Bose-Einstein Quantum Phase Transition in an Optical Lattice Model

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1. Introduction

Experiments [Greiner *et al.*] seem to have verified a 1989 prediction [M. Fisher *et al.*] that it is possible to have a *phase transition* from *Bose-Einstein condensation (BEC) of a gas of atoms* to *no BEC of the atoms* — by varying the strength of a periodic optical potential (called *optical lattice*). This means that for a large potential strength there is no BEC — even at zero temperature.

The disappearance of BEC is accompanied by a transition to a 'Mott-insulator' of well-localized atoms. This is a *quantum mechanical phase transition* since it is not energy-entropy driven.

The interaction between atoms is essential for this effect because BEC *always* occurs at sufficiently low T for non-interacting particles.

2. Model and Main Results

For $\Lambda \subset \mathbb{Z}^d$ a cubic lattice, $\mathcal{H} = \mathcal{F}(\mathbb{C}^{|\Lambda|})$. Our model is described by the Hamiltonian

$$H = -\frac{1}{2}\sum_{\langle xy \rangle}(a_x^\dagger a_y + a_x a_y^\dagger) + \lambda \sum_x (-1)^x a_x^\dagger a_x$$

$$+ U \sum_x a_x^\dagger a_x (a_x^\dagger a_x - 1).$$

Here $\sum_{\langle xy \rangle}$ is a sum over nearest neighbor sites. Hence the first term is just the lattice Laplacian. $a_x^\dagger a_x$ counts the number of atoms at x.

The optical lattice gives rise to a potential $\lambda(-1)^x$ which alternates in sign between the A and B sublattices. The inter-atomic on-site repulsion is U, and we take $U = \infty$.

For $U = \infty$, $\mathcal{H}$ reduces to $\mathcal{H} = \bigotimes_{x\in\Lambda} \mathbb{C}^2$, and H can be written as a spin XY Hamiltonian [Matsubara-Matsuda, 1956]

$$H = -\sum_{\langle xy\rangle}(S_x^1 S_y^1 + S_x^2 S_y^2) + \lambda \sum_x (-1)^x S_x^3.$$

BEC is equivalent to long-range spin order.

The matrix representations are:

$$a_x^\dagger \leftrightarrow \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},\; a_x \leftrightarrow \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},\; a_x^\dagger a_x \leftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$

for each $x \in \Lambda$. The correspondence with the spin $1/2$ matrices is thus

$$a_x^\dagger = S_x^1 + \mathrm{i}S_x^2 = S_x^+, \quad a_x = S_x^1 - \mathrm{i}S_x^2 = S_x^-,$$

and hence $a_x^\dagger a_x = S_x^3 + \frac{1}{2}$.

If $\lambda = 0$ but $U < \infty$ this is the *Bose-Hubbard model*. Then all sites are equivalent and the lattice represents the attractive sites of the optical lattice. In our case the adjustable parameter is λ instead of U and for large λ the atoms will try to localize on the B sublattice.

In our model, the number of particles is always half the number of lattice sites, i.e, there is *half-filling*. More precisely,

$$\langle \hat{N} \rangle = \frac{\mathrm{Tr}\left(\sum_{x \in \Lambda} a_x^\dagger a_x \right) e^{-\beta H}}{\mathrm{Tr} e^{-\beta H}} = \tfrac{1}{2} |\Lambda|.$$

This corresponds, physically, to one particle per site in the Bose-Hubbard model.

By a variety of methods we can prove:

1. Existence of BEC if $T = 1/\beta$ and λ are both small. I.e., one large eigenvalue (of order $|\Lambda|$) of the one-body density matrix

$$\gamma(x,y) = \langle a_x^\dagger a_y \rangle = \frac{\mathrm{Tr} a_x^\dagger a_y e^{-\beta H}}{\mathrm{Tr} e^{-\beta H}}$$

with corresponding condensate wave function $\phi(x) = \mathrm{const.}$

2. Exponential decay of correlation functions (and hence *absence of BEC*) if either T or λ is big enough, i.e.,

$$\gamma(x,y) \leq C e^{-c|x-y|}.$$

In particular, this applies to the ground state $T = 0$ for λ big enough.

3. Mott insulator phase, characterized by a gap, i.e., a jump in the chemical potential, for parameter region described in item 2 above. More precisely, there is a cusp in the dependence of the ground state energy on the number of particles. There is no such gap whenever there is BEC.

4. The interparticle interaction is essential for items 2 and 3. **Non-interacting bosons always display BEC** for low, but positive T (depending on λ, of course).

5. For all $T \geq 0$ and all $\lambda > 0$ the diagonal part of the one-body density matrix

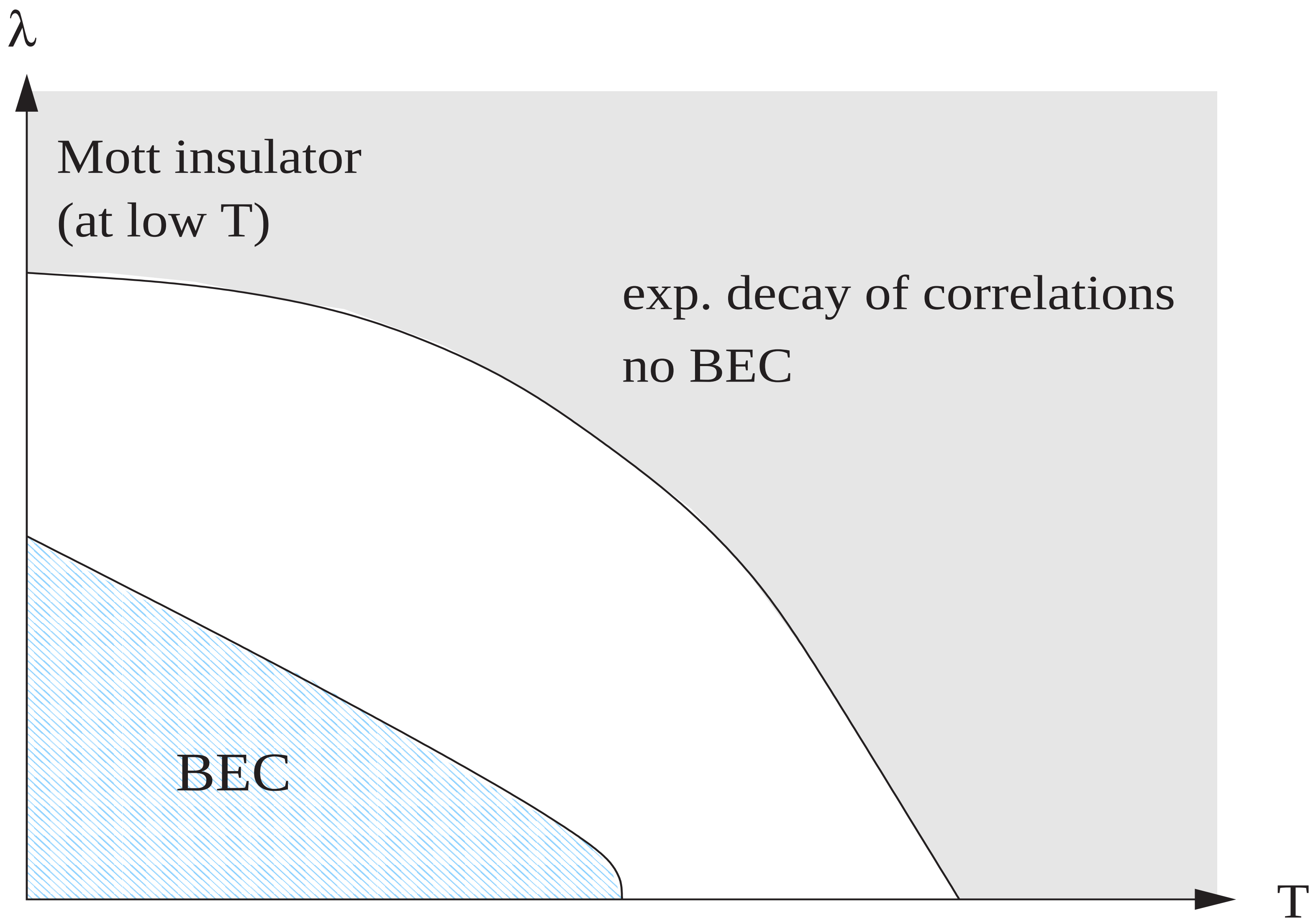
$$\varrho(x) = \langle a_x^\dagger a_x \rangle$$

is **not constant**. Its value on the A-sublattice is strictly less than on the B-sublattice. In contrast, if there is BEC the off-diagonal long-range order is constant, i.e.,

$$\gamma(x, y) = \langle a_x^\dagger a_y \rangle \approx \text{const.}$$

for large $|x - y|$.

Schematic λ-T-phase diagram at half-filling:



3. Proof of BEC for small λ and T

Consider the Fourier transform of $S_x^\#$,

$$\widetilde{S}_p^\# = |\Lambda|^{-1/2} \sum_x S_x^\# \exp(\mathrm{i}p \cdot x).$$

Then

$$\gamma(x,y) = \sum_{p \in \Lambda^*} \exp(\mathrm{i}p \cdot (x-y)) \langle \widetilde{S}_p^1 \widetilde{S}_{-p}^1 + \widetilde{S}_p^2 \widetilde{S}_{-p}^2 \rangle$$

and the behavior for $|x-y| \to \infty$ is determined by the $p=0$ contribution.

We use reflection positivity, as in the proof [Dyson-Lieb-Simon, 1978] of long-range order for the Heisenberg model, to obtain the *infrared bound*

$$(\widetilde{S}_p^1, \widetilde{S}_{-p}^1) \leq \frac{k_\mathrm{B} T}{2 \sum_{i=1}^d (1 - \cos(p_i))}$$

for the Duhamel two-point function, defined by

$$(A,B) = \int_0^1 \mathrm{Tr} \left(A e^{-s\beta H} B e^{-(1-s)\beta H} \right) ds / \mathrm{Tr} e^{-\beta H}.$$

Reflection positivity means that, for any operator F on the 'left',

$$\langle F\overline{\theta(F)}\rangle \geq 0,$$

with $\theta(F)$ the natural reflected operator, together with a (unitary) particle-hole transformation.

The crucial idea ('Gaussian domination') is: Define, for a real valued function h on Λ,

$$Z(h) = \mathrm{Tr}\exp\left[-\beta K(h)\right],$$

with the modified Hamiltonian

$$\begin{aligned} K(h) \quad &= \quad \sum_{\langle xy\rangle}\left(\tfrac{1}{2}(S_x^1 - S_y^1 - h_x + h_y)^2 - S_x^2 S_y^2\right) \\ &\quad +\lambda\sum_x (-1)^x S_x^3. \end{aligned}$$

Then $Z(h) \leq Z(0)$. The infrared bound follows from $d^2 Z(\varepsilon h)/d\varepsilon^2 \leq 0$.

The next step is to relate the Duhamel two point function to the thermal expectation value. This involves convexity arguments and estimations of double commutators, leading to an upper bound on the contribution from $p \neq 0$:

$$\sum_{p \neq 0} \langle \widetilde{S}^1_p \widetilde{S}^1_{-p} + \widetilde{S}^2_p \widetilde{S}^2_{-p} \rangle \leq c(\lambda, T)|\Lambda|$$

with $c(\lambda, T) < \frac{1}{2}$ for λ and T small enough.

On the other hand, we have the sum rule

$$\sum_{p \in \Lambda^*} \langle \widetilde{S}^1_p \widetilde{S}^1_{-p} + \widetilde{S}^2_p \widetilde{S}^2_{-p} \rangle = \frac{|\Lambda|}{2}.$$

Thus the long range order, $|\Lambda|^{-1} \langle \widetilde{S}^1_0 \widetilde{S}^1_0 + \widetilde{S}^2_0 \widetilde{S}^2_0 \rangle$, is bounded away from zero, uniformly in $|\Lambda|$, for λ and T small enough.

4. Absence of BEC for large λ or T, and the Mott insulator phase

The main results are: If either

(i) $\lambda \geq 0$ and $k_B T > d/(2 \ln 2)$, or

(ii) $T \geq 0$ and $\lambda \geq 0$ such that $\lambda + |e(\lambda)| > d$,

with $e(\lambda)$ the ground state energy per site, then there is exponential decay of correlations:

$$\gamma(x, y) \leq (\text{const.}) \exp(-\kappa |x - y|)$$

for some $\kappa > 0$.

Moreover, the chemical potential has a jump at half-filling (at $T = 0$), i.e.,

$$E(N - k) + E(N + k) - 2E(N) \geq |k|(\lambda + |e(\lambda)| - d)$$

for $N = \frac{1}{2}|\Lambda|$ and all $k \in \mathbb{Z}$.

The proof is based on a path integral representation of the one-particle density matrix, that follows from the Dyson expansion of the exponential of the Hamiltonian $H = H_0 + W$, with H_0 the hopping part and W the optical lattice potential.

We picture each path configuration ω by a collection of disjoint loops or curves in $\Lambda \times [0, \beta]$, describing the paths of 'quasi-particles':

The occupation number at site x of a 'quasi-particle' is defined to be

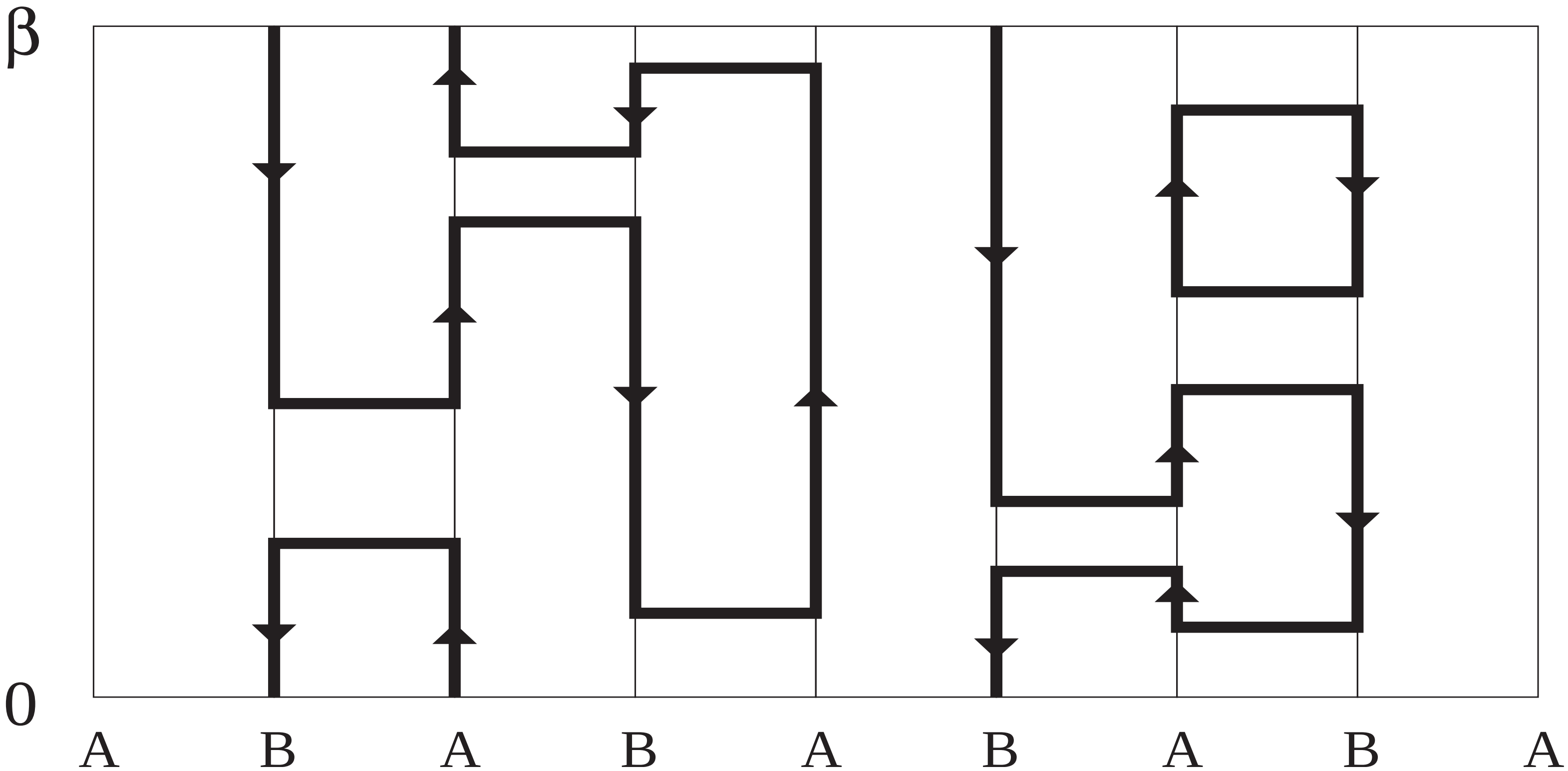
$$n_x = \tfrac{1}{2} + (-1)^x S_x^3.$$

Thus $n_x = 1$ means presence of a particle if x is on the A-sublattice (potential maximum) and absence if x is on the B-sublattice (potential minimum).

The potential energy is

$$W = \lambda \sum n_x.$$

Particles created on A-sites moves **"upward in time"**, but **"downward"** in time if they are created on B-sites.



Let $|\omega|$ denote the total length in the time direction of the loops of quasi-particles associated with ω, i.e.,

$$|\omega| = \sum_x \int dt \, n_x(\omega(t)).$$

We have

$$\operatorname{Tr} e^{-\beta H} = \int v(d\omega) e^{-\lambda|\omega|}$$

where the integral is over all configurations of disjoint oriented loops. Here $v(d\omega)$ is the path measure associated with the hopping H_0. Hence long paths are suppressed if λ is large.

The trace for fixed particle number $N = \frac{1}{2}|\Lambda| + k$ is analogously obtained by restricting to such configurations with total winding number k.

Likewise, for $x \neq y$,

$$\operatorname{Tr} a_x^\dagger a_y e^{-\beta H} = \int_{\partial\omega = \delta_{(x,0)} - \delta_{(y,0)}} v(d\omega) e^{-\lambda|\omega|}$$

where $\partial\omega = \delta_{(x,0)} - \delta_{(y,0)}$ means that ω contains exactly one curve connecting x and y (both at 'time'=0) and otherwise closed loops.

The one-particle density matrix can thus be written

$$\gamma(x,y) = \frac{\int_{\partial\omega=\delta_{(x,0)}-\delta_{(y,0)}} v(d\omega)e^{-\lambda|\omega|}}{\int v(d\omega)e^{-\lambda|\omega|}}.$$

Using a factorization of the path space measure together with reflection positivity one obtains

$$\gamma(x,y) \leq \int_{\mathcal{B}(x,y)} v(d\gamma)e^{-(\lambda-f)|\gamma|}$$

where $f < 0$ is the free energy per site and $\mathcal{B}(x,y)$ is the set of configurations that consist of exactly one curve, γ, connecting x and y and no other curves.
This can be further estimated by some random walk arguments, leading to exponential decay,

$$\gamma(x,y) \sim e^{-\kappa|x-y|}$$

provided

$$\frac{d}{\lambda - f}\left(1 - e^{-\beta(\lambda-f)}\right) < 1.$$

The proof of the energy gap is based on an estimate for the ratio

$$\frac{\mathrm{Tr}\,\mathcal{P}_k e^{-\beta H}}{\mathrm{Tr}\,\mathcal{P}_0 e^{-\beta H}}$$

where $\mathcal{P}_k$ projects onto states in Fock space with particle number $N = \frac{1}{2}|\Lambda| + k$.
The integral for the numerator is over configurations ω with a non-trivial winding number k. Each such configuration includes a collection of 'non-contractible' loops with total length at least $\beta|k|$. The relative weight of such loops and also the 'entropy' of such long loops can be estimated. The result is a bound

$$\frac{\mathrm{Tr}\,\mathcal{P}_k e^{-\beta H}}{\mathrm{Tr}\,\mathcal{P}_0 e^{-\beta H}} \leq \mathrm{const.} \left(\frac{|\Lambda|}{|k|}\right)^{|k|} \left(e^{1-\mathrm{const.}\,\beta}\right)^{|k|}$$

which gives for $\beta \to \infty$

$$E(N+k) - E(N) \geq \mathrm{const.}\,|k|$$

independently of $|\Lambda|$.

In the BEC phase there is *no gap* for adding particles beyond half filling (in the thermodynamic limit). In fact, the ground state energy per site in the thermodynamic limit satisfies

$$0 \leq e(\varrho) - e(\tfrac{1}{2}) \leq \mathrm{const.}\,(\varrho - \tfrac{1}{2})^2$$

Thus there is no cusp at $\varrho = 1/2$.
The proof is by a variational calculation with the test states

$$|\psi_y\rangle = e^{\mathrm{i}\varepsilon S^2_{\mathrm{tot}}}(S^1_y + \tfrac{1}{2})|0\rangle.$$

These have excess particle number $k \approx \varepsilon|\Lambda|$ but the energy increase is only $\sim \varepsilon^2|\Lambda|$.

The disappearance of BEC and the energy gap (jump in the chemical potential) for large λ are an effect of the interparticle interaction. For the noninteracting lattice gas the one-particle energy spectrum $\varepsilon(p)$ can easily be determined and satisfies

$$\varepsilon(p) - \varepsilon(0) \sim \tfrac{1}{2} d(d^2 + \lambda^2)^{-1/2} |p|^2$$

for small p. Hence there is BEC for all λ if $d \geq 3$ and small T (depending on the density). Note that the condensate wave function is *not* constant in this case. (It is the ground state of $-\frac{1}{2}\Delta + (-1)^x$.)

With the hard core interaction the condensate *wave function is* constant, but it can be proved that the local *particle density* oscillates with the period of the optical potential.