrm{d}y \\ &\cdot yn_q\sum_{j=-\infty}^{\infty}\delta_{-j}\left(\frac{n_q}{2} + \frac{1}{2}L_{jq}\right)\delta_j \\ &+ \frac{\hbar\mu\xi^2}{g}\int_0^{\mu\beta} \mathrm{d}s \int \mathrm{d}y \cdot yn_q\sum_{j=-\infty}^{\infty}\zeta_{1-j}(-2L_{jq})\zeta_{1j} \\ &+ \frac{\hbar\mu\xi^2}{g}\int_0^{\mu\beta} \mathrm{d}s \int \mathrm{d}y \cdot yn_q\sum_{j=-\infty}^{\infty}\zeta_{1-j}\left(\frac{\partial}{\partial s} + \frac{4qj}{y^2}\right)\delta_j.\end{aligned} \tag{4.12}$$

This action can be further simplified. Define

$$\hat{L}_{jq} = \left[-\frac{1}{y}\frac{\partial}{\partial y}\left(y\frac{\partial}{\partial y}\right) + \frac{j^2}{y^2}\right] + \left(\frac{q^2}{y^2} - \frac{1-n_q}{2}\right). \tag{4.13}$$

Suppose $F$ and $f$ are related by $F = \frac{f}{\sqrt{n_q}}$; then $L_{jq}$ and $\hat{L}_{jq}$ are related by

$$L_{jq}F = \frac{1}{\sqrt{n_q}}\hat{L}_{jq}f. \tag{4.14}$$

Define the covariant differential operator,

$$D_{s,jq} = \frac{\partial}{\partial s} - \frac{4qj}{y^2}, \tag{4.15}$$

which can be seen as the time derivative in a frame corotating with the vortex. With the transformation of the fluctuations,

$$\delta_j = \frac{\hat{\delta}_j}{\sqrt{n_q}}, \qquad \zeta_{1j} = \frac{\hat{\zeta}_{1j}}{\sqrt{n_q}}, \tag{4.16}$$

action (4.12) is then rewritten as

$$\begin{aligned}\mathcal{S}(q) \approx \mathcal{F}_0(q) &+ \frac{\hbar\mu\xi^2}{g}\int_0^{\mu\beta} \mathrm{d}s \int \mathrm{d}y \cdot y\sum_{j=-\infty}^{\infty} \\ &\times\left[\hat{\delta}_{-j}\frac{n_q + \hat{L}_{jq}}{2}\hat{\delta}_j - \hat{\zeta}_{1-j}(2\hat{L}_{jq})\hat{\zeta}_{1j} + \hat{\zeta}_{1-j}D_{s,jq}\hat{\delta}_j\right].\end{aligned} \tag{4.17}$$

From (4.5) and (4.6), or from action (4.17), the equations of motion in terms of the new operators are

$$(n_q + \hat{L}_{jq})\hat{\delta}_j = D_{s,-jq}\hat{\zeta}_{1j}, \tag{4.18}$$

$$4\hat{L}_{jq}\hat{\zeta}_{1j} = D_{s,jq}\hat{\delta}_j. \tag{4.19}$$

## 5. Lifetime of the condensate

Consider a Bose gas confined to a region of size $L$. We define as our system a part of the Bose gas with linear size $l$ smaller than $L$ but greater than the healing length $\xi$, i.e. $L \gg l \gg \xi$. The Bose gas within this system is interacting with other atoms outside, which act as a reservoir of energy, particle number and angular momentum. Therefore the total vorticity $q$ of our system is not conserved. The equilibrium state is described by the partition function [49]

$$\mathcal{Z} = \sum_{q=-\infty}^{\infty} \int \mathrm{d}\delta\, \mathrm{d}\zeta_1 \int D[\delta] D[\zeta_1] \exp\left(-\frac{\mathcal{S}(q)}{\hbar}\right), \qquad (5.1)$$

where the periodic boundary conditions [50] $\delta = \delta(0) = \delta(\mu\beta)$ and $\zeta_1 = \zeta_1(0) = \zeta_1(\mu\beta)$ have been incorporated in the evaluation of the path integral.

Setting an upper cutoff at $y = \Lambda$, the Euclidean action (essentially the free energy divided by $k_B T$) of the system with no vortex is obtained by putting $n_0 = 1$ in (4.4)

$$\mathcal{F}(0) = -\frac{\pi\hbar\xi^2\mu^2\beta}{g} \int_0^\Lambda \mathrm{d}y \cdot y = -\frac{\pi\hbar\xi^2\mu^2\beta}{g} \frac{\Lambda^2}{2}, \qquad (5.2)$$

and that with one vortex of vorticity $q$ is obtained after putting the asympotic expressions (3.11) and (3.13) in (4.4),

$$\begin{aligned} \mathcal{F}(q) &= -\frac{\pi\hbar\xi^2\mu^2\beta}{g} \int_0^\Lambda \mathrm{d}y \cdot y n_q^2 \\ &\approx -\frac{\pi\hbar\xi^2\mu^2\beta}{g} \left(\frac{\Lambda^2}{2} - 4q^2 \ln \Lambda\right), \end{aligned} \qquad (5.3)$$

as at small $y$ the integral vanishes in both cases. As a result, adding a vortex means adding an amount of the Euclidean action

$$\Delta\mathcal{F}(q) = \frac{4\pi\hbar\xi^2\mu^2\beta q^2}{g} \ln \Lambda. \qquad (5.4)$$

Suppose $K_0$ is the fluctuation factor calculated from the path integral in (5.1) around the $q = 0$ configuration, and $K_0 K_1$ is that around the $q = 1$ configuration. If $\kappa_{jq}^{\alpha\,2}$'s are the eigenvalues of $\hat{L}_{jq}$, then the partition function of the $q = 0$ case is given by [51]

$$K_0 = \prod_{\alpha,j} \frac{1}{2\sinh \frac{\sqrt{4\kappa_{j0}^{\alpha\,2}(1+\kappa_{j0}^{\alpha\,2})}\mu\beta}{2}}. \qquad (5.5)$$

For $q = 1$, the translation invariance of the vortices gives rise to the existence of the zero modes [52]. We know that we can generate solutions with $\omega = 0$ by simply moving the vortex around. Since the vortex is already rotation invariant, it is enough to consider a vortex centred at $x = R$. The displaced vortex solution is given by $n = n_q(y')$, $\zeta = q\varphi'$, where

$$y' = \sqrt{y^2 + R^2 - 2yR\cos\varphi}, \qquad y'\sin\varphi' = y\sin\varphi. \qquad (5.6)$$

For small $R$ we have

$$y' = y - R\cos\varphi, \qquad \varphi' = \varphi + \frac{R}{y}\sin\varphi, \qquad (5.7)$$

and the deviation from the centred vortex is

$$\bar{\zeta}_1 = \frac{qR}{y}\sin\varphi, \qquad \bar{\delta} = -R\frac{1}{n_q}\frac{\mathrm{d}n_q}{\mathrm{d}y}\cos\varphi. \qquad (5.8)$$

Then the zero-mode action $S_0$ is given by

$$S_0 \approx S[\bar{\delta}, \bar{\zeta}_1]. \qquad (5.9)$$

If $\hat{\Lambda}_0$ is the operator for $q = 0$ and $\hat{\Lambda}_1$ for $q = 1$, then the fluctuation factor is given by

$$K_1 = \left[\frac{\det \hat{\Lambda}_0}{\det \hat{\Lambda}_1}\right]^{\frac{1}{2}} = \sqrt{\frac{S_0}{2\pi\hbar}} \left[\frac{\det \hat{\Lambda}_0}{\det' \hat{\Lambda}_1}\right]^{\frac{1}{2}}, \qquad (5.10)$$

where the second equality is due to the existence of a zero mode because of the translational invariance of the vortices [41, 42], and det′ is the determinant excluding the zero mode. The ratio of the determinants is given by the Gelfand–Yaglom theorem [53, 54].

Now consider the situation where more than one vortex is formed. In the dilute gas approximation the vortices are assumed to be far apart so adding $n$ vortices of vorticity $q = 1$ increases the Euclidean action by $n\Delta\mathcal{F}(1)$ [40, 41]. From a statistical ensemble of different numbers of vortices $n$, the partition function is given by

$$\begin{aligned} \mathcal{Z} &\approx \mathrm{e}^{-\frac{\mathcal{F}_0(0)}{\hbar}} \sum_{n=0}^{\infty} \int \mathrm{d}^2 y_1 \int \mathrm{d}^2 y_2 \ldots \int \mathrm{d}^2 y_n \cdot \frac{1}{n!} K_0 (K_1)^n\, \mathrm{e}^{-n\frac{\Delta\mathcal{F}}{\hbar}} \\ &= K_0 \exp\left(-\frac{\mathcal{F}_0(0)}{\hbar} + \Lambda^2 K_1\, \mathrm{e}^{-\frac{\Delta\mathcal{F}}{\hbar}}\right), \end{aligned} \qquad (5.11)$$

where the integrations over the space have an upper cutoff $\Lambda^2$, and the factor $\frac{1}{n!}$ is due to the indistinguishability of the vortices. The decay probability per unit time of the configuration from $q = 0$ to 1 is [40]

$$\Gamma = -\frac{2}{\hbar}\mathrm{Im}\mathcal{F} = \frac{1}{\hbar\beta}\mathrm{Im}(K_1)\, \mathrm{e}^{-\frac{\Delta\mathcal{F}(1)}{\hbar} + 2\ln\Lambda}. \qquad (5.12)$$

From the expression of the decay probability, the BKT transition temperature can be read off from the exponential factor since the formation occurs at a reasonable rate as $\mathrm{e}^{-\frac{\Delta\mathcal{F}}{\hbar} + 2\ln\Lambda} \sim 1$. It is given by

$$T_{\mathrm{BKT}} \approx \frac{2\pi\xi^2\mu^2}{gk_B} = \frac{\pi\hbar^2\rho_0}{2mk_B}, \qquad (5.13)$$

where the definition of the healing length $\xi$ in (2.9) is used and $\rho_0 = \mu/g$ [18] is the number density of the lowest macroscopically occupied state of the homogeneous configuration $n_0 = 1$. This agrees with the known results in the original BKT theory [5][4]. The correction due to non-homogeneous configuration in the transition temperature is given in [27, 55].

Because $K_1$ is given as the square root of the ratio of the determinants of two differential operators, we expect that it is of order 1. Then by dimensional analysis, $\Gamma \sim \frac{1}{\hbar\beta} \sim 13.1\ \mathrm{ms}^{-1}$.[5] The average time of vortex formation is then of the order of 0.08 ms. The numerical estimation of the vortex nucleation rate around the transition temperature with the estimated numerical parameters listed in section 2 is plotted as shown in figure 2. The vortex formation is very slow below the transition temperature but it increases drastically when the temperature increases past the critical point.

[4] Another way of writing the equation is $\rho_0\lambda^2 = 4$ [20], where $\lambda = \sqrt{\frac{2\pi\hbar^2}{mk_B T}}$ is the thermal length.

[5] The cutoff is the dimensionless length of the size of the Bose gas, which is set to be $\Lambda = \sqrt{\frac{R_\perp}{\xi}} \sim 40$.

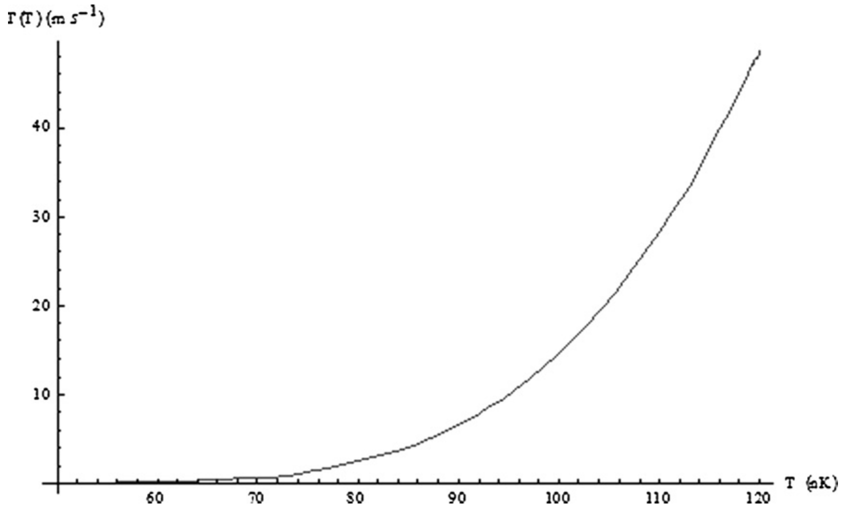


**Figure 2.** The rate of vortex nucleation around the BKT transition temperature.

## 6. Computing the imaginary part of the free energy

The expression for the decay rate in (5.12) shows that under the dilute gas approximation the stability of the canonical equilibrium hinges on whether the path integral over fluctuations around a one-vortex configuration is complex.

Recall that the action for a linearized fluctuation is given by (4.17), where the $\hat{L}_{jq}$ operators are defined in (4.13). We perform the Gaussian path integration over $\zeta_1$ to obtain

$$\mathcal{S}(q) \approx \mathcal{F}_0(q) + \frac{\hbar\mu\xi^2}{g}\int_0^{\mu\beta} \mathrm{d}s \int \mathrm{d}y \cdot y \sum_{j=-\infty}^{\infty} \times \left[\hat{\delta}_{-j}\frac{n_q + \hat{L}_{jq}}{2}\hat{\delta}_j + \frac{1}{8}\left(\hat{L}_{jq}^{-1}D_{s,-jq}\hat{\delta}_{-j}\right)\left(D_{s,jq}\hat{\delta}_j\right)\right]. \tag{6.1}$$

If the $\hat{L}_{jq}$ operators are positive definite, it is clear that the path of steepest descent away from the stationary point corresponds to real $\delta_j$, and the path integral is real.

This is indeed so when we are considering fluctuations around a homogeneous configuration, namely $q = 0$, $n_q = 1$. In this case, the eigenvectors of $\hat{L}_{j0}$ are Bessel functions of order $j$. The requirement that the Euclidean action must be finite means that we only need to consider eigenfunctions which do not diverge at infinity and are regular at the origin. The only Bessel functions satisfying these conditions are of the form $J_j[\kappa y]$ corresponding to a positive eigenvalue $\kappa^2$. Thus, we conclude that the no-vortex state is stable at zero temperature, when the no-vortex configuration is the only finite action extremal point in the partition function.

Let us see if this argument carries over for nonzero $q$. For simplicity, we set $q = 1$ (however, we shall leave $q$ explicit). We seek finite action solutions to the equation

$$\hat{L}_{jq}F_{jq}^{\kappa}(y) = -\kappa^2 F_{jq}^{\kappa}(y), \tag{6.2}$$

with real $\kappa$. The further change of variables,

$$F_{jq}^{\kappa}(y) = \frac{f_{jq}^{\kappa}(y)}{\sqrt{y}}, \tag{6.3}$$

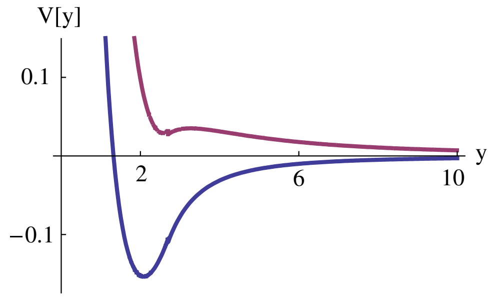


**Figure 3.** The effective potential (6.5) for $j = 1$ (upper curve) and $j = 0$ (lower curve). We have used the profile in figure 1 to compute $n_q$. We see that for $j = 1$ there can be no negative energy state, even more so for larger values of $j$. For $j = 0$, on the other hand, the potential is negative for large enough values of $y$. The existence of a negative energy state is shown by the Bohr–Sommerfeld condition as in (6.6).

reduces the left-hand side to a Schrödinger operator

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}y^2} + V_{jq}(y)\right] f_{jq}^{\kappa}(y) = -\kappa^2 f_{jq}^{\kappa}(y), \tag{6.4}$$

where

$$V_{jq}(y) = \frac{j^2 + q^2 - \frac{1}{4}}{y^2} - \frac{1}{2}(1 - n_q(y)). \tag{6.5}$$

Therefore, the question of whether the Euclidean action for linearized fluctuations around an isolated vortex is positive definite becomes whether a one-dimensional particle of mass $1/2$ in potential (6.5) admits a negative energy state. Now, the potential happens to be everywhere positive for all $j > 0$, so we may discard this possibility outright unless $j = 0$ (see figure 3).

In the $j = 0$ case there is a well-defined potential well, and we must investigate whether it is deep enough to support a bound state. One possibility is to check the Bohr–Sommerfeld condition, namely whether there is a value of $\kappa$ such that

$$\int_{y_-}^{y_+} \mathrm{d}y\sqrt{-\kappa^2 - V_{01}(y)} = \frac{\pi}{2}, \tag{6.6}$$

where $y_\pm$ are the classical turning points, namely the roots of $\kappa^2 + V_{01}(y) = 0$. The answer turns out to be yes though just barely. Under the approximation given in figure 1 for the density profile, the Bohr–Sommerfeld condition is satisfied for $\kappa = 0.024$. The turning points are located at $y_- = 1.32$ and $y_+ = 21.2$. Bohr–Sommerfeld quantization would also predict bound excited states; however, these states fall beneath the accuracy of our approximations, and they may be considered artefacts. For example, according to Bohr–Sommerfeld quantization the first excited state appears at $\kappa = 4 \times 10^{-5}$, with the outer turning point at $y = 12\,500$. This is beyond the intended size of the original homogeneous patch, because from the numerical estimation in section 2, the size of the patch in the dimensionless unit is $\sqrt{\frac{R_\perp}{\xi}} \sim 40$, which is far less than 12 500.[6]

Observe that not only have we shown that the Euclidean action for axially symmetric perturbations of the isolated vortex is not positive definite, but we have also characterized the eigenvector corresponding to the direction in configuration space where it becomes negative. Since $n_q$ does not commute with $\hat{L}_{01}$, this eigenvector does not correspond to an actual solution of the linearized fluctuations. However, its existence is enough to show that the free energy acquires an imaginary part.

## 7. Summary and discussions

In this work we have calculated the rate of decay of an effectively homogeneous 2D Bose gas (described by $V(\mathbf{x}) = 0$), in the form of $A\,\mathrm{e}^{-\frac{B}{T}}$, which complies with the well-known Arrhenius law. The prefactor $A$ is proportional to the imaginary part of the fluctuation factor of the free energy of a one-vortex configuration in the path integral. It is known that this imaginary part is due to the negative eigenvalue of the fluctuation operator belonging to the eigenvector that defines the direction the fluctuation spontaneously grows along (in real time). The qualitative features are like those in the decay of a metastable state due to classical fluctuations [38] and barrier penetration due to quantum fluctuations around the instanton solution of the Euclidean action [40]. We find that the imaginary part comes from the axially symmetric modes for nonzero vorticity configurations. As a result, we conclude that while at $T = 0$, the gas without any vortex is stable, the canonical ensemble of different numbers of vortices of the gas is unstable at any finite temperature.

Using the fact that at the BKT transition $A\,\mathrm{e}^{-\frac{B}{T}} \sim 1$ we derived the BKT transition temperature $T_{\mathrm{BKT}}$ in terms of the number density of the homogeneous phase given in (5.13). This expression derived via thermal field theory provides a more quantitative alternative to that originally derived from thermodynamics considerations of the competition between the energy and the entropy of a vortex [5]. It is known that isolated free vortices are formed in the normal phase above the BKT temperature. Hence the decay rate calculated here is also the rate of vortex formation. Our calculations show how it increases with temperature. The probability of the creation of vortex pairs in a trapped gas increases with temperature as well, as indicated by simulation studies with the PGPE [24].

In the experiments, measurements on the gas are made some time after the confining potential is abruptly turned off. In Dalibard group's experiment there are more isolated free vortices (measured by the dislocation of interference pattern of two planes of gas) at higher temperature after 20 ms time of flight (TOF) [32]. Our results are consistent with this finding in that the rate of isolated vortex formation increases with temperature. In Phillips group's experiment [34], they observed different characteristics on the density profile below and above the BKT temperature after 10 ms TOF, which is at a rate slower than the rate of the formation of isolated vortices. However, since we have assumed a homogeneous, time-independent configuration as starting point, this should factor in the comparison of our results with experiments. Further studies to bridge these gaps are desirable.

[6] This series of excited states is due to the fact that the integral in (6.6) diverges logarithmically when $\kappa \mapsto 0$. However, the Bohr–Sommerfeld approximation breaks down in this limit. This can be seen by approximating the density profile as $n_1 = 1 - 2/y^2$ for $y > \sqrt{2}$, $n_1 = 0$ otherwise. In this case the Bohr–Sommerfeld integral displays the same small-$\kappa$ behaviour, but (6.4) may be solved analytically and shows no bound states. The existence of a negative energy solution to (6.4) depends critically on the effective potential being deeper than just $1/y^2$, and may be confirmed by independent perturbative calculations.

## Acknowledgments

K-yH thanks Professor Theodore Kirkpatrick for his interest and support, and Anand Ramanathan for useful descriptions of the Phillips group's experiment. This work is supported in part by CONICET, ANPCyT and University of Buenos Aires (Argentina), grants from NIST in the cold atom program, NSF in the ITR program and under grant no DMR-09-01902 to the University of Maryland.

## References

[1] Mermin N D and Wagner H 1966 Absence of ferromagnetism or antiferromagnetism in one- or two-dimensional isotropic Heisenberg models *Phys. Rev. Lett.* **17** 1133

[2] Hohenberg P C 1967 Existence of long-range order in one and two dimensions *Phys. Rev.* **158** 383

[3] Coleman S 1973 There are no Goldstone bosons in two dimensions *Commun. Math. Phys.* **31** 259

[4] Berezinskii V L 1971 Destruction of long-range order in one-dimensional and two-dimensional systems having a continuous symmetry group: I. Classical systems *Sov. Phys.—JETP* **32** 493

[5] Kosterlitz J M and Thouless D J 1973 Ordering, metastability and phase transitions in two-dimensional systems *J. Phys. C: Solid State Phys.* **6** 1181

[6] Al Khawaja U, Andersen J O, Proukakis N P and Stoof H T C 2002 Low-dimensional Bose gases *Phys. Rev.* A **66** 013615

[7] How P-T and LeClair A 2010 Critical point of the two-dimensional Bose gas: an *S*-matrix approach *Nucl. Phys.* B **824** 415

[8] Gräter M and Wetterich C 1995 Kosterlitz–Thouless phase transition in the two-dimensional linear $\sigma$ model *Phys. Rev. Lett.* **75** 378

[9] Gersdorff G V and Wetterich C 2001 Nonperturbative renormalization flow and essential scaling for the Kosterlitz–Thouless transition *Phys. Rev.* B **64** 054513

[10] Floerchinger S and Wetterich C 2009 Superfluid Bose gas in two dimensions *Phys. Rev.* A **79** 013601
[11] Popov V N 1973 Quantum vortices and phase transitions in Bose systems *Sov. Phys.—JETP* **37** 341
[12] Popov V N 1987 *Functional Integrals and Collective Excitations* (Cambridge: Cambridge University Press) chapter 8
[13] Chu H-C and Williams G A 2000 Quenched Kosterlitz–Thouless superfluid transition *Phys. Rev. Lett.* **86** 2585
[14] Arovas D P and Auerbach A 2008 Quantum tunneling of vortices in two-dimensional superfluids *Phys. Rev.* B **78** 094508
[15] Lindner N H, Auerbach A and Arovas D P 2008 Vortex quantum dynamics of two-dimensional lattice bosons *Phys. Rev. Lett.* **102** 070403
[16] Joseph Wang C-C, Duine R A and MacDonald A H 2010 Quantum vortex dynamics in two-dimensional neutral superfluids *Phys. Rev.* A **81** 013609
[17] Gross E P 1963 Hydrodynamics of a superfluid condensate *J. Math. Phys.* **4** 195
[18] Ginzburg V L and Pitaevskii L P 1958 On the theory of superfluidity *Sov. Phys.—JETP* **34** 858
[19] Pu H, Law C K, Eberly J H and Bigelow N P 1999 Coherent disintegration and stability of vortices in trapped Bose condensates *Phys. Rev.* A **59** 1533
[20] Prokof'ev N, Ruebenacker O and Svistunov B 2001 Critical point of a weekly interacting two-dimensional Bose gas *Phys. Rev. Lett.* **87** 270402
[21] Prokof'ev N and Svistunov B 2002 Two-dimensional weakly interacting Bose gas in the fluctuation region *Phys. Rev.* A **66** 043608
[22] Davis M J, Morgan S A and Burnett K 2002 Simulations of thermal Bose fields in the classical limit *Phys. Rev.* A **66** 053618
[23] Hutchinson D A W and Blakie P B 2006 Phase transitions in ultra-cold two-dimensional Bose gases *Int. J. Mod. Phys.* B **20** 5224
[24] Simula T P and Blakie P B 2006 Thermal activation of vortex–antivortex pairs in quasi-two-dimensional Bose–Einstein condensates *Phys. Rev. Lett.* **96** 020404
[25] Shumayer D and Hutchinsin D A W 2007 Thermodynamically activated vortex-dipole formation in a two-dimensional Bose–Einstein condensate *Phys. Rev.* A **75** 015601
[26] Simula T P, Davis M J and Blakie P B 2008 Superfluidity of an interacting trapped quasi-two-dimensional Bose gas *Phys. Rev.* A **77** 023618
[27] Holzmann M, Chevallier M and Krauth W 2008 Semiclassical theory of the quasi-two-dimensional trapped Bose gas *Europhys. Lett.* **82** 30001
[28] Bisset R N, Baillie D and Blakie P B 2009 Analysis of the Holzmann–Chevallier–Krauth theory for the trapped quasi-two-dimensional Bose gas *Phys. Rev.* A **79** 013602
[29] Bisset R N, Davis M J, Simula T P and Blakie P B 2009 Quasi-condensation and coherence in the quasi-two-dimensional trapped Bose gas *Phys. Rev.* A **79** 033626
[30] Bisset R N and Blakie P B 2009 Quantitative test of the mean-field description of a trapped two-dimensional Bose gas *Phys. Rev.* A **80** 045603
[31] Bisset R N and Blakie P B 2009 Transition region properties of a trapped quasi-two-dimensional degenerate Bose gas *Phys. Rev.* A **80** 035602
[32] Hadzibabic Z, Krüger P, Cheneau M, Battelier B and Dalibard J 2007 Berezinskii–Kosterlitz–Thouless crossover in a trapped atomic gas *Nature* **441** 1118
[33] Krüger P, Hadzibabic Z and Dalibard J 2007 Critical point of an interacting two-dimensional atomic Bose gas *Phys. Rev. Lett.* **99** 040402
[34] Cladé P, Ryu C, Ramanathan A, Helmerson K and Phillips W D 2009 Observation of a 2D Bose gas: from thermal to quasi-condensate to superfluid *Phys. Rev. Lett.* **102** 170401
[35] Calzetta E and Hu B-L 2008 *Nonequilibrium Quantum Field Theory* (Cambridge: Cambridge University Press) chapter 13.3
[36] Rubakov V 2002 *Classical Theory of Gauge Fields* (Princeton, NJ: Princeton University Press)
[37] Langer J S 1968 Theory of nucleation rates *Phys. Rev. Lett.* **21** 973
[38] Langer J S 1969 Statistical theory of the decay of metastable states *Ann. Phys.* **54** 258
[39] Coleman S 1977 Fate of the false vacuum: semiclassical theory *Phys. Rev.* D **15** 2929
[40] Callan C G Jr and Coleman S 1977 Fate of the false vacuum: II. First quantum corrections *Phys. Rev.* D **16** 1762
[41] Coleman S 1985 *Aspects of Symmetry* (Cambridge: Cambridge University Press) chapter 7
[42] Affleck I K and De Luccia F 1979 Induced vacuum decay *Phys. Rev.* D **20** 3168
[43] Affleck I 1981 Quantum-statistical metastability *Phys. Rev. Lett.* **46** 388
[44] Haldane F D M 1981 Effective harmonic-fluid approach to low-energy properties of one-dimensional quantum fluids *Phys. Rev. Lett.* **47** 1840
[45] Calzetta E, Hu B L and Rey A M 2006 Bose–Einstein-condensate superfluid-Mott-insulator transition in an optical lattice *Phys. Rev.* A **73** 023610
[46] Hadzibabic Z and Dalibard J 2009 Two-dimensional Bose fluids: an atomic physics perspective, arXiv:0912.1490
[47] Lifshitz L M and Pitaevskii L P 1990 *Statistical Physics, Part 2 (Course of Theoretical Physics* vol 9*)* (Oxford: Pergamon) chapter 30
[48] Barnett R, Chen E and Refael G 2010 Vortex synchronization in Bose–Einstein condensates: a time-dependent Gross–Pitaevskii equation approach *New J. Phys.* **13** 043004
[49] Altland A and Simons B 2006 *Condensed Matter Field Theory* (Cambridge: Cambridge University Press) chapter 9
[50] Negele J W and Orland H 1998 *Quantum Many-Particle Systems* (New York: Perseus) chapter 2.2
[51] Feynman R P 1972 *Statistical Mechanics* (Reading, MA: Addison-Wesley) chapter 3
[52] Rajaraman R 1987 *Solitons and Instantons* (New York: Elsevier) chapter 10
[53] Gelfand I M and Yaglom A M 1960 Integration in functional spaces and its applications in quantum physics *J. Math. Phys.* **1** 48
[54] Dunne G V 2008 Functional determinants in quantum field theory *J. Phys. A: Math. Theor.* **41** 304006
[55] Holzmann M and Krauth W 2008 Kosterlitz–Thouless transition of the quasi two-dimensional trapped Bose gas *Phys. Rev. Lett.* **100** 190402