

Bose–Hubbard Model in the Rotating Frame of Reference

T.P. POLAK*

Faculty of Physics, Adam Mickiewicz University of Poznań, Umultowska 85, 61-614 Poznań, Poland

AND T.K. KOPEĆ

Institute for Low Temperatures and Structure Research, Polish Academy of Sciences

POB 1410, 50-950 Wrocław 2, Poland

Following a novel experimental arrangement which can rotate a two-dimensional optical lattice at frequencies up to several kilohertz we discuss the ground state of the two-dimensional Bose–Hubbard Hamiltonian, relevant for rotating gaseous Bose–Einstein condensates, by employing U(1) quantum rotor approach and the topologically constrained path integral. Ultracold atoms in such a rotating lattice can be used for the direct quantum simulation of strongly correlated systems under large effective magnetic fields. We derive an effective quantum action for the Bose–Hubbard model, which enables a non-perturbative treatment of the zero-temperature phase transition in the rotating frame. We calculate the ground-state phase diagram, analytically deriving maximum repulsive energy for several rational values of the frustration rotation parameter $f = 0, 1/2, 1/3, 1/4,$ and $1/6$ for the square and triangular lattice. Performed calculations revealed strong non-monotonical dependence of the critical ratio of the kinetic energy to the repulsive on-site energy, that separates the global coherent from the insulating state, on topology of the lattice.

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1. Introduction

Systems of ultracold atoms confined in optical lattices [1–3] facilitate an experimental environment, where a rich variety of quantum many-body models can be implemented in a wide range of spatial dimensions, geometries, and particle interactions. Surprisingly, the quantum phase transitions in systems under uniform magnetic field can be also analyzed considering rotating Bose–Einstein condensates [4–6] trapped in a two-dimensional (2D) lattice potential. In a frame of reference rotating about the z -axis with angular velocity Ω the kinetic term in Hamiltonian is equivalent to that of a particle of charge q experiencing a magnetic field B with $qB = 2m\Omega$, where m is the mass of the particle [7, 8]. This connection shows that the Coriolis force in the rotating frame plays the same role as the Lorentz force on a charged particle in a uniform magnetic field [9, 10]. The presence of angular velocity induces vortices in the system described by the rotation frustration parameter f ($\equiv ma^2\Omega/\pi\hbar$, with a being the lattice spacing).

The aim of this work is to study the superfluid to Mott-insulator zero-temperature phase transition by means of the Bose–Hubbard (BH) model in two-dimensional rotating optical condensates with different geometries. We address the question of evolution of the ground state phase

diagram for the system with various angular velocities for square and triangular lattices. To elucidate the quantum phase transition in optical lattices, where the kinetic energy scale is less than the dominating interaction energy and angular velocity is comparable to the recoil energy, we have adopted a theoretical approach for strongly interacting fermions [11] to the BH model in a way to include the effects of particle number fluctuations and make the qualitative phase diagrams more quantitative [12].

The outline of the paper is as follows first, we introduce the model Hamiltonian and the effects of rotation are discussed. Next, we derive an effective U(1) action in the quantum rotor representation and present the resulting phase diagrams for two-dimensional square and triangular Bose–Hubbard systems in rotating frame. Finally, we summarize our results.

2. Model

In optical lattices the two main energy scales are set by the hopping amplitude proportional to t (that sets the kinetic energy scale for bosons) due to the particles tunneling, and the on-site interaction $U > 0$. The competition between the kinetic energy, which is gained by delocalizing bosons over lattice sites and the repulsive interaction energy, which disfavors having more than one particle at any given site, can be modeled by the following quantum Bose–Hubbard Hamiltonian [13]:

* corresponding author; e-mail: tpolak@amu.edu.pl

$$\mathcal{H} = \frac{U}{2} \sum_{\mathbf{r}} n_{\mathbf{r}} (n_{\mathbf{r}} - 1) - \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} t_{\mathbf{r}\mathbf{r}'} a_{\mathbf{r}}^{\dagger} a_{\mathbf{r}'} - \mu \sum_{\mathbf{r}} n_{\mathbf{r}}, \quad (1)$$

where $a_{\mathbf{r}}^{\dagger}$ and $a_{\mathbf{r}'}$ stand for the bosonic creation and annihilation operators that obey the canonical commutation relations $[a_{\mathbf{r}}, a_{\mathbf{r}'}^{\dagger}] = \delta_{\mathbf{r}\mathbf{r}'}$, $n_{\mathbf{r}} = a_{\mathbf{r}}^{\dagger} a_{\mathbf{r}}$ is the boson number operator on the site \mathbf{r} , and the chemical potential μ controls the number of bosons. Here, $\langle \mathbf{r}, \mathbf{r}' \rangle$ identifies summation over the nearest-neighbor sites. Furthermore, $t_{\mathbf{r}\mathbf{r}'}$ is the hopping matrix element with dispersion $t_{\mathbf{k}}^{\square, \Delta}$.

In the fast rotation regime the physics of the Bose–Einstein condensates is very reminiscent of that of charged particle in magnetic field. An angular velocity enters the Hamiltonian Eq. (1) through the Peierls phase factor according to

$$t_{\mathbf{r}\mathbf{r}'} \rightarrow t_{\mathbf{r}\mathbf{r}'} \exp\left(\frac{2\pi i}{\kappa} \int_{\mathbf{r}}^{\mathbf{r}'} \mathbf{A} \cdot d\mathbf{l}\right), \quad (2)$$

where $\mathbf{A}(\mathbf{r}) = \boldsymbol{\Omega} \times \mathbf{r}$ is the equivalent of a magnetic vector appearing from the rotation and $\kappa = h/m$ is the quantum circulation unit. Thus, the phase shift on each site is determined by the vector potential $\mathbf{A}(\mathbf{r})$ and in typical experimental situations can be entirely ascribed to the external magnetic field/angular velocity. From Eq. (2) it follows that the properties of the system will be periodic with a period corresponding to $f = \pi \hbar \Omega / 2E_{\text{R}}$ per plaquette. Of special interest are the values of the angular momentum which correspond to rational numbers of $f = 1/2, 1/3, 1/4, \dots$

3. Description of the method

We write the partition function of the system switching from the particle-number representation to the conjugate phase representation of the bosonic degrees of freedom using the bosonic path-integral over the complex fields $a_{\mathbf{r}}(\tau)$ depending on the “imaginary time” $0 \leq \tau \leq \beta \equiv 1/k_{\text{B}}T$ with T being the temperature

$$\mathcal{Z} = \int [\mathcal{D}\bar{a}\mathcal{D}a] \exp\left(-\int_0^{\beta} d\tau \mathcal{H}(\tau) - \sum_{\mathbf{r}} \int_0^{\beta} d\tau \bar{a}_{\mathbf{r}}(\tau) \frac{\partial}{\partial \tau} a_{\mathbf{r}}(\tau)\right). \quad (3)$$

We decouple the interaction term in Eq. (1) by a Gaussian integration over the auxiliary scalar potential fields in which periodic parts $V'_{\mathbf{r}}(\tau) \equiv V'_{\mathbf{r}}(\tau + \beta)$ couple to the local particle number through the Josephson-like relation $\dot{\phi}_{\mathbf{r}}(\tau) = V'_{\mathbf{r}}(\tau)$, where

$$\dot{\phi}_{\mathbf{r}}(\tau) \equiv \frac{\partial \phi_{\mathbf{r}}(\tau)}{\partial \tau} = e^{-\phi_{\mathbf{r}}(\tau)} \frac{1}{i} \frac{\partial}{\partial \tau} e^{\phi_{\mathbf{r}}(\tau)}. \quad (4)$$

Next, we perform the local gauge transformation to the *new* bosonic variables

$$\begin{bmatrix} a_{\mathbf{r}}(\tau) \\ \bar{a}_{\mathbf{r}}(\tau) \end{bmatrix} = \begin{bmatrix} e^{i\phi_{\mathbf{r}}(\tau)} & 0 \\ 0 & e^{-i\phi_{\mathbf{r}}(\tau)} \end{bmatrix} \begin{bmatrix} b_{\mathbf{r}}(\tau) \\ \bar{b}_{\mathbf{r}}(\tau) \end{bmatrix}, \quad (5)$$

that removes the imaginary term $-i \int_0^{\beta} d\tau \dot{\phi}_{\mathbf{r}}(\tau) n_{\mathbf{r}}(\tau)$ from all the Fourier modes except at zero frequency. We

parametrize the boson fields $b_{\mathbf{r}}(\tau) = b_0 + b'_{\mathbf{r}}(\tau)$ and incorporate fully our calculations to the phase fluctuations governed by the gauge group $U(1)$. Assuming nonfluctuating amplitude at low temperatures $b_{\mathbf{r}}(\tau) = b_0$, we drop the correction, which was proved to be justified in the large U/t limit we are interested in [12, 14]. It is very convenient to define the order parameter $\Psi_{\text{B}} \equiv \langle a_{\mathbf{r}}(\tau) \rangle = \langle b_{\mathbf{r}}(\tau) \exp(i\phi_{\mathbf{r}}(\tau)) \rangle = b_0 \psi_{\text{B}}$, which signals the emergence of the superfluid phase (SF) and vanishes in the Mott-insulator (MI) state. The explicit value of the amplitude b_0 can be obtained from minimization of the Hamiltonian $\partial \mathcal{H}(b_0) / \partial b_0 = 0$. The SF state is characterized by spontaneous breaking of the $U(1)$ symmetry of the Bose–Hubbard Hamiltonian. Let us note that a nonzero value of the amplitude b_0 is *not sufficient* for superfluidity. To achieve this, also the phase variables ϕ must become stiff and coherent, which implies $\psi_{\text{B}} \neq 0$. In the symmetry broken state, with a finite expectation value of $a_{\mathbf{r}}(\tau)$, different phases ϕ_1, \dots, ϕ_n of the condensate lead to degenerate ground states. By integrating out the auxiliary static field $V_{\mathbf{r}0}$ we calculate the partition function with an effective action expressed in the form of the propagator \hat{G} :

$$\mathcal{Z} = \int [\mathcal{D}\phi] e^{-\sum_{\mathbf{r}} \int_0^{\beta} d\tau \left[\frac{1}{2U} \dot{\phi}_{\mathbf{r}}^2(\tau) + \frac{1}{i} \frac{\bar{\mu}}{U} \dot{\phi}_{\mathbf{r}}(\tau) \right] + \text{Tr} \ln \hat{G}^{-1}}, \quad (6)$$

where $\bar{\mu}/U = \mu/U + 1/2$ is the shifted reduced chemical potential. In the above $\exp(-\text{Tr} \ln \hat{G}^{-1}) \equiv \det \hat{G}$. Expanding the trace of the logarithm we have finally an effective action expressed *only* in the *phase* fields variable

$$\mathcal{S}_{\text{phase}}[\phi] = \int_0^{\beta} d\tau \left\{ \sum_{\mathbf{r}} \left[\frac{1}{2U} \dot{\phi}_{\mathbf{r}}^2(\tau) + \frac{1}{i} \frac{\bar{\mu}}{U} \dot{\phi}_{\mathbf{r}}(\tau) \right] - \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} e^{i\phi_{\mathbf{r}}(\tau)} J_{\mathbf{r}\mathbf{r}'} e^{-i\phi_{\mathbf{r}'}(\tau)} \right\}, \quad (7)$$

where the phase stiffness coefficient is given by $J_{\mathbf{r}\mathbf{r}'} = b_0^2 t_{\mathbf{r}\mathbf{r}'}$. Following as usual [11, 12] the quantum rotor approach we evaluate order parameter ψ_{B} in the thermodynamic limit $N \rightarrow \infty$ by the saddle point method $\delta \mathcal{F} / \delta \lambda = 0$ and the unimodular condition of the $U(1)$ phase variables translates into the equation

$$1 - \psi_{\text{B}}^2 = \frac{1}{N\beta} \sum_{\mathbf{k}, \nu} \frac{1}{\lambda - J_{\mathbf{k}} + \gamma^{-1}(\omega_{\nu})}. \quad (8)$$

The phase boundary is determined by the divergence of the order parameter susceptibility $\lambda_0 - J_{p/q}^{\text{max}} + \gamma^{-1}(\omega_{\nu=0}) = 0$ which determines the critical value of the Lagrange parameter $\lambda = \lambda_0$, that stays constant in the whole global coherent phase. To proceed, it is desirable to introduce the density of states for a 2D lattice in the rotating frame in the form $\rho_{p/q}^{\square, \Delta}(\xi) = \frac{1}{N} \sum_{\mathbf{k}} \delta(\xi - t_{\mathbf{k}}^{\square, \Delta} / t)$ with $t_{\mathbf{k}}^{\square, \Delta}$ being the Fourier transform of the hopping matrix elements. In this context the quantity $J_{p/q}^{\text{max}}$ represents the maximum of the spectrum described by the DOS. The problem of computing of $\rho_{p/q}^{\square, \Delta}(\xi)$ reduces effectively to the solution of the Harper equation relevant, e.g., to tight binding electrons on a two-dimensional lat-

tice with an uniform magnetic flux per unit plaquette. With the help of the above and after summation over the Bose–Matsubara frequency ω_ν , the superfluid state order parameter becomes

$$1 - \psi_B^2 = \frac{1}{2} \int_{-\infty}^{+\infty} \frac{\rho_{p/q}^{\square, \Delta}(\xi) d\xi}{\sqrt{2\xi \left(2z \frac{t}{U} + \frac{\mu}{U} + \frac{1}{2} \right) \frac{t}{U} + v^2 \left(\frac{\mu}{U} \right)}}. \quad (9)$$

In Eq. (9) $v(\mu/U) = \text{frac}(\mu/U) - 1/2$, where $\text{frac}(x) = x - [x]$ is the fractional part of the number and $[x]$ is the floor function which gives the greatest integer less than or equal to x ; $\xi = J_{p/q}^{\max} - \xi$ where $J_{p/q}^{\max}$ stands for the maximum value of the dispersion spectrum $t_{\mathbf{k}}^{\square, \Delta}$ and z is the lattice coordination number.

4. Phase diagrams

In Fig. 1 the zero-temperature phase diagram of the homogeneous Bose–Hubbard model Eq. (1) calculated from Eq. (9) is shown schematically as a function of t/U , with the density controlled by a chemical potential μ/U . At $U/t \rightarrow 0$, the kinetic energy dominates and the ground state is a delocalized superfluid, described by nonzero value of the superfluid order parameter $\Psi_B \neq 0$. At small values of t/U , interactions dominate and one obtains a series of MI lobes with fixed integer filling $n_B = 1, 2, \dots$ [12, 13]. The transition between the SF and MI phases is associated with the loss of long-range order. Let us introduce the notation for the maximum of the critical value for parameter t/U (as a function of the normalized chemical potential μ/U) at the tip of the first ($n_B = 1$) MI lobe for different lattices and frustration parameters f as follows: $x_f^{\square, \Delta} \equiv \max[(t/U)_{\text{crit}}]_f^{\square, \Delta}$. The ground state of the rotating Bose–Einstein condensates on a triangular lattice appears to be most stable against the effect of rotation. The stability comes from the higher values of the repulsive energy for the triangular lattice. However, if the rotation frustration parameter is $f = 1/3$ and $1/2$, the ratio $x_f^{\Delta}/x_f^{\square}$ of the energy needed to cause loss of the global coherent state changes character and is higher for triangular lattice unlike the cases with $f = 0, 1/6$ and $1/4$ (see Fig. 1). Behavior of the maximum repulsive energy $x_f^{\square, \Delta}$ in the rotating system with $f \neq 0$ taken for special value of the $\mu/U = 1/2$ is non-monotonical in both square and triangular lattice (Fig. 2 and Fig. 3).

5. Conclusions

We calculated the phase diagram using the quantum rotor approach with exactly evaluated density of states for two-dimensional lattices with rational magnetic flux/rotation frustration parameter $f = p/q$ for a number of values $f = 1/q$. In systems that are in the global coherent state at $f = 0$, but with the ratio t/U close to the critical value $(t/U)_{\text{crit}}$, a rotation can be used to drive the condensates into the MI state. We compare the maximum of the critical value for t/U parameter (as a function of the normalized chemical potential μ/U) at the tip of the

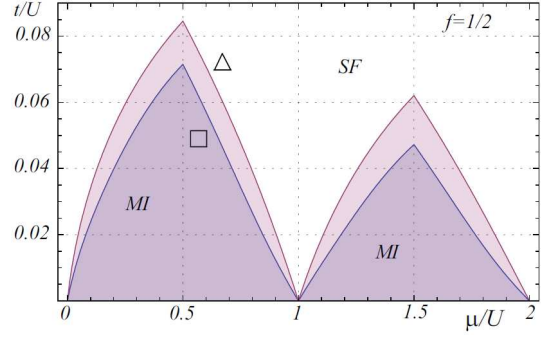


Fig. 1. Phase diagram for square \square and triangular Δ lattice (number of particles per lattice site is $n_B = 1$ inside the first and $n_B = 2$ inside the second lobe, respectively) with rotation frustration parameter $f = 1/2$. Within the lobes the MI phase takes place with $\Psi_B = 0$.

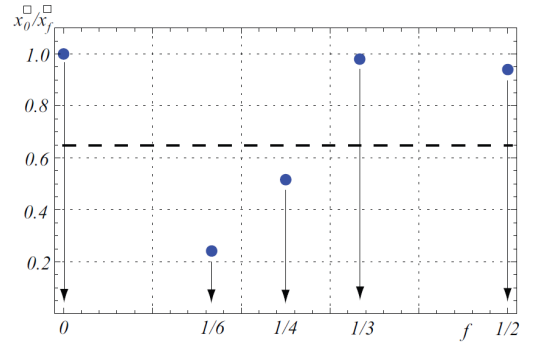


Fig. 2. The maximum of the critical value for t/U parameter (as a function of the normalized chemical potential μ/U) at the tip of the first ($n_B = 1$) MI lobe $x_0^{\square}/x_f^{\square}$ for rotating square lattice. The vertical dashed line marks the ratio of the maximum of the critical value for t/U parameter for the second to first lobe $x_0^{\square}(n_B = 2)/x_0^{\square}(n_B = 1)$.

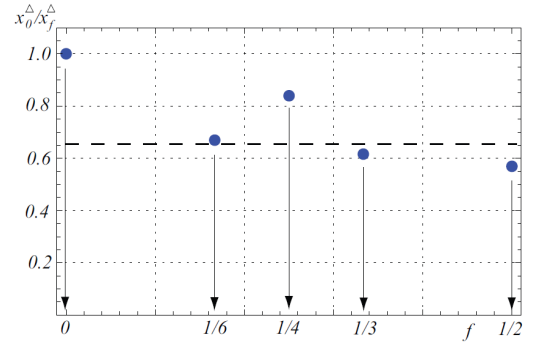


Fig. 3. The maximum of the critical value for t/U parameter (as a function of the normalized chemical potential μ/U) at the tip of the first ($n_B = 1$) MI lobe $x_0^{\Delta}/x_f^{\Delta}$ for rotating triangular lattice. The vertical dashed line marks the ratio of the maximum of the critical value for t/U parameter for the second to first lobe $x_0^{\Delta}(n_B = 2)/x_0^{\Delta}(n_B = 1)$.

first ($n_B = 1$) MI lobe for square lattice with several numerical and analytical works and found them in a good agreement. Note that the dependence of the $x_f^{\square,\Delta}/x_0^{\square,\Delta}$ on frustration parameter f is non-monotonical (Fig. 2 and Fig. 3). The critical values of the energy needed to drive a rotating condensate out of a global coherent state change by varying the frustration parameter and strongly depend on topology of the lattice.

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References

- [1] D. Jaksch, C. Bruder, J.I. Cirac, C.W. Gardiner, P. Zoller, *Phys. Rev. Lett.* **81**, 3108 (1998).
- [2] M. Greiner, O. Mandel, T. Esslinger, T.W. Hänsch, I. Bloch, *Nature* **415**, 39 (2002).
- [3] M. Greiner, I. Bloch, O. Mandel, T.W. Hänsch, T. Esslinger, *Phys. Rev. Lett.* **87**, 160405 (2001).
- [4] I. Coddington, P.C. Haljan, P. Engels, V. Schweikhard, S. Tung, E.A. Cornell, *Phys. Rev. A* **70**, 063607 (2004).
- [5] S. Tung, V. Schweikhard, E.A. Cornell, *Phys. Rev. Lett.* **97**, 240402 (2006).
- [6] V. Schweikhard, S. Tung, E.A. Cornell, *Phys. Rev. Lett.* **99**, 030401 (2007).
- [7] R. Bhat, B.M. Peden, B.T. Seaman, M. Krämer, L.D. Carr, M.J. Holland, *Phys. Rev. A* **74**, 063606 (2006).
- [8] R. Bhat, M. Krämer, J. Cooper, M.J. Holland, *Phys. Rev. A* **76**, 043601 (2007).
- [9] N.R. Cooper, *Adv. Phys.* **57**, 539 (2008).
- [10] A. Leggett, *Quantum Liquids*, Oxford, New York 2006.
- [11] T.K. Kopeć, *Phys. Rev. B* **70**, 054518 (2004).
- [12] T.P. Polak, T.K. Kopeć, *Phys. Rev. B* **76**, 094503 (2007).
- [13] M.P.A. Fisher, P.B. Weichman, G. Grinstein, D.S. Fisher, *Phys. Rev. B* **40**, 546 (1989).
- [14] A.P. Kampf, G.T. Zimanyi, *Phys. Rev. B* **47**, 279 (1993).