# Physics 7450: Solid State Physics 2

# Lecture 3: Bosonic matter

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## Abstract

In these lectures, starting with a review of second- and coherent-state path-integral quantization, we will formulate a quantum field theory of bosonic matter and will study its thermodynamics and correlation functions. We will explore the transition to Bose-Einstein condensation (BEC) of noninteracting bosons. Including interactions, we will study the properties of a superfluid and a phase transition into it within a mean-field theory, quantum "hydrodynamics", Bogoluibov theory and Lee-Huang-Yang expansion of a weakly interacting Bose gas.

# I. INTRODUCTION

- Bose gases thermodynamics and BEC
- Bogoluibov theory of a superfluid
- Lee-Huang-Yang thermodynamics
- Ginzburg-Landau theory and Landau's quantum hydrodynamics
- XY model, 2d order, vortices and the Kosterlitz-Thouless transition

The goal of these notes is to study a macroscopic number of interacting bosonic particles, as for example realized in ultra-cold atomic gases, e.g., $Rb^{87}$ that realized first Bose-Einstein condensate (BEC) in 1995 in JILA, and in low-temperature $He^4$ liquid, a strongly interacting, much older "cousin", whose superfluidity occurs below 2.172 Kelvin as was discovered by Pyotr Kapitsa and John Allen and Don Misener in 1937.

This is a fascinating systems exhibiting a wealth of phenomena the basis of which will be able with the ideas developed below. As we will see, the key ingredients are a macroscopic number of particle obeying quantum Bose statistics, that manifests itself at low temperatures (determined primarily by density and particle mass), and interactions.

As we will see shortly, because of their weak interactions, the description of a Bose gas is amenable to a detailed microscopic analysis. In contrast, strong interactions in liquid Helium preclude its detailed analytical description, though significant progress has been made through quantum Monte Carlo and other numerical methods. Nevertheless, significant understanding of Helium phenomenology has been developed at a qualitative level using a combination of symmetry based phenomenological description of Landau and Ginzburg and extrapolation of the weakly interacting Bose gas.

# II. SECOND QUANTIZATION

## A. Motivation and qualitative arguments

A direct attack on this problem is via (the so called) "first quantization", by simply generalizing Schrödinger's equation to $N$ particles,

$$H\Psi_{\{\mathbf{k}_i\}}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = E_{\{\mathbf{k}_i\}}\Psi_{\{\mathbf{k}_i\}}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N), \tag{1}$$

with an $N$-body Hamiltonian

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2}\sum_{i\neq j} V(|\mathbf{r}_i - \mathbf{r}_j|) \tag{2}$$

of $2N$ phase-space coordinates satisfying the canonical commutation relation $[r_i^\alpha, p_j^\beta] = i\hbar\delta_{\alpha\beta}\delta_{ij}$ and with the many-body eigenstates characterized by a set of quantum numbers $\mathbf{k}_1, \mathbf{k}_2, \ldots$ and a symmetrization constraint

$$\Psi_{\{\mathbf{k}_i\}}(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_i, \ldots, \mathbf{r}_j, \ldots \mathbf{r}_N) = \Psi_{\{\mathbf{k}_i\}}(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_j, \ldots, \mathbf{r}_i, \ldots \mathbf{r}_N)$$

encoding the bosonic quantum statistics.

While this formulation is in principle sufficient[4], for an interacting case it is quite clumsy to work with. One can appreciate this by recalling a quantization of a harmonic oscillator, where one can shed the complexity of the series solution and Hermite polynomial algebra of the first-quantized coordinate formulation by transitioning to the so-called "second-quantized" reformulation in terms of creation and annihilation operators, $a = \frac{1}{\sqrt{2}}(x + ip)$, $a^\dagger = \frac{1}{\sqrt{2}}(x - ip)$, satisfying bosonic commutation relation $[a, a^\dagger] = 1$. The corresponding Hamiltonian is given by $H = \hbar\omega_0 a^\dagger a = \hbar\omega_0 \hat{n}$ and eigenstates $|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle$ written in the occupation basis $n$.

A first-quantization description in terms of individual particles' coordinates $\mathbf{r}_i$ is akin to a Lagrangian description of fluids and crystals, which is particularly challenging here because of the quantum indistinguishability of Bose particles. As we will see below, an elegant "fix" is the quantum analog of the Eulerian description, where instead, the many-body state is characterized by dynamical field variables (such as particle and momentum densities $n(\mathbf{r}, t)$, $g(\mathbf{r}, t)$) at each spatial coordinate $\mathbf{r}$ (a passive label rather than a dynamic variable), not associated with any specific particle.

## B. Canonical second-quantization

### 1. *Fock states*

Given that in the second-quantization formulation creation and annihilation operators convert $N$-particle states to $N \pm 1$-particle states, we generalize the usual, fixed particle number Hilbert space $\mathcal{H}_N$ to Fock space $\mathcal{H}_F = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \ldots \oplus \mathcal{H}_N \oplus \ldots$. In the first-quantized formulation the many-body basis set can be conveniently taken as a (symmetried for bosons) product of single-particle eigenstates $|\mathbf{k}\rangle$ with coordinate space wavefunctions $\psi_{\mathbf{k}}(\mathbf{r}_i) = \langle \mathbf{r}_i|\mathbf{k}\rangle$. Instead, in the second-quantized formulation we take the many-body basis set to be

$$|\{n_{\mathbf{k}_i}\}\rangle = |n_{\mathbf{k}_1}, n_{\mathbf{k}_1}, \ldots, n_{\mathbf{k}_N}, \ldots\rangle = \prod_{\mathbf{k}_i} |n_{\mathbf{k}_i}\rangle,$$

a direct product of eigenstates $|n_{\mathbf{k}}\rangle = \frac{1}{\sqrt{n_{\mathbf{k}}!}}(a^\dagger_{\mathbf{k}})^{n_{\mathbf{k}}}|0\rangle$ labelled by the occupation number of a single-particle eigenstate $\mathbf{k}$. The immediate advantage of this description is that, by construction, particles in the same single particle state $\mathbf{k}$ are identical, with only the occupation numbers $n_{\mathbf{k}_i}$ labelling the many-body state and symmetrization automatically encoded in the bosonic commutation relation

$$[a_{\mathbf{k}_1}, a^\dagger_{\mathbf{k}_2}] = \delta_{\mathbf{k}_1,\mathbf{k}_2}. \tag{3}$$

The $N$-particle wavefunction is then given by the projection of the Fock state onto $N$-particle coordinate eigenstate

$$\Psi_{\{\mathbf{k}_i\}}(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = \langle \mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N|\{n_{\mathbf{k}_i}\}\rangle,$$

latter given by

$$|\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\rangle = \prod_i^N \psi(\mathbf{r}_i)|0\rangle,$$

where

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}, \qquad a_{\mathbf{k}} = \frac{1}{\sqrt{V}}\int d^d r \psi(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}}$$

destroys a boson at coordinate $\mathbf{r}$, satisfies a canonical commutation relation with its hermitian conjugate creation field,

$$[\psi(\mathbf{r}), \psi(\mathbf{r}')^\dagger] = \delta^d(\mathbf{r} - \mathbf{r}'). \tag{4}$$

dictated by (3), and gives the number density operator

$$\begin{aligned} n(\mathbf{r}) &= \psi(\mathbf{r})^\dagger \psi(\mathbf{r}), & (5)\\ &= \frac{1}{V}\sum_{\mathbf{q}}\left(\sum_{\mathbf{k}} a^\dagger_{\mathbf{k}} a_{\mathbf{k}+\mathbf{q}}\right) e^{i\mathbf{q}\cdot\mathbf{r}} \equiv \frac{1}{\sqrt{V}}\sum_{\mathbf{q}} \tilde{n}(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{r}}. & (6) \end{aligned}$$

and its Fourier transform $\tilde{n}(\mathbf{q})$.

### 2. Hamiltonian

To construct the 2nd-quantized Hamiltonian we first note that by analogy with a single harmonic oscillator and phonon fields studied in Lectures 2, in momentum basis $\mathbf{k}$ the many-body energy eigenvalue is given by

$$E_{\{\mathbf{k}\}} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} n_{\mathbf{k}},$$

where in the case of nonrelativistic bosons $\epsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}$ is an energy eigenvalue of a single particle Hamiltonian $\hat{h} = \frac{-\hbar^2 \nabla^2}{2m}$

$$\hat{h}|\mathbf{k}\rangle = \epsilon_{\mathbf{k}}|\mathbf{k}\rangle$$

in a momentum eigenstate state $|\mathbf{k}\rangle = a^\dagger_{\mathbf{k}}|0\rangle$, where $|0\rangle$ is particle vacuum, $a_{\mathbf{k}}|0\rangle = 0$.

Thus the 2nd-quantized one-body Hamiltonian is given by

$$\hat{H} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \hat{n}_{\mathbf{k}} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} a^\dagger_{\mathbf{k}} a_{\mathbf{k}}, \tag{7}$$

$$= \int d^d r \psi^\dagger(\mathbf{r}) \hat{h} \psi(\mathbf{r}) = \int d^d r \psi^\dagger(\mathbf{r}) \frac{-\hbar^2 \nabla^2}{2m} \psi(\mathbf{r}), \tag{8}$$

where in the second line we expressed the Hamiltonian in terms of the field operators using Fourier representation. More generally a 2nd-quantized one-body operator $H$, corresponding to a 1st-quantized one-body operator $\hat{h}$ in a single-particle basis $|\alpha\rangle$ is given by

$$H = \sum_{\alpha\beta} a^\dagger_\alpha h_{\alpha\beta} a_\beta, \tag{9}$$

where $a^\dagger_\alpha$ creates a particle in a single particle state $|\alpha\rangle$ and $h_{\alpha\beta} = \langle\alpha|\hat{h}|\beta\rangle$ is the corresponding matrix element.

Armed with the many-body Hamiltonian, using the Heisenberg equation of motion together with the commutation relation, (4), we obtain the equation for the Heisenberg field operators $\psi(\mathbf{r}, t)$

$$i\hbar\partial_t \psi = [\psi, H], \tag{10}$$

$$= [\psi, \int d^d r' \psi^\dagger(\mathbf{r}') \hat{h} \psi(\mathbf{r}')], \tag{11}$$

$$= \frac{-\hbar^2 \nabla^2}{2m} \psi(\mathbf{r}), \tag{12}$$

that when Fourier transformed (or equivalently by writing the Heisenberg equation for $a_{\mathbf{k}}(t)$ and $a^\dagger_{\mathbf{k}}(t)$) can be straightforwardly solved to give

$$a_{\mathbf{k}}(t) = a_{\mathbf{k}} e^{-i\epsilon_{\mathbf{k}} t/\hbar}, \quad a^\dagger_{\mathbf{k}}(t) = a^\dagger_{\mathbf{k}} e^{i\epsilon_{\mathbf{k}} t/\hbar}.$$

The equation of motion for $\psi(\mathbf{r})$ can also be obtained from a many-body action $S$

$$\begin{aligned} S[\psi^\dagger, \psi] &= \int dt d^d r \left[\Pi \partial_t \psi - \mathcal{H}\right], && (13)\\ &= \int dt d^d r \left[\psi^\dagger \left(i\hbar\partial_t + \frac{\hbar^2}{2m}\nabla^2\right)\psi\right], && (14)\\ &= \int dt d^d r \left[\psi^\dagger \left(i\hbar\partial_t - \hat{h}\right)\psi\right], && (15)\end{aligned}$$

via an Euler-Lagrange equation extremizing the action, $\frac{\delta S}{\delta\psi^\dagger(\mathbf{r})} = 0$. The momentum field $\Pi(\mathbf{r}) = i\hbar\psi^\dagger(\mathbf{r})$ conjugate to $\psi(\mathbf{r})$ can be identified from the commutation relation (4), consistent with its canonical definition as $\Pi(\mathbf{r}) = \frac{\delta S}{\delta \partial_t \psi(\mathbf{r})}$. In the last action, above we made an obvious generalization of the action for an arbitrary single-particle Harmiltonian $\hat{h}$, that in addition to the kinetic energy generically also has a single particle potential as e.g., due to a trapping potential or an optical lattice potential in the context of trapped atomic gases.

Above Heisenberg field operator equation (12) is formally equivalent to a single-particle Schrödinger's equation, but with a very distinct physical interpretation. In contrast to the latter, here $\psi(\mathbf{r})$ is a quantum field operator and $\mathbf{r}$ is simply a spatial label for infinite number of operators, one for each point $\mathbf{r}$. This equation is a quantized version of a classical field equation akin to the phonon field equation for sound and Maxwell's field equation for the electromagnetic field.

The two-body interaction in (2) can also be straightforwardly written in the 2nd-quantized form using the second-quantized form for the number density $n(\mathbf{r}) = \sum_i \delta^d(\mathbf{r} - \mathbf{r}_i)$ from Eq. (5)

$$\begin{aligned} \hat{H}_{int} &= \frac{1}{2}\sum_{i\neq j} V(|\mathbf{r}_i - \mathbf{r}_j|) = \frac{1}{2}\int_{\mathbf{r},\mathbf{r}'} n(\mathbf{r}) V(|\mathbf{r} - \mathbf{r}'|) n(\mathbf{r}), && (16)\\ &= \frac{1}{2}\int_{\mathbf{r},\mathbf{r}'} V(|\mathbf{r} - \mathbf{r}'|)\psi^\dagger(\mathbf{r})\psi(\mathbf{r})\psi^\dagger(\mathbf{r}')\psi(\mathbf{r}'), && (17)\\ &= \frac{1}{2}\int_{\mathbf{r},\mathbf{r}'} V(|\mathbf{r} - \mathbf{r}'|)\psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}')\psi(\mathbf{r}')\psi(\mathbf{r}) + \frac{1}{2}V(0)\int_{\mathbf{r}}\psi^\dagger(\mathbf{r})\psi(\mathbf{r}), && (18)\end{aligned}$$

where typically we choose to normal order the operators, so as to avoid counting particle self-interaction. Thus normal-ordering allows to avoid the last term, above.

More generally the second-quantization prescription for a two-body operator $V^{(2)} = \frac{1}{2}\sum_{i\neq j} V(\mathbf{r}_i, \mathbf{r}_j)$ written in a general basis $V^{(2)} = \frac{1}{2}\sum_{\alpha,\beta,\gamma\delta} |\alpha\rangle|\beta\rangle\langle\alpha\beta|V(\mathbf{r}_1, \mathbf{r}_2)|\gamma\delta\rangle\langle\gamma|\langle\delta|$ is given by a normal-ordered form

$$\hat{V}^{(2)} = \frac{1}{2}\sum_{\alpha,\beta,\gamma\delta} V_{\alpha\beta,\gamma\delta} a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma, \tag{19}$$

where $V_{\alpha\beta,\gamma\delta} = \langle\alpha\beta|V|\gamma\delta\rangle$ is the two-particle matrix element and in the last equality we commuted $a_\gamma$ and $a_\delta$ that is inconsequential for bosons but is a more convenient form for anticommuting fermions.

### C. Path-integral quantization

Inspired by Dirac's beautiful on role of the action in quantum mechanics, Richard Feynman developed a path-integral quantization method[5] complementary to the Schrödinger equation and noncommuting operators Heisenberg formalism.

As a warmup we begin with a phase-space path-integral formulation of a single particle quantum mechanics. We will then generalize it to a many-body system, simplest formulated in terms of a coherent states path-integral.

#### *1. phase-space path-integral*

A central object in formulation of quantum mechanics is the unitary time evolution operator $\hat{U}(t)$ that relates a state $|\psi(t)\rangle$ at time $t$ to the $|\psi(0)\rangle$ at time 0,

$$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle.$$

Given that $|\psi(t)\rangle$ satisfies the Schrödinger's equation, the formal solution is given by $\hat{U}(t) = e^{-\frac{i}{\hbar}Ht}$. In a 1d coordinate representation, we have

$$\langle x_f|\psi(t)\rangle = \int_{-\infty}^{\infty} dx_0 \langle x_f|\hat{U}(t)|x_0\rangle\langle x_0|\psi(0)\rangle, \tag{20}$$

$$\psi(x_N, t) = \int_{-\infty}^{\infty} dx_0 U(x_N, x_0; t)\psi(x_0, 0), \tag{21}$$

where we defined $x_f \equiv x_N$, $x_i \equiv x_0$, $t = t_N = N\epsilon$, $t_0 = 0$. Our goal then is to find an explicit expression for the evolution operator, equivalent to a solution of the Schrödinger's.

To this end we employ the so-called Trotter decomposition of the evolution operator $\hat{U}(t_N)$ in terms of the infinitesimal evolution over time $t/N = \epsilon$:

$$\hat{U}(t_N) \;=\; e^{-\frac{i}{\hbar}\hat{H}t} = \left(e^{-\frac{i}{\hbar}\hat{H}\frac{t}{N}}\right)^N = \underbrace{\hat{U}(\epsilon)\hat{U}(\epsilon)\ldots\hat{U}(\epsilon)}_{N}. \tag{22}$$

$$\tag{23}$$

In coordinate representation, we have

$$\begin{aligned}
U(x_N, x_0; t_N) \;&=\; \langle x_N|\hat{U}(\epsilon)\hat{U}(\epsilon)\ldots\hat{U}(\epsilon)|x_0\rangle, && (24)\\
&= \prod_{n=1}^{N-1}\left[\int_{-\infty}^{\infty} dx_n\right]\langle x_N|\hat{U}(\epsilon)|x_{N-1}\rangle\langle x_{N-1}|\hat{U}(\epsilon)|x_{N-2}\rangle\ldots\langle x_{n+1}|\hat{U}(\epsilon)|x_n\rangle\ldots\langle x_1|\hat{U}(\epsilon)|x_0\rangle, &&\\
&= \prod_{n=1}^{N-1}\left[\int_{-\infty}^{\infty} dx_n\langle x_n|\hat{U}(\epsilon)|x_{n-1}\rangle\right] = \prod_{n=1}^{N-1}\left[\int_{-\infty}^{\infty} dx_n\langle x_n|e^{-\frac{i}{\hbar}(\frac{\hat{p}^2}{2m}+V(\hat{x}))\epsilon}|x_{n-1}\rangle\right], && (25)\\
&= \prod_{n=1}^{N-1}\left[\int_{-\infty}^{\infty} dx_n\langle x_n|e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}}|x_{n-1}\rangle e^{-\frac{i}{\hbar}V(x_{n-1})\epsilon}\right], && (26)\\
&= \prod_{n=1}^{N-1}\left[\int_{-\infty}^{\infty} dx_n dp_n\langle x_n|e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}}|p_n\rangle\langle p_n|x_{n-1}\rangle e^{-\frac{i}{\hbar}V(x_{n-1})\epsilon}\right], && (27)\\
&= \prod_{n=1}^{N-1}\left[\int_{-\infty}^{\infty} dx_n dp_n e^{\frac{i}{\hbar}\left[p_n(x_n-x_{n-1})-\frac{p_n^2}{2m}-V(x_{n-1})\right]\epsilon}\right], && (28)\\
&\equiv \int\!\!\int \mathcal{D}x(t)\mathcal{D}p(t)e^{\frac{i}{\hbar}S[x(t),p(t)]}, && (29)\\
&\equiv \int_{x(0)=x_i}^{x(t)=x_f}\mathcal{D}x(t)e^{\frac{i}{\hbar}S[x(t)]}, && (30)
\end{aligned}$$

where we took the continuum limit $\epsilon \to 0$, defined a functional integral $\int\mathcal{D}x(t)\ldots \equiv \prod_{n=1}^{N-1}\left[\int_{-\infty}^{\infty}dx_n\right]\ldots$, and the phase-space and coordinate actions are given by

$$S[x(t), p(t)] \;=\; \int_0^t dt\big[p\dot{x} - \frac{p^2}{2m} - V(x)\big], \tag{31}$$

$$S[x(t)] \;=\; \int_0^t dt\big[\frac{1}{2}m\dot{x}^2 - V(x)\big]. \tag{32}$$

In going from phase-space to coordinate space path-integral, (30), we performed the Gaussian integrals over the momenta $p_n = p(t_n)$. The a graphical visualization of the path-integral is given in Fig.1.

The advantage of the path integral formulation is that it allows us to work with commuting functions rather than noncommuting operators. It also very powerful for semi-classical

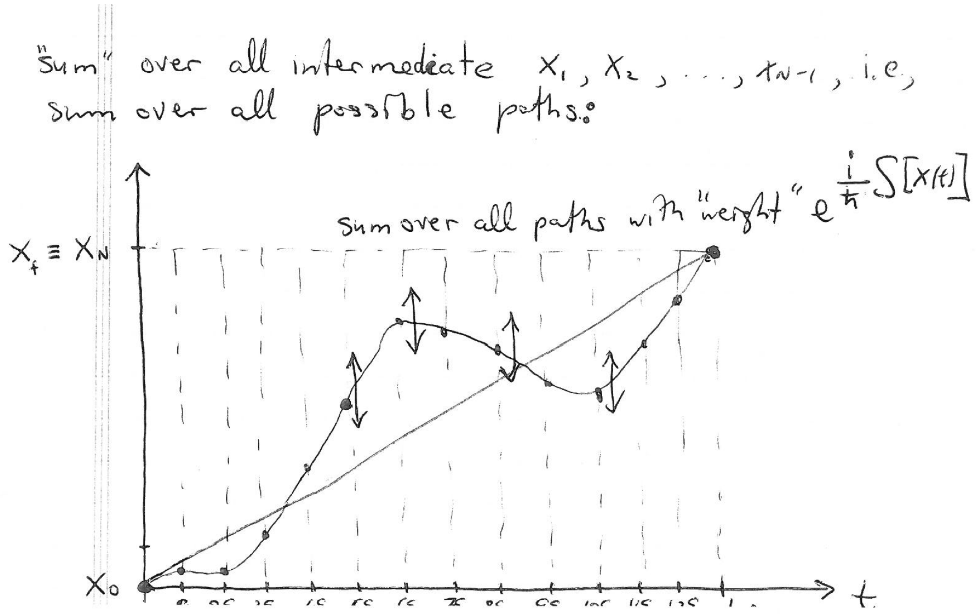


FIG. 1: A graphical illustration of a coordinate path integral for an evolution operator in one dimension.

analysis with classical $\hbar \to 0$ limit emerges as its saddle point that extremizes the action. As discussed in great detail in Feynman and Hibbs[5] and references therein, most problems in quantum mechanics and field theory can be reproduced using this approach, often much more efficiently. However, some problmes are much more amenable to treatment through the operator formalism (e.g., spin quantization).

For a vanishing potential, the path integral becomes Gaussian and the evolution operator is easily computed[5] by a number of methods (for example via a direct Gaussian integration of (28), a saddle-point solution, exact in this case, or by a solution of the Schrödinger's equation), giving

$$U_0(x_f, x_i; t) = \Big(\frac{m}{2\pi i\hbar t}\Big)^{1/2} e^{\frac{i}{\hbar}\frac{m}{2}(x_f - x_i)^2/t}.$$

This is why Gaussian integrals play such a crucial role in theoretical physics.

We now turn to a seemingly distinct problem of a quantum partition function for this system given by a trace of the density matrix $\hat{\rho}(\beta) = e^{-\beta\hat{H}}$

$$Z = \mathrm{Tr} e^{-\beta\hat{H}} = \int_{-\infty}^{\infty} dx_0 \langle x_0|e^{-\beta\hat{H}}|x_0\rangle = \int_{x(0)=x(\beta\hbar)} \mathcal{D}x(\tau) e^{-\frac{1}{\hbar}S_E[x(\tau)]}, \tag{33}$$

where

$$S_E[x(\tau)] = \int_0^{\beta\hbar} d\tau \big[\frac{1}{2}m\dot{x}^2 + V(x)\big],$$

obtained by repeating Trotter decomposition of the previous analysis, but here applying it to imaginary time $0 \leq \tau = it < \beta\hbar$, with the maximum imaginary time given by $\tau = \beta\hbar$. The saddle-point Euler-Lagrange equation for $S_E$ corresponds to a particle moving in an inverted potential $-V(x)$. We note that this Euclidean action can also be obtained directly from the real action (32) by replacement $it = \tau$ with compact imaginary time $\beta\hbar$. Immediately, we can also obtain an analog of the Schrödinger's equation in imaginary time, satisfied by the density matrix

$$\partial_\beta \hat{\rho}(\beta) = -\hat{H}\hat{\rho}(\beta).$$

We note that correlation functions computed with a path integral automatically give time-ordered ones (operators are arranged in later ones appearing to the left),

$$\mathrm{Tr}\left[T\left(x(\tau_1)\ldots x(\tau_n)\hat{\rho}(\beta)\right)\right] = \int \mathcal{D}x(\tau)x(\tau_1)\ldots x(\tau_n)e^{-\frac{1}{\hbar}S_E[x(\tau)]} \tag{34}$$

as it is only these time-ordered operators are arranged in the necessary order to apply the Trotter decomposition to a correlation function.

Finally, generalizing this single variable coordinate path-integral to many variables, its formulation for quantum field theory is straightforward. For example, a quantum partition function for a phonon field $\mathbf{u}(\mathbf{r})$ in a continuum of an isotropic model is given by

$$Z = \int_{\mathbf{u}(\mathbf{r},0)=\mathbf{u}(\mathbf{r},\beta\hbar)} \mathcal{D}\mathbf{u}(\mathbf{r},\tau)e^{-\frac{1}{\hbar}S_E[\mathbf{u}(\mathbf{r},\tau)]}, \tag{35}$$

where

$$S_E[\mathbf{u}(\mathbf{r},\tau)] = \int_0^{\beta\hbar} d\tau d^d r\left[\frac{1}{2}\rho(\partial_\tau \mathbf{u})^2 + \frac{1}{2}\mu(\boldsymbol{\nabla}\mathbf{u})^2\right].$$

We observe that in a path-integral formulation a $d$-dimensional quantum field theory looks like a path integral of an effective "classical" theory in $d+1$ dimensions with the extra imaginary time dimension confined to a slab $0 \leq \tau < \beta\hbar$.

At zero temperature $\beta\hbar \to \infty$, leading to a classical like path-integral in all $d+1$ dimensions. In contrast, at high temperature, $\beta\hbar \to 0$, the field $\mathbf{u}$ becomes $\tau$ independent (otherwise the time-derivatives cost too much action and are suppressed) and the partition function reduces to that of a $d$-dimensional classical one

$$Z \to Z_{cl} = \int \mathcal{D}\mathbf{u}(\mathbf{r})e^{-\beta\int d^d r \frac{1}{2}\mu(\boldsymbol{\nabla}\mathbf{u})^2}$$

over time-independent classical phonon field $\mathbf{u}(\mathbf{r})$ with a Boltzmann weight controlled by the elastic energy. This is indeed as expected, as quantum fluctuations are insignificant at high temperature.

### 2. coherent states path-integral

From the derivation of the coordinate path-integral above, it is quite clear that other equivalent representations are possible, determined by the basis set of the resolution of identity in the Trotter decomposition. One particularly convenient representation is that of coherent states $|z\rangle$

$$|z\rangle = e^{-\frac{1}{2}|z|^2} e^{za^\dagger}|0\rangle = e^{-\frac{1}{2}|z|^2}\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}|n\rangle \tag{36}$$

labelled by a complex number $z$. From the canonical commutation relation $[a, a^\dagger] = 1$ it is clear that $e^{za^\dagger}$ is an operator (analogously to $e^{\frac{i}{\hbar}cp}$ for $x$) that shifts $a$'s eigenvalue of the vacuum state $|0\rangle$ by $z$, leading to coherent state's key property

$$a|z\rangle = z|z\rangle.$$

These states are overcomplete with nontrivial overlap given by

$$\langle z_1|z_2\rangle = e^{-\frac{1}{2}|z_1|^2} e^{-\frac{1}{2}|z_2|^2} e^{\bar{z}_1 z_2}$$

and resolution of identity

$$\hat{1} = \frac{d^2 z}{2\pi i}|z\rangle\langle z| \tag{37}$$

where $\frac{d^2 z}{2\pi i} \equiv \frac{d\mathrm{Re}z d\mathrm{Im}z}{\pi}$.

Armed with these properties, we derive a very useful coherent-state path-integral. Using the resolution of identity, (37), we deduce Trotter decomposition of the density matrix,

$$\langle z_f|e^{-\beta\hat{H}}|z_i\rangle = \langle z_N|e^{-\frac{\epsilon}{\hbar}\hat{H}}|z_{N-1}\rangle\langle z_{N-1}|e^{-\frac{\epsilon}{\hbar}\hat{H}}|z_{N-1}\rangle \ldots \langle z_j|e^{-\frac{\epsilon}{\hbar}\hat{H}}|z_{j-1}\rangle \ldots \langle z_1|e^{-\frac{\epsilon}{\hbar}\hat{H}}|z_0\rangle. \tag{38}$$

where $\epsilon = \beta\hbar/N$. The matrix element can be evaluated for $\epsilon \ll 1$, given by

$$\langle z_j|e^{-\frac{\epsilon}{\hbar}\hat{H}}|z_{j-1}\rangle = \langle z_j|z_{j-1}\rangle\left(1 - \frac{\epsilon}{\hbar}\frac{\langle z_j|\hat{H}|z_{j-1}\rangle}{\langle z_j|z_{j-1}\rangle}\right), \tag{39}$$

$$= \langle z_j|z_{j-1}\rangle e^{-\frac{\epsilon}{\hbar}\frac{\langle z_j|\hat{H}|z_{j-1}\rangle}{\langle z_j|z_{j-1}\rangle}} = \langle z_j|z_{j-1}\rangle e^{-\frac{\epsilon}{\hbar}H(\bar{z}_j, z_{j-1})}, \tag{40}$$

$$= e^{-\frac{1}{2}[\bar{z}_j(z_j - z_{j-1}) - z_{j-1}(\bar{z}_j - \bar{z}_{j-1})]} e^{-\frac{\epsilon}{\hbar}H(\bar{z}_j, z_{j-1})}. \tag{41}$$

where in the last line we simplified expression by taking the Hamiltonian $H[a^\dagger, a]$ to be normal-ordered (all $a^\dagger$s are to the left of $a$'s).

Putting this matrix element into the (42), we find

$$\langle z_f|e^{-\beta\hat{H}}|z_i\rangle = \int\prod_{j=1}^{N-1}\frac{d^2z_j}{2\pi i}e^{-\frac{1}{\hbar}S_E[\{\overline{z}_j,z_j\}]} = \int_{\overline{z}(\beta\hbar)=\overline{z}_f}^{z(0)=z_i}\mathcal{D}\overline{z}(\tau)\mathcal{D}z(\tau)e^{-\frac{1}{\hbar}S_E[\overline{z}(\tau),z(\tau)]}, \quad (42)$$

in the second equality we took the continuum limit $N\to\infty$, and the Euclidean action in discrete and continuous forms is respectively given by

$$\begin{aligned} S_E[\{\overline{z}_j,z_j\}] &= \sum_{j=1}^{N-1}\left[\frac{1}{2}\overline{z}_j(z_j-z_{j-1})-\frac{1}{2}z_j(\overline{z}_{j+1}-\overline{z}_j)+\frac{\epsilon}{\hbar}H(\overline{z}_j,z_{j-1})\right]\\ &\quad+\frac{1}{2}\overline{z}_f(z_f-z_{N-1})-\frac{1}{2}z_i(\overline{z}_1-\overline{z}_i), \quad (43)\\ S_E[\overline{z}(\tau),z(\tau)] &= \int_0^{\beta\hbar}d\tau\left[\frac{1}{2}(\overline{z}\partial_\tau z-z\partial_\tau\overline{z})+\frac{\epsilon}{\hbar}H[\overline{z}(\tau),z(\tau)]\right]\\ &\quad+\frac{1}{2}\overline{z}_f(z_f-z(\beta\hbar))-\frac{1}{2}z_i(\overline{z}(0)-\overline{z}_i), \quad (44)\end{aligned}$$

where the last terms involving $\overline{z}_f, z_i$ are boundary terms that can be important in some situations but not in the cases that we will consider.

With this single-particle formulation in place, it is straightforward to generalize it to many variables, and then by extension to a coherent-state path-integral formulation of a quantum field theory. Applying this to bosonic matter, with identification $a^\dagger, a\to\psi^\dagger,\psi$ and $\overline{z}(\tau),z(\tau)\to\overline{\psi}(\tau,\mathbf{r}),\psi(\tau,\mathbf{r})$

$$Z = \int\mathcal{D}\overline{\psi}(\tau,\mathbf{r})\mathcal{D}\psi(\tau,\mathbf{r})e^{-\frac{1}{\hbar}S_E[\overline{\psi}(\tau,\mathbf{r}),\psi(\tau,\mathbf{r})]}, \quad (45)$$

where the Euclidean bosonic action is given by

$$\begin{aligned} S_E[\overline{\psi}(\tau,\mathbf{r}),\psi(\tau,\mathbf{r})] &= \int_0^{\beta\hbar}d\tau d^dr\left[\frac{1}{2}\hbar\left(\overline{\psi}\partial_\tau\psi-\psi\partial_\tau\overline{\psi}\right)-\overline{\psi}\frac{\hbar^2\nabla^2}{2m}\psi\right], \quad (46)\\ &= \int_0^{\beta\hbar}d\tau d^dr\overline{\psi}(\hbar\partial_\tau-\frac{\hbar^2\nabla^2}{2m})\psi, \quad (47)\end{aligned}$$

with periodic boundary conditions on the bosonic field $\psi(0,\mathbf{r})=\psi(\beta\hbar,\mathbf{r})$ and its conjugate, allowing us to integrate by parts to obtain the second form above. The action can also be immediately obtained from the real-time action $S$, (145) by replacing $it\to\tau$. A huge advantage of this formulation is that it now allows us to calculation bosonic (time-ordered) correlation functions using simple Gaussian integrals over commuting "classical" $d+1$-dimensional fields, with the only price the extra imaginary time dimension, as compared to the classical $d$-dimensional statistical field theory.

Fourier transforming the coherent bosonic fields,

$$\psi(\tau,\mathbf{r}) = \frac{1}{\sqrt{\beta\hbar}}\sum_{\omega_n}\int\frac{d^dk}{(2\pi)^d}\psi(\omega_n,\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}-i\omega_n\tau},\quad \overline{\psi}(\tau,\mathbf{r}) = \frac{1}{\sqrt{\beta\hbar}}\sum_{\omega_n}\int\frac{d^dk}{(2\pi)^d}\overline{\psi}(\omega_n,\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{r}+i\omega_n\tau},$$

we obtain

$$S_E[\overline{\psi}(\omega_n,\mathbf{k}),\psi(\omega_n,\mathbf{k})] = \sum_{\omega_n}\int\frac{d^dk}{(2\pi)^d}\overline{\psi}(-i\hbar\omega_n+\epsilon_k)\psi, \tag{48}$$

where $\omega_n = \frac{2\pi}{\beta\hbar}n$ is the bosonic Matsubara frequency.

### D. Propagators and Wick's theorem

#### 1. *Scalar field theory*

For pedagogical clarity it is convenient to illustrate path-integral calculus with a field theory of a real scalar field $\phi(\mathbf{x})$ ($\mathbf{x}=(\tau,\mathbf{r})$), with Euclidean imaginary time action

$$S = \frac{1}{2}\int_{\mathbf{x}}\int_{\mathbf{x}'}\phi(\mathbf{x})\Gamma(\mathbf{x},\mathbf{x}')\phi(\mathbf{x}') - \int_{\mathbf{x}} j(\mathbf{x})\phi(\mathbf{x}),$$

with an external source field $j(\mathbf{x})$. Utilizing Gaussian integral calculus, the associated generating (partition) function is then given by

$$\begin{aligned} Z[j(\mathbf{x})] &= \int\mathcal{D}\phi(\mathbf{x})e^{-\frac{1}{2}\int_{\mathbf{x}}\int_{\mathbf{x}'}\phi(\mathbf{x})\Gamma(\mathbf{x},\mathbf{x}')\phi(\mathbf{x}')+\int_{\mathbf{x}}j(\mathbf{x})\phi(\mathbf{x})}, &(49)\\ &= e^{\frac{1}{2}\int_{\mathbf{x}}\int_{\mathbf{x}'}j(\mathbf{x})\Gamma^{-1}(\mathbf{x},\mathbf{x}')j(\mathbf{x}')}, &(50)\end{aligned}$$

where the $\Gamma^{-1}(\mathbf{x},\mathbf{x}')$ is an inverse of $\Gamma(\mathbf{x},\mathbf{x}')$. For a translationally invariant case $\Gamma(\mathbf{x}-\mathbf{x}')$, the inverse is computed by a Fourier transformation, namely $\Gamma^{-1}(\mathbf{x}-\mathbf{x}') = \int_{\mathbf{k}}\frac{1}{\tilde{\Gamma}(\mathbf{k})}e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}$.

Using $Z[j(\mathbf{x})]$ the correlators are straightforwardly computed by simply differentiating with respect to $j(\mathbf{x})$,

$$G(\mathbf{x},\mathbf{x}') = \langle\phi(\mathbf{x})\phi(\mathbf{x}')\rangle = \frac{1}{Z}\frac{\delta^2 Z[j(\mathbf{x})]}{\delta j(\mathbf{x})\delta j(\mathbf{x}')}\bigg|_{j=0}.$$

The "connected" correlation functions

$$\begin{aligned} G_c(\mathbf{x},\mathbf{x}') &= \langle\phi(\mathbf{x})\phi(\mathbf{x}')\rangle_c \equiv \langle\phi(\mathbf{x})\phi(\mathbf{x}')\rangle - \langle\phi(\mathbf{x})\rangle\langle\phi(\mathbf{x}')\rangle = \frac{1}{2}\langle[\phi(\mathbf{x})-\phi(\mathbf{x}')]^2\rangle, &(51)\\ &= \frac{\delta^2\ln Z[j(\mathbf{x})]}{\delta j(\mathbf{x})\delta j(\mathbf{x}')}\bigg|_{j=0} \equiv \frac{\delta^2 W[j(\mathbf{x})]}{\delta j(\mathbf{x})\delta j(\mathbf{x}')}\bigg|_{j=0}, &(52)\end{aligned}$$

where $W[j(\mathbf{x})]$ is a generating function for *connected* correlation functions, with disconnected parts cancelled by the differentiation of normalization $1/Z[j(\mathbf{x})]$.

Using $Z[j(\mathbf{x})]$ above we immediately obtain the powerful Wick's theorem valid for Gaussian fields only. Namely,

$$\begin{aligned}\langle\phi(\mathbf{x}_1)\phi(\mathbf{x}_2)\phi(\mathbf{x}_3)\ldots\phi(\mathbf{x}_{2n})\rangle &= \frac{1}{Z}\frac{\delta^{2n}Z[j(\mathbf{x})]}{\delta j(\mathbf{x}_1)\delta j(\mathbf{x}_2)\delta j(\mathbf{x}_3)\ldots\delta j(\mathbf{x}_{2n})}\Big|_{j=0},\\ &= G(\mathbf{x}_1,\mathbf{x}_2)G(\mathbf{x}_3,\mathbf{x}_4)\ldots G(\mathbf{x}_{2n-1},\mathbf{x}_{2n})\\ &\quad+\text{all other pairings of } \mathbf{x}_i,\mathbf{x}_j, \qquad (53)\end{aligned}$$

and vanishing for correlators odd number of fields.

Now above Wick's theorem directly applies to a *classical* statistical field theory. Thanks to a path-integral formulation of a quantum field (that maps it onto an effective $d+1$-dimensional classical statistical field theory), with a slight modification, the theorem also extends to a quantum field theory for time-ordered correlation functions in a ground state $|0\rangle$

$$\begin{aligned}\langle 0|T_\tau\left(\phi(\mathbf{x}_1)\phi(\mathbf{x}_2)\phi(\mathbf{x}_3)\ldots\phi(\mathbf{x}_{2n})\right)|0\rangle &= G(\mathbf{x}_1,\mathbf{x}_2)G(\mathbf{x}_3,\mathbf{x}_4)\ldots G(\mathbf{x}_{2n-1},\mathbf{x}_{2n})\\ &\quad+\text{all other pairings of } \mathbf{x}_i,\mathbf{x}_j, \qquad (54)\end{aligned}$$

A more general form of the quantum Wick's theorem at the level of operators is given by

$$\begin{aligned}T_\tau\left(\phi(\mathbf{x}_1)\phi(\mathbf{x}_2)\phi(\mathbf{x}_3)\ldots\phi(\mathbf{x}_n)\right) &= :\phi(\mathbf{x}_1)\phi(\mathbf{x}_2)\phi(\mathbf{x}_3)\phi(\mathbf{x}_4)\phi(\mathbf{x}_5)\ldots\phi(\mathbf{x}_n):\\ &= \overline{\phi(\mathbf{x}_1)\phi(\mathbf{x}_2)}:\phi(\mathbf{x}_3)\phi(\mathbf{x}_4)\phi(\mathbf{x}_5)\ldots\phi(\mathbf{x}_n):\\ &\quad+\text{all other } \textit{single} \text{ pair } (\mathbf{x}_i,\mathbf{x}_j) \text{ contraction}\\ &= \overline{\phi(\mathbf{x}_1)\phi(\mathbf{x}_2)}\,\overline{\phi(\mathbf{x}_3)\phi(\mathbf{x}_4)}:\phi(\mathbf{x}_5)\ldots\phi(\mathbf{x}_n):\\ &\quad+\text{all other } \textit{double} \text{ pair } (\mathbf{x}_i,\mathbf{x}_j),\ (\mathbf{x}_k,\mathbf{x}_l) \text{ contraction}\\ &= \overline{\phi(\mathbf{x}_1)\phi(\mathbf{x}_2)}\ldots\overline{\phi(\mathbf{x}_{n-1})\phi(\mathbf{x}_n)}\\ &\quad+\text{all other } n/2 \text{ pairs, if } n \text{ is even}\\ &= \overline{\phi(\mathbf{x}_1)\phi(\mathbf{x}_2)}\ldots\overline{\phi(\mathbf{x}_{n-2})\phi(\mathbf{x}_{n-1})}\,\phi(\mathbf{x}_n)\\ &\quad+\text{all other } (n-1)/2 \text{ pairs, if } n \text{ is odd}, \qquad (55)\end{aligned}$$

where the contraction of a pair of fields is defined to be

$$\overline{\phi(\mathbf{x}_1)\phi(\mathbf{x}_2)} \equiv T_\tau\left(\phi(\mathbf{x}_1)\phi(\mathbf{x}_2)\right) - :\phi(\mathbf{x}_1)\phi(\mathbf{x}_2):,$$

$: \hat{O} :$ is the normal ordered arrangments of operators with creation operators to the left of annihilation operators. Evaluation of the expectation value in the vacuum gives the path-integral expression, (53).

### 2. *Bosonic field theory*

Correlators and thermodynamics of a Gaussian bosonic field theory are controlled by the Euclidean action, (47),(48) for a path-integral computation and equivalently by the Hamiltonian (8) in a canonical computation.

The key correlator is the the time-ordered propagator

$$\begin{aligned} G(\tau, \mathbf{r}) &= \langle T_\tau(\psi(\tau, \mathbf{r})\psi^\dagger(0,0))\rangle = Z^{-1}\mathrm{Tr}[T_\tau(\psi(\tau, \mathbf{r})\psi^\dagger(0,0))e^{-\beta H}], \\ &= \langle \psi(\tau, \mathbf{r})\overline{\psi}(0,0)\rangle \end{aligned} \tag{56}$$

from which via Wick's theorem all other correlators can be obtained. In the first form the average is a trace over quantum many-body states with. In the second form it is its coherent-state path-integral equivalent, that automatically gives time-ordered correlators.

Using Heisenberg equation of motion for $\psi(\tau, \mathbf{k})$ with Hamiltonian (8), we have $\psi(\tau, \mathbf{k}) = \psi(\mathbf{k})e^{-\epsilon_k \tau/\hbar}$, from which the propagator is given by

$$\begin{aligned} G(\tau, \mathbf{r}) &= \frac{1}{V}\sum_{\mathbf{k}} e^{-\epsilon_k\tau/\hbar + i\mathbf{k}\cdot\mathbf{r}} Z^{-1}\sum_{n_{\mathbf{k}}=0}^{\infty}\langle n_{\mathbf{k}}| \left(\theta(\tau)a_{\mathbf{k}}a_{\mathbf{k}}^\dagger + \theta(-\tau)a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\right)|n_{\mathbf{k}}\rangle e^{-\beta\epsilon_k n_{\mathbf{k}}}, \\ &= \frac{1}{V}\sum_{\mathbf{k}} e^{-\epsilon_k\tau/\hbar + i\mathbf{k}\cdot\mathbf{r}}\left(\theta(\tau)\frac{e^{\beta\epsilon_{\mathbf{k}}}}{e^{\beta\epsilon_{\mathbf{k}}}-1} + \theta(-\tau)\frac{1}{e^{\beta\epsilon_{\mathbf{k}}}-1}\right) \end{aligned} \tag{57}$$

Equivalently, the result can be computed using coherent-state path-integral with the second form in (56)

$$\begin{aligned} G(\tau, \mathbf{r}) &= \frac{1}{\beta\hbar}\sum_{\omega_n,\omega_{n'}}\int\frac{d^dk}{(2\pi)^d}\int\frac{d^dk'}{(2\pi)^d}e^{-i\omega_n\tau + i\mathbf{k}\cdot\mathbf{r}}\langle\psi(\omega_n,\mathbf{k})\overline{\psi}(\omega_{n'},\mathbf{k}')\rangle, \\ &= \frac{1}{\beta\hbar}\sum_{\omega_n}\int\frac{d^dk}{(2\pi)^d}\frac{e^{-i\omega_n\tau + i\mathbf{k}\cdot\mathbf{r}}}{-i\omega_n + \epsilon_{\mathbf{k}}}, \end{aligned} \tag{58}$$

with the sum over bosonic Matsubara frequencies, $\omega_n = \frac{2\pi}{\beta\hbar}n$.

To evaluate the last sum we utilize a complex contour integral over a circle at $|z| \to \infty$

that vanishes for $\tau < 0$

$$0 = \frac{1}{2\pi i}\oint_C \frac{e^{-z\tau}}{-z+\epsilon_{\mathbf{k}}/\hbar}\frac{1}{e^{\beta\hbar z}-1}, \tag{59}$$

$$= \frac{1}{\beta\hbar}\sum_{\omega_n}\frac{e^{-i\omega_n\tau}}{-i\omega_n+\epsilon_{\mathbf{k}}/\hbar} - \frac{e^{-\epsilon_{\mathbf{k}}\tau/\hbar}}{e^{\beta\epsilon_{\mathbf{k}}}-1}. \tag{60}$$

Repeating this for $\tau > 0$, we find

$$0 = \frac{1}{2\pi i}\oint_C \frac{e^{-z\tau}}{-z+\epsilon_{\mathbf{k}}/\hbar}\frac{e^{\beta\hbar z}}{e^{\beta\hbar z}-1}, \tag{61}$$

$$= \frac{1}{\beta\hbar}\sum_{\omega_n}\frac{e^{-i\omega_n\tau}}{-i\omega_n+\epsilon_{\mathbf{k}}/\hbar} - \frac{e^{-\epsilon_{\mathbf{k}}\tau/\hbar+\beta\epsilon_{\mathbf{k}}}}{e^{\beta\epsilon_{\mathbf{k}}}-1}, \tag{62}$$

where to ensure the convergence of the contour integral for $Re(z) \to -\infty$ part, we introduced an additional factor of $e^{\beta\hbar z}$ in the numerator of the first equality.

Together these give

$$\frac{1}{\beta\hbar}\sum_{\omega_n}\frac{e^{-i\omega_n\tau}}{-i\omega_n+\epsilon_{\mathbf{k}}/\hbar} = \theta(\tau)\frac{e^{-\epsilon_{\mathbf{k}}\tau/\hbar+\beta\epsilon_{\mathbf{k}}}}{e^{\beta\epsilon_{\mathbf{k}}}-1} + \theta(-\tau)\frac{e^{-\epsilon_{\mathbf{k}}\tau/\hbar}}{e^{\beta\epsilon_{\mathbf{k}}}-1},$$

$$= e^{-\epsilon_{\mathbf{k}}\tau/\hbar}\left[\theta(\tau)\big(\frac{1}{e^{\beta\epsilon_{\mathbf{k}}}-1}+1\big) + \theta(-\tau)\frac{1}{e^{\beta\epsilon_{\mathbf{k}}}-1}\right], \tag{63}$$

$$= e^{-\epsilon_{\mathbf{k}}\tau/\hbar}\left[\theta(\tau)\big(n_{BE}(\beta\epsilon_{\mathbf{k}})+1\big) + \theta(-\tau)n_{BE}(\beta\epsilon_{\mathbf{k}})\right], \tag{64}$$

which when used inside (58) reproduces the canonical quantization result, (57).

## III. NONINTERACTING BOSE GAS: BOSE-EINSTEIN CONDENSATION

We now want to calculate the thermodynamics of a noninteracting Bose gas as for example found in dilute degenerate Bose gases laser and evaporatively cooled in JILA and nwo around the world. To fix the number of bosonic atoms to be $N$ it is convenient to work in the grand-canonical formulation of quantum statistical mechanics, using effective Hamiltonian $H_\mu = H - \mu N$, with the chemical potential $\mu$ tuned such that the expectation value of the atom number is given by the experimentally prescribed number $N$,

$$N = \int d^d r \langle \psi^\dagger(0,\mathbf{r})\psi(0,\mathbf{r}))\rangle = \int d^d r G(\tau \to 0^{-1}, \mathbf{r}), \tag{65}$$

$$= \sum_{\mathbf{k}} \frac{1}{e^{\beta(\epsilon_{\mathbf{k}}-\mu)} - 1}, \tag{66}$$

$$= V \int \frac{d^d k}{(2\pi)^d} \frac{1}{e^{\beta\varepsilon_{\mathbf{k}}} - 1}, \tag{67}$$

$$= V \frac{C_d}{2} \left(\frac{2m}{\hbar^2}\right)^{d/2} \int_0^\infty d\epsilon \frac{\epsilon^{d/2-1}}{e^{\beta(\epsilon-\mu)} - 1}, \tag{68}$$

where $\varepsilon_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu = \hbar^2 k^2/2m - \mu$, and in going to the last two lines we made (what will turn out to be) a crucial thermodynamic limit approximation, replacing sum over $\mathbf{k}$ by an integral; $1/C_d = 2^{d-1}\pi^{d/2}\Gamma(d/2)$.

At high temperature the gas should behave as a classical Boltzmann gas with a negative chemical potential. Indeed in that regime we can ignore 1 relative to the exponential and straightforwardly perform the integration. Solving for the chemical potential in terms of the density $n = N/V$ and temperature we obtaining the classical Boltzmann result:

$$\mu(T, n) = -k_B T \ln(n\lambda_T^d) = -k_B T \ln T/T_c, \quad \text{valid for } T >> T_c \tag{69}$$

where

$$\lambda_T = \left(\frac{2\pi\hbar^2}{mk_B T}\right)^{1/2}$$

is the thermal deBroglie wavelength and we deduced the crossover, degeneracy temperature scale

$$T_d = 4\pi \frac{\hbar^2 n^{2/d}}{2m}$$

above which this classical result is valid.

Because in 1d and 2d dimensions the integral diverges for $\mu = 0$ at the lower limit $\epsilon = 0$ (think about expanding the exponential for small $\beta(\epsilon - \mu)$), $N(\mu)$ and therefore $\mu(n, T)$ are smooth functions exhibiting no phase transitions. On the hand, as illustrated in Fig.3 for $d > 2$, the integral saturates at a finite value even for $\mu = 0$,

$$N(T_c) = V \frac{C_d}{2} \left(\frac{2mk_B T_c}{\hbar^2}\right)^{d/2} \int_0^\infty d\epsilon \frac{\epsilon^{d/2-1}}{e^\epsilon - 1} = V\zeta(d/2) \left(\frac{mk_B T_c}{2\pi\hbar^2}\right)^{d/2} \tag{70}$$

with the corresponding temperature, the BEC temperature:

$$k_B T_c = \zeta(d/2)^{-2/d} \left(\frac{2\pi\hbar^2 n^{2/d}}{m}\right),$$

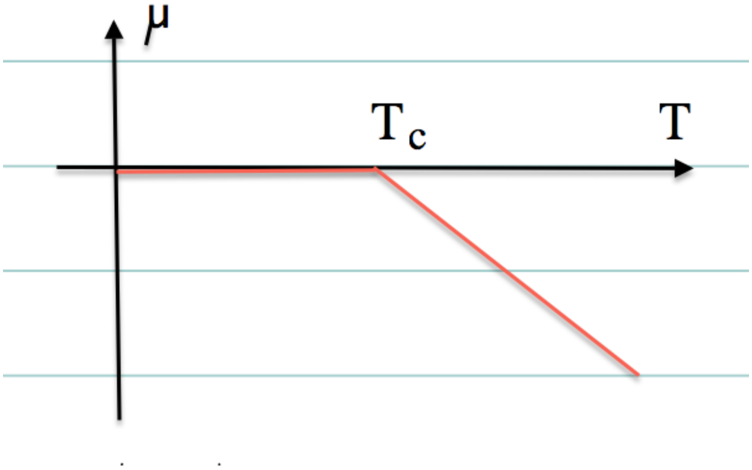


FIG. 2: Chemical potential in a noninteracting Bose gas as a function of temperature near the transition to Bose-Einstein condensation at temperature $T_c$.

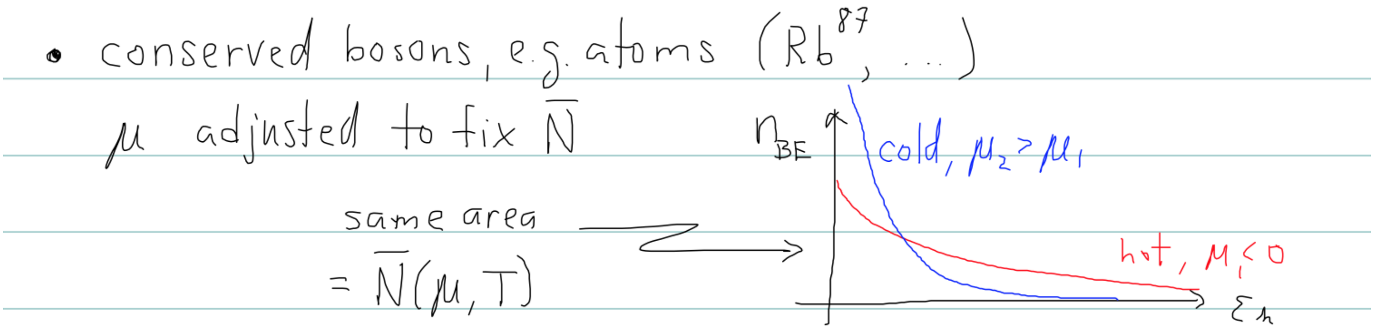


FIG. 3: A sketch of the Bose-Einstein momentum distribution function as a function of $k$ as $T$ is reduced toward $T_c$ from above.

where we used $\int_0^\infty d\epsilon \frac{\epsilon^{d/2-1}}{e^\epsilon - 1} = \Gamma(d/2)\zeta(d/2)$, valid for $d > 2$.

This saturations is a consequence of a density of states that vanishes more strongly with increased dimension and thus in $d > 2$ the integral does an inadequate job of accounting for the low $k$ states that at low $T < T_c$ is macroscopically occupied.

To account for the discreteness of states we separate out the occupation $N_0 = n_0 V$ of the single particle ground state $\mathbf{k} = 0$, the Bose Einstein condensate, obtaining for $T < T_c$

$$n_0(T) = n\left[1 - \left(\frac{T}{T_c}\right)^{d/2}\right], \quad \text{for } T < T_c \tag{71}$$

and vanishing for $T > T_c$. The number density of finite-temperature excitations is then given by the complement $n_{exc}(T) = n\left(\frac{T}{T_c}\right)^{d/2}$. We thus discovered the existence of a finite-temperature phase transition in an noninteracting Bose gas, between thermal and Bose-condensed states.

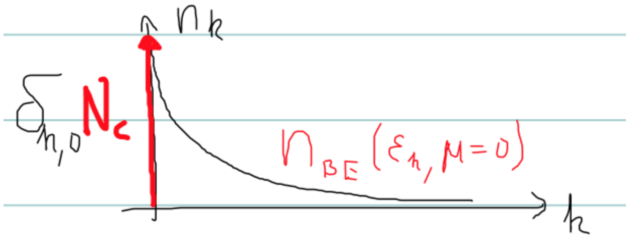


FIG. 4: A sketch of the Bose-Einstein momentum distribution function $n_k$ as a function of $k$ for $T < T_c$, illustrating the thermal finite $k$ and the condensate $k = 0$ components.

At $T = 0$ the BEC state is described by a many-body eigenstate

$$|\Psi_0\rangle = \left(a^\dagger_{\mathbf{k}=0}\right)^N |0\rangle \tag{72}$$

that corresponds to a wavefunction that is a product of the single-particle ground state wavefunction $\psi_0(\mathbf{r})$ occupied by each atom,

$$\Psi_0(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = \prod_{i=1}^{N} \psi_0(\mathbf{r}_i) = \frac{1}{V^{N/2}},$$

with last equality corresponding to the case of a box trap. In a harmonic isotropic trap, relevant to AMO experiments, instead $\psi_0(\mathbf{r}) \sim e^{-\frac{1}{2}r^2/r_0^2}$, with $r_0 = \sqrt{\hbar/(m\omega_{trap})}$ the trap's quantum oscillator length.

We note that without interactions the condensate $n_0(T)$ grows from zero, approaching total atomic density $n$ at $T = 0$. This last property is not generic and will not survive inclusion of atomic interactions. All other properties of this noninteracting system can be extensivelyl explored (see e.g.,[6]), but we instead turn our attention to the more interesting and nontrivial interacting Bose gas.

## IV. INTERACTING BOSE GAS

We now turn to the study of a weakly *interacting* Bose gas, a generalization of the previous noninteracting BEC study.

Utilizing second-quantization formulation from Sec.(II), we consider interacting bosons, described by a grand-canonical Hamiltonian:

$$\begin{aligned} H_\mu &= \int_{\mathbf{r}} \left[\psi^\dagger(\frac{-\hbar^2\nabla^2}{2m} - \mu)\psi + \frac{g}{2}\psi^\dagger\psi^\dagger\psi\psi\right], \\ &= \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \frac{g}{2V}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}} a^\dagger_{\mathbf{k}_1+\mathbf{q}/2} a^\dagger_{-\mathbf{k}_1+\mathbf{q}/2} a_{\mathbf{k}_2+\mathbf{q}/2} a_{-\mathbf{k}_2+\mathbf{q}/2}, \end{aligned} \tag{73}$$

where $\varepsilon_k = \epsilon_k - \mu = \hbar^2 k^2/2m - \mu$, and $\psi(\mathbf{r}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}$. Above, we have taken the interaction to be short-ranged, $V(r) = g\delta^d(\mathbf{r})$, characterized by a parameter ("pseudo-potential") $g \equiv 4\pi\hbar^2 r_0/m$ (that for many atoms can be tunable using external magnetic field through the magic of Feshbach resonances), with $r_0 = 1/\Lambda$ the microscopic range of the interatomic potential (van der Waals for neutral atoms), usually on the order a few tens of atomic units. This "bare" interaction parameter $g$ controls the renormalized interaction coupling $g_R$, according to

$$g_R^{-1} = g^{-1} + \int \frac{d^dk}{(2\pi)^d}\frac{1}{2\epsilon_k} = g^{-1} + m\Lambda/(2\pi^2\hbar^2),$$

related to the two-atom scattering length $a_s$ via $g_R = 4\pi\hbar^2 a_s/m$, and in the last equality the integral was evaluating in three dimensions, $d = 3$.

### A. Mean-field Ginzburg-Landau theory

Having studied the non-interacting case in the previous section, we anticipate a possibility of Bose-condensation at low temperatures by splitting the bosonic field operator $\psi(\mathbf{r}) = \Psi_0(\mathbf{r}) + \phi(\mathbf{r})$ into a c-number condensate field $\Psi_0(\mathbf{r})$ and the bosonic quantum fluctuations (bosonic excitations out of the condensate) field, $\phi(\mathbf{r})$. In terms of the Fourier modes (momentum operators) this correspoinds to $a_{\mathbf{k}} = a_0\delta_{\mathbf{k},0} + a_{\mathbf{k}\neq 0}$, with $\Psi_0 = a_0/\sqrt{V}$ a constant. More generally, however, say in a trap, $\Psi_0(\mathbf{r})$ is single-particle ground state wavefunction that is spatially dependent.

In the complementary coherent-state formulation, above decomposition is equivalently understood as the condensation into a macroscopic coherent state $|\Psi_0\rangle = e^{\Psi_0(\mathbf{r})a_0^\dagger}|0\rangle$, that unlike all other single-particle states $\alpha \neq 0$ states exhibits a finite expectation value of $a_0|\Psi_0\rangle = \Psi_0(\mathbf{r})|\Psi_0\rangle$.

Inserting this decomposition into the many-body Hamiltonian, (73), we obtain $H_\mu =$

$H_{mft}[\Psi_0(\mathbf{r})] + \delta H_\mu$, where

$$
\begin{aligned}
H_{mft}[\Psi_0(\mathbf{r})] &= \int_{\mathbf{r}} \left[ \overline{\Psi}_0 (\frac{-\hbar^2 \nabla^2}{2m} - \mu) \Psi_0 + \frac{g}{2} |\Psi_0|^4 \right], \\
&= V \left[ -\mu |\Psi_0|^2 + \frac{g}{2} |\Psi_0|^4 \right], \qquad (74)
\end{aligned}
$$

where in the second line we specialized to a box trap for which the condensate is spatially uniform. In the presence of a trap $\Psi_0(\mathbf{r})$ would be the lowest eigenstate of the single-particle Hamiltonian. $\delta H_\mu$ is the fluctuations part that will study in the subsequent subsection.

### B. Normal-to-superfluid phase transition

Minimizing $H_{mft}[\Psi_0(\mathbf{r})]$ (that exhibits the famous "Mexican-hat" potential, Fig.5) over $\Psi_0$ we find

$$\Psi_0 = 0, \quad \text{for } \mu < 0, \qquad (75)$$

$$\Psi_0 = |\Psi_0| e^{i\varphi} = \sqrt{\mu/g} e^{i\theta}, \quad \text{for } \mu > 0, \qquad (76)$$

where $\theta$ is an arbitrary phase (there is a global $U(1)$ gauge symmetry of the Hamiltonian associated with atom number conservations) that without loss of generality we take to be $\theta = 0$. Thus this mean-field theory immediately captures the thermal-to-superfluid (BEC) phase transition as a function of the chemical potential controlable through density $n$, temperature, $T$ and interaction, $g$, equivalent to our analysis for BEC in the previous subsection.

Evaluating $H_{mft}$ at above $\Psi_0$ we find at this mean-field approximation the grand-canonical ground state energy is

$$
\begin{aligned}
E_\mu^{mft} &\equiv H_{mft}[\Psi_0] = -V\mu^2/g, \quad \mu > 0,\, T < T_c, \qquad (77) \\
&= 0, \quad \mu < 0,\, T > T_c, \qquad (78)
\end{aligned}
$$

clearly exhibiting a singularity in its second derivative with $\mu$ or equivalently with $T$ at $T = T_c$, characteristic of the second order transition. This negative condensation energy is what drives the phase transition. We note that at finite temperature this is a transition from a thermal normal gas to a Bose-condensed superfluid. At zero temperature, it is driven by the chemical potential or bosonic density, $n$, taking place at zero atom density. It then represents in a sense trivial vacuum-to-superfluid transition. Thus, we learn that in the

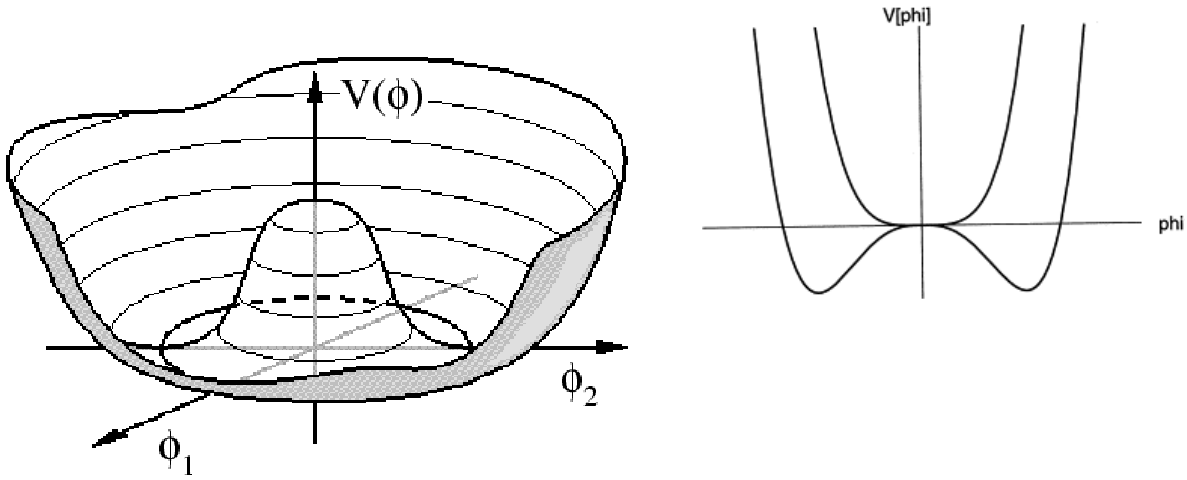


FIG. 5: A Mexican-hat potential and its cross-section controlling the normal-to-superfluid phase transition. Massive (gapped) amplitude (Higg's) and gapless Goldstone mode excitations respectively correspond to radial and azimuthal fluctuations about $\Psi_0$.

*continuum*, at $T = 0$ and any nonzero density, bosons always form a superfluid ground state.

The order parameter for this transition is the condensate field $\Psi_0$, that also exhibits a square-root singularity characteristic of mean-field approximation, as illustrated in Fig.6.

## V. LOW-ENERGY BOGOLUIBOV THEORY OF A SUPERFLUID

We now turn to the nontrivial effects of fluctuations about the above mean-field solution $\Psi_0$. Since this is an expansion small fluctuations, it is only valid for weak interactions, characterized by small "gas parameter" $na_s^3 \ll 1$.

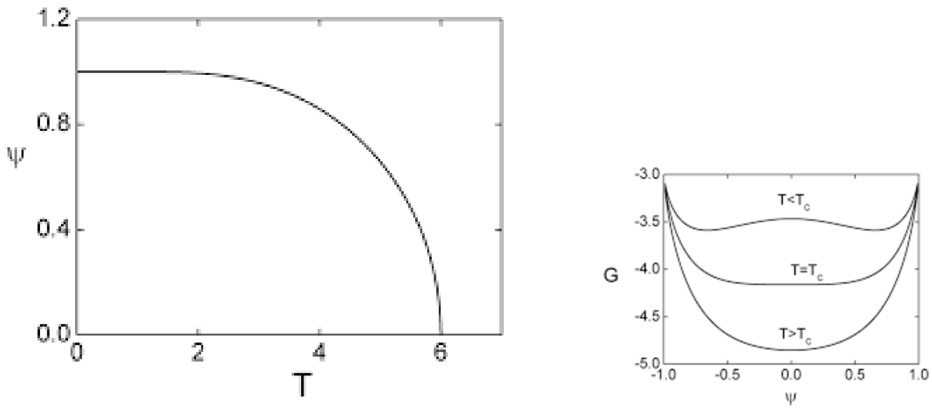


FIG. 6: Behavior of the order parameter $\Psi_0$ as a function of control parameter $\mu$ or temperature $T$. On the right is the cross-section of the corresponding ground-state energy $E_\mu(\mu)$ exhibiting transition from single minimum at $\Psi_0 = 0$ to a minimum at a finite $|\Psi_0| > 0$.

## A. Bogoluibov's creation-annihilation operator description

### 1. *Hamiltonian*

With above field decomposition, $\delta H_\mu$ is the Hamiltonian that controls fluctuations $\phi(\mathbf{r})$ about the condensate $\Psi_0$. Limiting it to quadratic order in $\phi(\mathbf{r})$, i.e., ignoring quasi-particle interactions we obtain the quadratic Bogoluibov Hamiltonian:

$$\delta H_\mu \approx \int_{\mathbf{r}} \left[\phi^\dagger \hat{\varepsilon}\phi + \frac{gn_0}{2}\left(4\phi^\dagger\phi + \phi\phi + \phi^\dagger\phi^\dagger\right)\right], \tag{79}$$

$$= \frac{1}{2}\int_{\mathbf{r}} \begin{pmatrix} \phi^\dagger & \phi \end{pmatrix} \begin{pmatrix} \hat{\epsilon} - \mu + 2gn_0 & gn_0 \\ gn_0 & \hat{\epsilon} - \mu + 2gn_0 \end{pmatrix} \begin{pmatrix} \phi \\ \phi^\dagger \end{pmatrix} - \frac{1}{2}\sum_{\mathbf{k}\neq 0}(\epsilon_k - \mu + 2gn_0), \tag{80}$$

$$= -\frac{1}{2}\sum_{\mathbf{k}\neq 0}(\epsilon_k + gn_0) + \frac{1}{2}\int_{\mathbf{r}} \begin{pmatrix} \phi^\dagger & \phi \end{pmatrix} \begin{pmatrix} \hat{\epsilon} + gn_0 & gn_0 \\ gn_0 & \hat{\epsilon} + gn_0 \end{pmatrix} \begin{pmatrix} \phi \\ \phi^\dagger \end{pmatrix}, \tag{81}$$

$$= -\frac{1}{2}\sum_{\mathbf{k}\neq 0}\tilde{\varepsilon}_k + \frac{1}{2}\sum_{\mathbf{k}\neq 0} \begin{pmatrix} a_{\mathbf{k}}^\dagger & a_{-\mathbf{k}} \end{pmatrix} \begin{pmatrix} \tilde{\varepsilon}_k & gn \\ gn & \tilde{\varepsilon}_k \end{pmatrix} \begin{pmatrix} a_{\mathbf{k}} \\ a_{-\mathbf{k}}^\dagger \end{pmatrix} \tag{82}$$

where $\tilde{\varepsilon}_k = \epsilon + gn_0$, the constant part comes from the commutation relation, above we used mean-field expression $\mu = gn_0 = g|\psi_0|^2$, obtained from minimization of $H_{mft}(n_0)$, (76), to eliminate $\mu$ in favor of condensate density $n_0$, and within this Bogoluibov weak coupling approximation, in the last expression we safely replaced $n_0$ by $n$.

For completeness we also note that in a canonical ensemble (fixed $N$, rather than the chemical potential, $\mu$) we can obtain the same Bogoluibov Hamiltonian utilizing expansion $a_{\mathbf{k}} = a_0\delta_{\mathbf{k},0} + a_{\mathbf{k}\neq 0}$, with $a_0^\dagger a_0 = N_0$, obtaining

$$\begin{aligned} H_N &\approx \frac{g}{2V}N_0^2 + \frac{1}{2}\sum_{\mathbf{k}\neq 0}\left[\epsilon_k a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + 2gn_0 a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + gn_0 a_{-\mathbf{k}}a_{\mathbf{k}} + h.c.\right], && (83)\\ &\approx \frac{g}{2V}N^2 + \frac{1}{2}\sum_{\mathbf{k}}{}' \left[(\epsilon_k + gn)a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + gna_{-\mathbf{k}}a_{\mathbf{k}} + h.c.\right]. && (84) \end{aligned}$$

where in going to second line we eliminating $N_0$ in favor of $N$ using the total atom constraint, $N = N_0 + \sum_{\mathbf{k}\neq 0} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$,

### 2. Diagonalization

In contrast to the fermionic *unitary* Bogoluibov transformation, for bosons $\Phi_k = (a_k, a_{-k}^\dagger)$ the transformation to Bogoluibov *bosonic* quasi-particles, $\Psi_k = (\alpha_k, \alpha_{-k}^\dagger)$

$$\begin{aligned} \begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix} &= \begin{pmatrix} u_k & v_k \\ v_k^* & u_k^* \end{pmatrix} \begin{pmatrix} \alpha_k \\ \alpha_{-k}^\dagger \end{pmatrix} && (85)\\ \Phi_k &= U_k\Psi_k && (86) \end{aligned}$$

must be nonunitary to preserve commutation relation, $[a_{\mathbf{k}}, a_{\mathbf{k}'}^\dagger] = \delta_{\mathbf{k},\mathbf{k}'}$, corresponding to $[\Phi_{i\mathbf{k}}, \Phi_{j\mathbf{k}'}^\dagger] = \sigma_{ij}^z\delta_{\mathbf{k},\mathbf{k}'}$, and giving

$$U\sigma_z U^\dagger = \sigma_z = U^\dagger\sigma_z U, \tag{87}$$

with $|u_k|^2 - |v_k|^2 = 1$ and $\sigma^z$ the third Pauli matrix. This constraint can be resolved by parametrization $u_k = \cosh\chi_k$, $v_k = \sinh\chi_k$, with "angle" $\chi_k$.

With above parameterization the diagonalization can be done by a direct substitution in $\delta H_\mu$ and demanding a vanishing of the coefficients of the off-diagonal terms in $\Psi_i^\dagger\Psi_j$. We leave this approach for homework.

Equivalently, a more formal matrix diagonalization can be carried out using

$$h_{ij}U_{js} = E_s\sigma_{ij}^z U_{js}, \tag{88}$$

for the Bogoluibov Hamiltonian matrix

$$h = \begin{pmatrix} \tilde{\varepsilon}_k & gn \\ gn & \tilde{\varepsilon}_k \end{pmatrix} \tag{89}$$

This is equivalent to

$$(h_{ij} - E_s\sigma^z_{ij})U_{js} = 0, \tag{90}$$

which demands a vanishing of the corresponding determinant

$$\begin{vmatrix} \varepsilon_k - E_s & gn \\ gn & \varepsilon_k + E_s \end{vmatrix} = 0, \tag{91}$$

giving $E_s = \pm\sqrt{\varepsilon^2 - g^2n^2} = \pm E$ for two $s = 1, 2$ corresponding to $\pm 1$.

We note that this $E_{1,2} \pm E$ eigenvalue structure of the pseudo-eigenvalue problem Eq. (88) is intrinsic in the bosonic Bogoluibov Hamiltonian form ($\Delta_R = Re(gn)$, $\Delta_I = Im(gn)$):

$$h = \varepsilon \mathbb{1} + \Delta_R\sigma_x + \Delta_I\sigma_y,$$

which has a symmetry

$$\sigma_x h \sigma_x = h^*.$$

Using this it is easy to see that eigenvectors come in $\pm E$ pairs: $e_+ = u$ and $e_- = \sigma_x u^*$,

$$\begin{aligned} hU &= E\sigma_z U, \\ \sigma_x h^* \sigma_x(\sigma_x U^*) &= E\sigma_x\sigma_z\sigma_x\sigma_x U^*, \\ h(\sigma_x U^*) &= (-E)\sigma_z(\sigma_x U^*), \end{aligned} \tag{92}$$

Utilizing this in the many-body Hamiltonian we obtain,

$$\begin{aligned} H_\mu &\approx E_0 - \frac{1}{2}\sum_{\mathbf{k}\neq 0}\tilde{\varepsilon}_k + \frac{1}{2}\sum_{\mathbf{k}\neq 0}\Phi_i^\dagger h_{ij}\Phi_j, \qquad (93) \\ &\approx E_0 - \frac{1}{2}\sum_{\mathbf{k}\neq 0}\tilde{\varepsilon}_k + \frac{1}{2}\sum_{\mathbf{k}\neq 0}\Psi_t^\dagger U_{ti}^\dagger h_{ij} U_{js}\Psi_s, \\ &\approx E_0 - \sum_{\mathbf{k}\neq 0}\tilde{\varepsilon}_k + \frac{1}{2}\sum_{\mathbf{k}\neq 0}\Psi_t^\dagger U_{ti}^\dagger \sigma^z_{ij} U_{js} E_s \Psi_s, \\ &\approx E_0 - \frac{1}{2}\sum_{\mathbf{k}\neq 0}\tilde{\varepsilon}_k + \frac{1}{2}\sum_{\mathbf{k}\neq 0}\Psi_t^\dagger \sigma^z_{ts} E_s \Psi_s, \\ &\approx E_0 - \frac{1}{2}\sum_{\mathbf{k}\neq 0}\tilde{\varepsilon}_k + \frac{1}{2}\sum_{\mathbf{k}\neq 0} E\Psi_t^\dagger \sigma^z_{tn}\sigma^z_{ns}\Psi_s, \\ &\approx E_0 - \frac{1}{2}\sum_{\mathbf{k}\neq 0}\tilde{\varepsilon}_k + \frac{1}{2}\sum_{\mathbf{k}\neq 0} E\Psi_s^\dagger\Psi_s. \end{aligned} \tag{94}$$

which then reduces to

$$H_\mu \approx \epsilon_0 N + \frac{g}{2V}N^2 - \frac{1}{2}\sum_k(\tilde{\varepsilon}_k - E_k) + \sum_k E_k \alpha^\dagger_{\mathbf{k}}\alpha_{\mathbf{k}}, \tag{95}$$

where

$$E_k = \sqrt{\tilde{\varepsilon}_k^2 - g^2 n^2} = \sqrt{\epsilon_k^2 + 2gn\epsilon_k} = c_s\hbar k\sqrt{1+\xi^2 k^2}, \tag{96}$$

$$\approx \begin{cases} \epsilon_k + \mu = \frac{\hbar^2 k^2}{2m} + \mu, & \text{for } \epsilon_k \gg \mu = gn, \text{ or equivalently } k\xi \gg 1, \\ \sqrt{2gn\epsilon_k} = c_s\hbar k, & \text{for } \epsilon_k \ll \mu = gn, \text{ or equivalently } k\xi \ll 1, \end{cases}, \tag{97}$$

where $\tilde{\varepsilon}_k = \epsilon_k + gn$, zeroth-sound velocity $c_s = \sqrt{gn/m}$ and correlation length $\xi = \hbar/\sqrt{4mgn}$. We note that while at high momenta the dispersion remains nonrelativistic, but shifted up by the chemical potential, at low momenta, a linear zeroth sound emerges ("More Is Different", P. A. Anderson). While there are numerous indirect observations of this, an explicit Bogoluibov dispersion has been explicitly measured via Bragg spectroscopy in degenerate bosonic $Rb^{87}$ atoms by Steinhauer[7], as illustrated in Fig.7 In the presence of strong in-

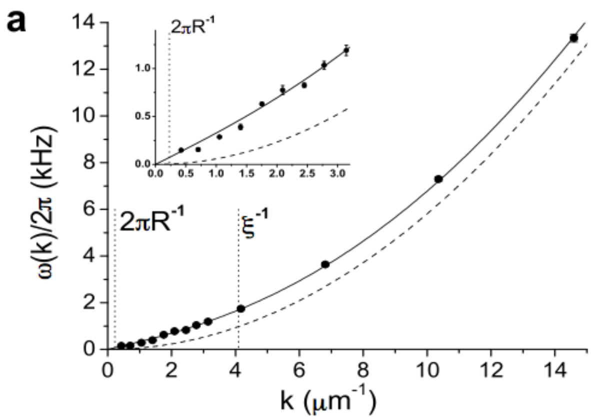


FIG. 7: Bogoluibov spectrum measured in a degenerate cloud of $Rb^{87}$ bosonic atoms by Steinhauer[7].

teractions, one also expects the so-called "roton minimum" in the spectrum rather than a monotonic crossover found in Bogoluibov's weakly interacting system. The minimum represents short-scale strong atom-atom correlations of a liquid as is found for example in liquid Helium-4 and discussed extensively by Richard Feynman.

The coherence factors in the transformation matrix $U$ that diagonalizes the Bogoluibov

Hamiltonian are given by

$$
\begin{aligned}
u_k^2 &= \frac{1}{2}(\frac{\tilde{\varepsilon}_k}{E_k}+1), && (98)\\
v_k^2 &= \frac{1}{2}(\frac{\tilde{\varepsilon}_k}{E_k}-1). && (99)
\end{aligned}
$$

The many-body ground state is then given by $|\Psi_0\rangle = e^{\Psi_0(\mathbf{r})a_0^\dagger}|n_\alpha = 0\rangle$, where in contrast to the pure mean-field result above, here the vacuum $|n_\alpha = 0\rangle$ is a vacuum of Bogoluibov quasi-particles, $\alpha_\mathbf{k}|n_\alpha = 0\rangle = 0$ rather than simply a true vacuum of atoms, $a_\mathbf{k}|0\rangle = 0$.

### *3. Physical observables*

From this we find the ground state energy in Bogoluibov approximation ($\epsilon_0 = 0$) is given by the constant part of the total Hamiltonian above,

$$
\begin{aligned}
E_{gs} &= \frac{1}{2}Vgn^2 - \frac{1}{2}\sum_k(\tilde{\varepsilon}_k - E_k), && (100)\\
&= V\left[\frac{1}{2}gn^2 - \int\frac{d^3k}{(2\pi)^3}E_k v_k^2\right], && (101)
\end{aligned}
$$

and

$$
\begin{aligned}
\mu &= \frac{\partial E_{gs}}{\partial N},\\
&= gn - \frac{g}{2}\int\frac{d^3k}{(2\pi)^3}\left[1 - \frac{\epsilon_k}{E_k}\right],\\
&= gn\left[1 - \frac{1}{8\pi^2}\left(\frac{2m}{n^{2/3}\hbar^2}\right)^{3/2}\int d\epsilon\epsilon^{1/2}\left(1 - \frac{\epsilon}{\sqrt{\epsilon^2 + 2gn\epsilon}}\right)\right],
\end{aligned}
\tag{102}
$$

These integrals are UV divergent. However, we expect this dependence on the short-scale cutoff to be eliminated once it is reexpressed in terms of the physical scattering length $a_s$. This then should give Lee-Yang-Huang expression for the chemical potential, that is an expansion in $na_s^3$. For $\mu$ this is indeed the case:

$$
\begin{aligned}
\frac{\mu}{g_R} &= n\left[1-\frac{1}{8\pi^2}\left(\frac{2m}{n^{2/3}\hbar^2}\right)^{3/2}\int d\epsilon\epsilon^{1/2}\left(1-\frac{\epsilon}{\sqrt{\epsilon^2+2gn\epsilon}}-\frac{\mu}{\epsilon}\right)\right], \\
&= n\left[1-\frac{1}{8\pi^2}\left(\frac{2m}{n^{2/3}\hbar^2}\right)^{3/2}\int d\epsilon\epsilon^{1/2}\left(1-\frac{\epsilon}{\sqrt{\epsilon^2+2g_Rn\epsilon}}-\frac{g_Rn}{\epsilon}\right)\right], \\
&= n\left[1+\frac{\sqrt{2}}{3\pi^2}\left(\frac{2mg_Rn}{n^{2/3}\hbar^2}\right)^{3/2}\right], \\
&= n\left[1+\frac{32}{3\sqrt{\pi}}(na_s^3)^{1/2}\right], \qquad (103)
\end{aligned}
$$

This can alternatively be calculated by computing the grand-canonical ground state energy $E_{gs}(\mu)$ and using $n=-\partial E_{gs}/\partial\mu$, together with $g-a_s$ relation and the $\Psi_0(\mu)$ saddle-point dependence. Equivalently, from $\mu(n)=\partial\varepsilon_{gs}(n)/\partial n$, we can obtain

$$
\varepsilon_{gs} = \frac{1}{2}g_Rn^2\left[1+\frac{128}{15\sqrt{\pi}}(na_s^3)^{1/2}\right]. \qquad (104)
$$

From above we can also calculation "depletion" $N_d$ of the $k=0$ state, namely the number of atoms promoted by the repulsive interactions into $\mathbf{k}\neq 0$ single particle states,

$$
\begin{aligned}
N_d &= \sum_k \langle a_k^\dagger a_k\rangle, \\
&= \sum_k \langle (u_k^*\alpha_k^\dagger + v_k^*\alpha_k)(u_k\alpha_k + v_k\alpha_k^\dagger)\rangle, \\
&= \sum_k \left[|v_k|^2 + (|u_k|^2+|v_k|^2)n_{BE}(T)\right], \\
&= N\frac{8}{3\sqrt{\pi}}(na_s^3)^{1/2}, \quad \text{at } T=0, \qquad (105)
\end{aligned}
$$

We note that in contrast to the noninteracting BEC limit, here even at $T=0$ because of repulsive interactions not all atoms reside in the $k=0$ single-particle state. We stress, that despite of this condensate depletion, one can show that at $T=0$, all $N$ atoms participate in the superfluid state, as for example gauged by the superflow momentum density $p$ that at $T=0$ is given by $p=n_sv_s$, with $n_s=n$ (total atom density), not $n_0$ condensate fraction that is less than $n$.

At $T=0$ we also find that the atom momentum distribution function is given by

$$
\begin{aligned}
n_k &= |v_k|^2, \\
&= \frac{1}{2}\left(\frac{\varepsilon_k}{E_k}-1\right), \\
{}_{k\to\infty} &\approx \frac{C}{k^4}, \qquad (106)
\end{aligned}
$$

where the Tan's "contact" $C = 16\pi^2 n^2 a_s^2$ at this level of approximation, is the amplitude of the universal high momentum $1/k^4$ tail.

## VI. DENSITY-PHASE (POLAR) OPERATOR REPRESENTATION

It is useful to complement about description by a density-phase representation of fluctuations about the superfluid state, still working in the Hamiltonian approach. Using

$$\psi(\mathbf{r}) = \sqrt{n_0 + \pi(\mathbf{r})}e^{i\theta(\mathbf{r})}, \tag{107}$$

inside the $H_\mu$, with density and phase fluctuations satisfying the canonical commutation relation, $[\theta(\mathbf{r}), \pi(\mathbf{r}')] = -i\delta(\mathbf{r} - \mathbf{r}')$, we obtain

$$H_\mu = -\frac{1}{2}gn_0^2 V + \int_{\mathbf{r}} \left[\frac{\hbar^2}{8mn_0}|\nabla\pi|^2 + \frac{\hbar^2 n_0}{2m}|\nabla\theta|^2 + \frac{g}{2}\pi^2\right], \tag{108}$$

where we dropped the nonlinearities in $\pi(\mathbf{r})$ and used the relation $\mu = n_0 g$, valid at harmonic order. In Fourier space as usual this can be written as independent oscillators with "momentum" field $\pi_k$ and "coordinate" field $\theta_k$

$$\delta H_\mu = \sum_{\mathbf{k}} \left[\frac{\hbar^2}{2M_k}\pi_{-k}\pi_k + \frac{1}{2}M_k\Omega_k^2\theta_{-k}\theta_k\right], \tag{109}$$

where $k$-dependent effective "mass" and "frequency" are given by

$$M_k = \left(\frac{k^2}{4mn_0} + \frac{g}{\hbar^2}\right)^{-1}, \tag{110}$$

$$\Omega_k = \sqrt{\left(\frac{k^2}{4mn_0} + \frac{g}{\hbar^2}\right)\frac{\hbar^2 k^2 n_0}{m}}, \tag{111}$$

$$= \hbar^{-1}\sqrt{\epsilon_k(\epsilon_k + 2gn_0)} = E_k/\hbar, \tag{112}$$

the latter indeed gives the Bogoluibov excitation spectrum $E_k$.

Introducing complex fields, that correspond to the Bogoluibov creation and annihilation operators

$$\theta_k = \frac{\theta_0}{\sqrt{2}}\left(\alpha_{-k}^\dagger + \alpha_k\right), \tag{113}$$

$$\pi_k = \frac{1}{i\sqrt{2}\theta_0}\left(\alpha_{-k}^\dagger - \alpha_k\right), \tag{114}$$

$$\tag{115}$$

inheriting creation-annihilation commutation relation, $[\alpha_k, \alpha^\dagger_{k'}] = \delta_{k,k'}$, the Hamiltonian reduces to

$$\begin{aligned}
\delta H_\mu &= \sum_{\mathbf{k}} \left[ \frac{-\hbar^2}{4M_k\theta_0^2} \left(\alpha^\dagger_k - \alpha_{-k}\right)\left(\alpha^\dagger_{-k} - \alpha_k\right) + \frac{1}{4} M_k \Omega_k^2 \theta_0^2 \left(\alpha^\dagger_k + \alpha_{-k}\right)\left(\alpha^\dagger_{-k} + \alpha_k\right)\right], \\
&= \sum_{\mathbf{k}} \left[ \left(\frac{1}{4} M_k \Omega_k^2 \theta_0^2 + \frac{\hbar^2}{4M_k\theta_0^2}\right)\left(\alpha^\dagger_k \alpha_k + \alpha_{-k}\alpha^\dagger_{-k}\right) + \left(\frac{1}{4} M_k \Omega_k^2 \theta_0^2 - \frac{\hbar^2}{4M_k\theta_0^2}\right)\left(\alpha^\dagger_{-k}\alpha^\dagger_k + \alpha_{-k}\alpha_k\right)\right], \\
&= \sum_{\mathbf{k}} E_k \left(\alpha^\dagger_k \alpha_k + \frac{1}{2}\right),
\end{aligned} \tag{116}$$

where we chose angle scale to be

$$\theta_0 = \sqrt{\frac{\hbar}{M_k \Omega_k}} = \sqrt{\frac{1}{2n_0}\frac{E_k}{\epsilon_k}}$$

so as to eliminate $\alpha_k$ quanta nonconserving cross terms and reduce the Hamiltonian to a standard form. This form for $\theta_0$ is indeed the effective quantum oscillator "length", characterizing the size of rms fluctuations of $\theta_k$ in the ground state. Namely the ground-state wavefunction for $\theta_k$ is a Gaussian with width $\theta_0$.

It is interesting to note that even in $d \leq 2$, where at finite $T$ there is no condensate (as we will see later, by virtue of the Hohenberg-Mermin-Wagner-Coleman theorem), i.e., $n_0 = 0$, the quantum low-energy theory is still described by a Hamiltonian of the same form

$$\delta H = \int_{\mathbf{r}} \left[ \frac{\hbar^2 n_s}{2m} |\nabla\theta|^2 + \frac{\kappa^{-1}}{2} \delta\rho^2 \right], \tag{117}$$

where $n_s$ is the superfluid number density, that for a bulk Galilean-invariant (no lattice or disorder) superfluid at $T = 0$ is given by the total density, $n$. And the coupling controlling density fluctuations given by the compressibility $\kappa$.

## VII. COHERENT-STATE PATH-INTEGRAL FORMULATION

All of above can equivalently be rederived from the coherent state path-integral formulation, with the Euclidean action

$$\begin{aligned}
S_E &= \int d^d r d\tau \left[\overline{\psi}\hbar\partial_\tau \psi + \mathcal{H}[\overline{\psi}, \psi]\right], \\
&= \int d^d r d\tau \left[\overline{\psi}\left(\hbar\partial_\tau - \frac{\hbar^2\nabla^2}{2m} - \mu\right)\psi + \frac{1}{2} g\, \overline{\psi}\psi\overline{\psi}\psi\right].
\end{aligned} \tag{118}$$

## A. Coherent fields representation

Using condensate-fluctuations decomposition $\psi(\mathbf{r},\tau) = \Psi_0 + \phi(\mathbf{r},\tau)$, expanding the action to quadratic order and minimizing over $\Psi_0$ we obtain

$$\begin{aligned}
\delta S_E &\approx \int_{\mathbf{r},\tau} \left[ \overline{\phi} \left( \hbar\partial_\tau + \hat{\varepsilon} \right) \phi + \frac{g n_0}{2} \left( 4\overline{\phi}\phi + \phi\phi + \overline{\phi\phi} \right) \right], \qquad (119) \\
&= \frac{1}{2} \sum_{\omega_n} \int_{\mathbf{k}} \left( \overline{\phi}(\mathbf{k},\omega_n) \;\; \phi(-\mathbf{k},-\omega_n) \right) \begin{pmatrix} -i\hbar\omega_n + \tilde{\varepsilon}_k & gn \\ gn & i\hbar\omega_n + \tilde{\varepsilon}_k \end{pmatrix} \begin{pmatrix} \phi(\mathbf{k},\omega_n) \\ \overline{\phi}(-\mathbf{k},-\omega_n) \end{pmatrix}, \\
&\equiv \frac{\hbar}{2} \sum_{\omega_n} \int_{\mathbf{k}} \left( \overline{\phi}(\mathbf{k},\omega_n) \;\; \phi(-\mathbf{k},-\omega_n) \right)_i G^{-1}_{ij}(k,\omega_n) \begin{pmatrix} \phi(\mathbf{k},\omega_n) \\ \overline{\phi}(-\mathbf{k},-\omega_n) \end{pmatrix}_j, \qquad (120)
\end{aligned}$$

from which thermodynamics and correlation functions can be straightforwardly calculated using the coherent-state path integral.

Since $\delta S_E$ is harmonic (by construction), the Green's functions are obtained from simply inverting its matrix kernel, $G^{-1}$. This gives

$$G_{ij}(k,\omega_n) = \begin{pmatrix} \langle \phi_{\mathbf{k},\omega_n} \overline{\phi}_{\mathbf{k},\omega_n} \rangle & \langle \phi_{\mathbf{k},\omega_n} \phi_{-\mathbf{k},-\omega_n} \rangle \\ \langle \overline{\phi}_{\mathbf{k},\omega_n} \overline{\phi}_{-\mathbf{k},-\omega_n} \rangle & \langle \phi_{-\mathbf{k},-\omega_n} \overline{\phi}_{-\mathbf{k},-\omega_n} \rangle \end{pmatrix} = \frac{\hbar}{\hbar^2\omega_n^2 + E_k^2} \begin{pmatrix} i\hbar\omega_n + \tilde{\varepsilon}_k & -gn \\ -gn & -i\hbar\omega_n + \tilde{\varepsilon}_k \end{pmatrix}, \qquad (121)$$

where $E_k = \sqrt{\tilde{\varepsilon}_k^2 - g^2 n^2} = \sqrt{\epsilon_k^2 + 2gn\epsilon_k} = c\hbar k\sqrt{1+\xi^2 k^2}$ is by-now familiar Bogoluibov spectrum.

Specifically the two key (connected) Green's functions $G \equiv G_{11}$ and $G_{anom} \equiv G_{12}$

$$\begin{aligned}
G(\mathbf{r},\tau) &= \langle \psi(\mathbf{r},\tau) \overline{\psi}(0,0) \rangle - n_0, \qquad (122) \\
G_{anom}(\mathbf{r},\tau) &= \langle \psi(\mathbf{r},\tau) \psi(0,0) \rangle - n_0, \qquad (123) \\
& \qquad (124)
\end{aligned}$$

in Fourier space are given by

$$\begin{aligned}
G(\mathbf{k},\omega_n) &= \hbar \frac{i\hbar\omega_n + \tilde{\varepsilon}_k}{\hbar^2\omega_n^2 + E_k^2}, \qquad (125) \\
&= \frac{u_k^2}{-i\omega_n + E_k/\hbar} + \frac{v_k^2}{i\omega_n + E_k/\hbar}, \qquad (126) \\
G_{anom}(\mathbf{k},\omega_n) &= \hbar \frac{-gn}{\hbar^2\omega_n^2 + E_k^2}, \qquad (127) \\
&= \frac{-u_k v_k}{-i\omega_n + E_k/\hbar} + \frac{-u_k v_k}{i\omega_n + E_k/\hbar}, \qquad (128) \\
& \qquad (129)
\end{aligned}$$

with the pole giving the Bogoluibov spectrum in imaginary frequency, and corresponding residues given by the squares of previously found coherence factors $u_k, v_k$. We note that for $g \to 0$ limit, the correlators reduce to that of noninteracting bosons, with $G_{anom} = 0$.

### B. Density-phase fields representation

Above analysis is nicely complemented by the density-phase coherent-state representation, which as we will see has a somewhat more direct connection to the physical fluctuations of the superfluid state.

Starting with the Euclidean coherent-state action $S_E[\psi, \overline{\psi}]$ and expressing it in terms of "radial", $\pi(\mathbf{r}, \tau)$ and "azimuthal", $\theta(\mathbf{r}, \tau)$ fluctuations inside the Mexican-hat potential, Fig.5, defined by

$$\psi(\mathbf{r}, \tau) = \sqrt{n_0 + \pi(\mathbf{r}, \tau)} e^{i\theta(\mathbf{r}, \tau)}, \tag{130}$$

we find

$$\begin{aligned}
S_E[\pi(\mathbf{r}, \tau), \theta(\mathbf{r}, \tau)] &= \int d^d r d\tau \left[ i\hbar n \partial_\tau \theta + \frac{\hbar^2 n}{2m} |\boldsymbol{\nabla}\theta|^2 + \frac{\hbar^2}{8mn} |\boldsymbol{\nabla}\pi|^2 - \mu n + \frac{1}{2} g n^2 \right], \\
&\approx \int d^d r d\tau \left[ i\hbar \pi \partial_\tau \theta + \frac{\hbar^2 n_0}{2m} |\boldsymbol{\nabla}\theta|^2 + \frac{\hbar^2}{8mn_0} |\boldsymbol{\nabla}\pi|^2 + \frac{1}{2} g \pi^2 \right], \qquad (131) \\
&\approx \sum_{\omega_n} \int_{\mathbf{k}} \left[ \hbar\omega_n \pi(-\mathbf{k}, -\omega_n) \theta(\mathbf{k}, \omega_n) + \frac{\hbar^2 k^2}{2m} n_0 |\theta(\mathbf{k}, \omega_n)|^2 \right. \\
&\quad \left. + \frac{\hbar^2 k^2}{8mn_0} |\pi(\mathbf{k}, \omega_n)|^2 + \frac{1}{2} g |\pi(\mathbf{k}, \omega_n)|^2 \right], \qquad (132) \\
&= \frac{1}{2} \sum_{\omega_n} \int_{\mathbf{k}} \begin{pmatrix} \theta(-\mathbf{k}, -\omega_n) & \pi(-\mathbf{k}, -\omega_n) \end{pmatrix} \begin{pmatrix} \frac{n_0 \hbar^2 k^2}{m} & -\hbar\omega_n \\ \hbar\omega_n & \frac{\hbar^2 k^2}{4mn_0} + g \end{pmatrix} \begin{pmatrix} \theta(\mathbf{k}, \omega_n) \\ \pi(\mathbf{k}, \omega_n) \end{pmatrix}, \\
&\equiv \frac{\hbar}{2} \sum_{\omega_n} \int_{\mathbf{k}} \begin{pmatrix} \theta(-\mathbf{k}, -\omega_n) & \pi(-\mathbf{k}, -\omega_n) \end{pmatrix}_i D^{-1}_{ij}(\mathbf{k}, \omega_n) \begin{pmatrix} \theta(\mathbf{k}, \omega_n) \\ \pi(\mathbf{k}, \omega_n) \end{pmatrix}_j,
\end{aligned} \tag{133}$$

where we minimized $S_E$ over $n_0$ to eliminate $\mu$, expanded to quadratic order in $\pi, \theta$, ignored constant contributions, and defined the kernel $D^{-1}_{ij}(\mathbf{k}, \omega_n)$ that is the inverse of the $\pi, \theta$ correlator tensor. We note that in the superfluid phase by definition fluctuations of $\theta$ are small and $n$ field be a continuous field. In contrast, in the insulating state, where $\theta$ fluctuates wildly (multiples of $2\pi$) $n$ is quantized through the first "$p\dot{q}$", namely $n\partial_\tau\theta$ term.

Inverting $D^{-1}(\mathbf{k},\omega_n)$,

$$D(\mathbf{k},\omega_n) \;=\; \frac{\hbar}{\hbar^2\omega_n^2+E_k^2}\begin{pmatrix} \frac{\hbar^2k^2}{4mn_0}+g & \hbar\omega_n \\ -\hbar\omega_n & \frac{n_0\hbar^2k^2}{m}\end{pmatrix} \tag{134}$$

we immediately obtain all the relevant $\theta,\pi$ correlators. All of these exhibit a pole at imaginary frequency $E_k/\hbar$ set by the Bogoluibov spectrum.

A particularly interesting correlator $\pi-\pi$ as it gives the dynamic structure and density response functions,

$$S(\mathbf{r},\tau) \;=\; \langle n(\mathbf{r},\tau)n(0,0)\rangle - n^2 \approx \langle \pi(\mathbf{r},\tau)\pi(0,0)\rangle, \tag{135}$$

whose Fourier transform is

$$S(\mathbf{k},\omega_n) \;=\; D_{22}(\mathbf{k},\omega_n) = \hbar\frac{n_0\hbar^2k^2/m}{\hbar^2\omega_n^2+E_k^2} \tag{136}$$

To obtain the structure function at real frequency we Fourier transform back to imaginary time $\tau$ (using contour integration[1, 8] $\frac{1}{\beta\hbar}\sum_{\omega_n}\frac{e^{-i\omega_n\tau}}{\hbar^2\omega_n^2+E_k^2} = \frac{\cosh[(\beta\hbar/2-\tau)E_k/\hbar]}{2\hbar E_k\sinh[\beta E_k/2]},$)

$$\begin{aligned} S(\mathbf{k},\tau) \;&=\; \frac{1}{\beta\hbar}\sum_{\omega_n} S(\mathbf{k},\omega_n)e^{-i\omega_n\tau}, &(137)\\ &=\; \frac{n_0\hbar^2k^2}{2mE_k}\frac{e^{\beta E_k}e^{-E_k\tau/\hbar}+e^{E_k\tau/\hbar}}{e^{\beta E_k}-1}, &(138)\\ &=\; \frac{n_0\hbar^2k^2}{2mE_k}\left[(n_{BE}(E_k)+1)\,e^{-E_k\tau/\hbar}+n_{BE}(E_k)e^{E_k\tau/\hbar}\right], &(139)\end{aligned}$$

which immediately gives the static structure function

$$S(\mathbf{k},\tau=0) \;=\; \frac{n_0\hbar^2k^2}{2mE_k}\coth\left(\frac{\beta E_k}{2}\right), \tag{140}$$

satisfying Feynman's prediction at $T=0$; this formula was also independently derived by Abrikosov, Gorkov, Dzyaloshinskii. The static structure function was directly measured via Bragg spectroscopy in degenerate bosonic $\mathrm{Rb}^{87}$ atoms by Steinhauer[7], finding close agreement with the predictions of the Bogoluibov's theory, above.

We note that vanishing of $S(k)$ with vanishing momentum is a consequence of number conservation. As discussed by R.P. Feynman, in fact one can invert this relation, to extract the spectrum from the measured structure function. Since in a liquid strong short-scale atom-atom correlations are expected to give finite-width peaks in $S(k)$, remnants of melted crystal's Bragg peaks, this immediately implies a minimum in the spectrum of a superfluid, the so-called "roton minimum".

Analytically continuing to real time $t = -i\tau$

$$S(\mathbf{k}, t) \;=\; \frac{n_0\hbar^2 k^2}{2mE_k}\left[\left(n_{BE}(E_k)+1\right)e^{-iE_k t/\hbar} + n_{BE}(E_k)e^{iE_k t/\hbar}\right], \tag{141}$$

and Fourier transforming to real frequency $\omega$, we finally find the dynamic structure function, i.e., the density-density correlator at real-frequency and momentum,

$$\begin{aligned} S(\mathbf{k}, \omega) \;&=\; \int_{-\infty}^{\infty} dt S(\mathbf{k}, t)e^{-i\omega_n\tau}, & (142)\\ &=\; \frac{n_0\hbar^2 k^2}{2mE_k}\frac{2\pi}{e^{\beta E_k}-1}\left[e^{\beta E_k}\delta(\omega - E_k/\hbar) + \delta(\omega + E_k/\hbar)\right], & (143)\\ &=\; 2\pi\frac{n_0\hbar^2 k^2}{2mE_k}\left[\left(n_{BE}(E_k)+1\right)\delta(\omega - E_k/\hbar) + n_{BE}(E_k)\delta(\omega + E_k/\hbar)\right]. & (144)\end{aligned}$$

This result is consistent with the quantum fluctuation-dissipation theorem (that we will prove later), that relates the imaginary part of the retarded response function $\hbar\chi(\mathbf{k}, \omega) \equiv S(\mathbf{k}, \omega_n \to -i\omega + 0^+)$ and finite frequency correlation function $S(\mathbf{k}, \omega)$,

$$S(\mathbf{k}, \omega) = \frac{2\hbar}{1 - e^{-\beta\hbar\omega}} Im[\chi(\mathbf{k}, \omega)].$$

We next turn to the derivation of Landau's quantum "hydrodynamics".

### C. Quantum "hydrodynamics"

Using coherent-state path-integral we can gain further intuition about superfluid dynamics, by working with real-time action in density-phase representation and evaluating the path-integral via a saddle-point analysis. To this end, minimizing the action

$$\begin{aligned} S[\psi, \overline{\psi}] \;&=\; \int d^d r dt\left[\overline{\psi} i\hbar\partial_t\psi - \mathcal{H}[\overline{\psi}, \psi]\right], \\ &=\; \int d^d r dt\left[\overline{\psi}\left(i\hbar\partial_t + \frac{\hbar^2\nabla^2}{2m} + \mu\right)\psi - \frac{1}{2}g\,\overline{\psi}\psi\overline{\psi}\psi\right] & (145)\end{aligned}$$

over $\overline{\psi}$, we obtain the saddle-point equation of motion

$$i\hbar\partial_t\psi = \frac{-\hbar^2}{2m}\nabla^2\psi - \mu\psi + g\,\overline{\psi}\psi\psi,$$

that is referred by a variety of synonimous names, depending on the context, such as the Gross-Pitaevskii equation (GPE), the nonlinear Schrödinger's equation, and the Ginzburg-Landau equation.

Using a polar representation, $\psi(\mathbf{r},t)=\sqrt{n(\mathbf{r},t)}e^{i\theta(\mathbf{r},t)}$, GPE becomes

$$\frac{i\hbar}{2}\partial_t n-\hbar n\partial_t\theta \;=\; -\frac{\hbar^2}{2m}\left(-\frac{1}{4n}(\boldsymbol{\nabla}n)^2+\frac{1}{2}\nabla^2 n+i\boldsymbol{\nabla}n\cdot\boldsymbol{\nabla}\theta+in\nabla^2\theta-n(\nabla\theta)^2\right)-(\mu-gn)n. \tag{146}$$

Separating into real and imaginary parts we obtain

$$\partial_t n \;=\; -\frac{\hbar}{m}\boldsymbol{\nabla}n\cdot\boldsymbol{\nabla}\theta-\frac{\hbar}{m}n\nabla^2\theta, \tag{147}$$

$$\;=\; -\boldsymbol{\nabla}\cdot(n\frac{\hbar}{m}\boldsymbol{\nabla}\theta)\equiv-\boldsymbol{\nabla}\cdot(n\mathbf{v}), \tag{148}$$

$$\hbar\partial_t\theta+\frac{\hbar^2}{2m}(\nabla\theta)^2 \;=\; -\delta\mu(\mathbf{r}) \tag{149}$$

where $\delta\mu(\mathbf{r})=\frac{\hbar^2}{8mn^2}(\nabla n)^2-\frac{\hbar^2}{4mn}\nabla^2 n+\mu-gn$ is the effective chemical potential fluctuation about a uniform equilibrium value, and the superfluid velocity is as usual given by

$$\mathbf{v}=\frac{\hbar}{m}\boldsymbol{\nabla}\theta,$$

that in the absence of vortices (i.e., single-valued condensate wavefunction; see below) is irrotational

$$\boldsymbol{\nabla}\times\mathbf{v}=0.$$

These equations can equivalently be obtained by first expressing $S$ in terms of $\theta$ and $n$ and then minimizing over them, respectively. The first equation is then nothing more than the atom number continuity equation and the second one has a form of a Kardar-Parisi-Zhang (KPZ) equation for $\theta$ and is the Bernoulli's equation. Taking a gradient of this second equation and using the fact that $\mathbf{v}$ is irrotational, for which $\mathbf{v}\cdot\boldsymbol{\nabla}\mathbf{v}=\frac{1}{2}\boldsymbol{\nabla}v^2$ (from $\mathbf{v}\times\boldsymbol{\nabla}\times\mathbf{v}=0$) reduce it to the Euler equations for an inviscid irrotational fluid. Together these equations then take quantum "hydrodynami" form:

$$\partial_t n+\boldsymbol{\nabla}\cdot(n\mathbf{v}) \;=\; 0, \tag{150}$$

$$m(\partial_t\mathbf{v}+\mathbf{v}\cdot\boldsymbol{\nabla}\mathbf{v}) \;=\; -\boldsymbol{\nabla}\mu(\mathbf{r}). \tag{151}$$

We note that in the absence of any external inhomogeneous potentail, as required these equation are Galilean-invariant. Namely, changing coordinates to a moving frame $\mathbf{r}'=\mathbf{r}-\mathbf{v}_0 t$, gives the same equations but with a velocity of the fluid that's reduced to $\mathbf{v}'=\mathbf{v}-\mathbf{v}_0$, as expected in the moving $\mathbf{r}'$ frame:

$$
\begin{aligned}
\partial_t n - \mathbf{v}_0\cdot\boldsymbol{\nabla}' n + \boldsymbol{\nabla}'\cdot(n\mathbf{v}) &= 0,\\
\partial_t n + \boldsymbol{\nabla}'\cdot(n(\mathbf{v}-\mathbf{v}_0)) &= 0, \qquad (152)\\
m(\partial_t\mathbf{v} - \mathbf{v}_0\cdot\boldsymbol{\nabla}'\mathbf{v} + \mathbf{v}\cdot\boldsymbol{\nabla}\mathbf{v}) &= -\boldsymbol{\nabla}\mu(n),\\
m(\partial_t\mathbf{v} + (\mathbf{v}-\mathbf{v}_0)\cdot\boldsymbol{\nabla}(\mathbf{v}-\mathbf{v}_0)) &= -\boldsymbol{\nabla}\mu(n). \qquad (153)
\end{aligned}
$$

## VIII. SUPERFLUID STATE AT FINITE TEMPERATURE

### A. Classical XY model

As we discussed at various points of our analysis, at finite temperature, the coherent-state field theory reduces to a finite $\beta\hbar$ width slab in imaginary time. Thus at low energies the statistical quantum field theory characterized by a path-integral with action $S_E$ reduces to $\tau$-independent fields giving

$$
\begin{aligned}
Z &= \int \mathcal{D}\theta\mathcal{D}\pi e^{-\frac{1}{\hbar}\int d^d r\int_0^{\beta\hbar} d\tau[i\hbar n\partial_\tau\theta + cH[\pi,\theta]]} \approx \int \mathcal{D}\theta\mathcal{D}\pi e^{-\beta H[\pi,\theta]}, \qquad (154)\\
&\approx \int \mathcal{D}\theta\mathcal{D}\pi e^{-\beta\int_{\mathbf{r}}\left[\frac{\hbar^2 n}{2m}|\boldsymbol{\nabla}\theta|^2+\frac{1}{2}g\pi^2\right]}, \qquad (155)\\
&\approx \int \mathcal{D}\theta e^{-\beta\int_{\mathbf{r}}\frac{1}{2}K|\boldsymbol{\nabla}\theta|^2}, \qquad (156)
\end{aligned}
$$

where neglected $\tau$ derivatives and integrated out the gapped "radial" density mode (momentum field, canonically conjugate to $\theta$), inconsequentially absorbing the resulting constant into the measure of integration. The classical Hamiltonian is given by

$$
H \approx \frac{K}{2}\int_{\mathbf{r}}|\boldsymbol{\nabla}\theta|^2 = \frac{\rho_s}{2}\int_{\mathbf{r}} v_s^2, \qquad (157)
$$

where in mean-field theory the stiffness $K$ and superfluid mass density $\rho_s$ are givey by

$$
K = \frac{\hbar^2 n}{m}, \quad \rho_s = mn,
$$

and $v_s = \frac{\hbar}{m}\boldsymbol{\nabla}\theta$.

Using equipartition (or equivalently simply performing Gaussian integrals over $\theta$) we find

$$
\theta_{rms}^2 = \langle\theta(\mathbf{r})\theta(\mathbf{r})\rangle = \int\frac{d^d k}{(2\pi)^d}\frac{k_B T}{Kk^2} \sim \begin{cases} \frac{k_B T}{K}\frac{1}{a^{d-2}}, & \text{for } d>2,\\ \frac{k_B T}{K}L^{2-d}, & \text{for } d<2,\\ \frac{k_B T}{K}\ln(L/a), & \text{for } d=2,\end{cases}, \qquad (158)
$$

where $L \gg r$ is the system size IR cutoff and $\Lambda^{-1} = a \gg r$ is the UV lattice cutoff. Thus we observe (as with did for acoustic lattice vibrations in lectures 2) that while for $d > 2$ the superfluid state is stable at nonzero $T$, despite its thermal fluctuations, at $d \le 2$ the superfluid state is destabilized by thermal fluctuations, with $\theta_{rms}$ diverging with system size; that is no matter how low $T$ is, for system large enough phase fluctuations are a large fraction of $2\pi$ and therefore superfluid is unstable. This is a consequence of the Hohenberg-Mermin-Wagner-Coleman theory that forbids spotaneous breaking of a continuous symmetry ($U(1)$ here) in $d \le 2$.

### B. Superfluid film: 2d classical XY model

We now examine in more detail the marginal 2d case of a finite temperature superfluid film. While the $\theta_{rms}$ diverges in films, we examine a more refined correlation function that measures the difference in phase fluctuations at points separated by distance $r$:

$$C(\mathbf{r}) = \frac{1}{2}\langle(\theta(\mathbf{r}) - \theta(0))^2\rangle = \langle\theta(\mathbf{r})\theta(\mathbf{r}) - \theta(\mathbf{r})\theta(0)\rangle, \tag{159}$$

$$= \int \frac{d^2k}{(2\pi)^2}\frac{k_B T}{K k^2}\left(1 - e^{i\mathbf{k}\cdot\mathbf{r}}\right), \tag{160}$$

$$= \frac{k_B T}{2\pi K}\ln(r/a), \quad \text{for } r \gg a, \tag{161}$$

and growing quadratically with $r/a$ for $r \ll a$, where the continuum limit is not really well-defined anyway.

#### 1. *quasi-long-range order*

We can now calculate the bosonic propagator for a superfluid film

$$\langle\psi(r)\overline{\psi}(0)\rangle \approx n\langle e^{i(\theta(\mathbf{r})-\theta(0))}\rangle \sim e^{-C(\mathbf{r})}, \tag{162}$$

$$\sim \frac{1}{(r/a)^\eta} \to |\langle\psi(r)\rangle|^2 \sim |\Psi_0|^2 \to 0, \quad \text{for } r \gg a, \tag{163}$$

which shows that even in the (supposedly) superfluid state in 2d (in contrast to $d > 2$), the order parameter $\Psi_0$ vanishes, there is no long-range order and the system exhibits what we call a "quasi-long-range" order,[11–13] i.e., correlations fall off as a power-law, with exponent

$$\eta = \frac{k_B T}{2\pi K},$$

observations that go back all the way to Peierles and Landau in mid 1930s.

As noted by Berezinskii and by Kosterlitz and Thouless[13], amazingly, this does *not* imply absence of a normal-superfluid phase transition in finite temperature films. The reason is that it is quite straightforward to show that in the truly normal phase $\psi$ correlations are short-ranged, falling off exponentially in a fully disordered high $T$ state. Since we have just rigorously demonstrated that inside the superfluid film they fall off as a power-law, with an arbitrary small exponent $\eta(T \to 0) \to 0$, it is clear that there must be a genuine phase transition, that separations these two qualitatively distinct behaviors.

### *2. vortices and the Kosterlitz-Thouless (KT) transition*

As was further recognized by Berezinskii and by Kosterlitz and Thouless[13], in fact this transition is of topological nature as it is between two qualitatively distinct *disordered* states. The two states are distinguished by the nature of vortices, being bound into dipole pairs and unbound into a weakly-correlated two-component vortex plasma.

We will not pursue a full detailed analysis of this Kosterlitz-Thouless (KT) transition[9, 13], as it requires a renormalization group treatment, that takes into account screening of vortex-vortex interaction by vortex dipoles. However, much of the basic idea can be understood more simply by considering the competition between energy and entropy of a vortex-antivortex gas.

To this end, we note that a 2d vortex is defined by $\theta(\mathbf{r})$ that satisfies the Euler-Lagrange equation and the topological circulation condition

$$\nabla^2\theta = 0, \tag{164}$$

$$\boldsymbol{\nabla} \times \boldsymbol{\nabla}\theta = 2\pi\delta^2(\mathbf{r})\hat{z}, \tag{165}$$

in contrast to the earlier assumption of the irrotational flow condition. The second equation can be understood from a more basic conditionof applying Stokes theorem to a $2\pi$ vorticity integral equation

$$\oint \boldsymbol{\nabla}\theta \cdot d\mathbf{r} = 2\pi \to \int d^2r\boldsymbol{\nabla} \times \boldsymbol{\nabla}\theta = 2\pi \int d^2r\delta^2(\mathbf{r}), \tag{166}$$

$$\int_0^{2\pi} v_v(r)\hat{\boldsymbol{\varphi}} \cdot \hat{\boldsymbol{\varphi}} r d\varphi = 2\pi, \tag{167}$$

$$v_v(r)r2\pi = 2\pi, \tag{168}$$

which leads to the solution $\boldsymbol{\nabla}\theta = \frac{\hat{\boldsymbol{\varphi}}}{r}$.

Altenratively, as for a Coulomb problem of electrostatic charges, these pair of equations are easily solved by $\theta(\mathbf{r}) = \theta_s(\mathbf{r}) + \theta_v(\mathbf{r})$ with the smooth (single-valued) deformation part, $\theta_s = 0$ and

$$\begin{aligned} \theta_v(\mathbf{r}) &= \varphi = \arctan(y/x), && (169)\\ \boldsymbol{\nabla}\theta_v(\mathbf{r}) &= \frac{\hat{\mathbf{z}}\times\mathbf{r}}{r^2} = \frac{1}{r}(-y,x) \equiv \frac{\hat{\boldsymbol{\varphi}}}{r}, && (170)\\ \mathbf{v}_v(\mathbf{k}) \equiv \boldsymbol{\nabla}\theta_v(\mathbf{k}) &= -2\pi i\frac{\hat{\mathbf{z}}\times\mathbf{k}}{k^2}, && (171) \end{aligned}$$

with $\varphi$ the polar angle coordinate and the later form obviously satisfying the Euler-Lagrange Laplace's equation, $\nabla^2\theta = 0$, corresponding to $\mathbf{k}\cdot\boldsymbol{\nabla}\theta_v(\mathbf{k}) = 0$.

The corresponding single vortex energy is then given by

$$\begin{aligned} E_v &= \frac{1}{2}K\int d^2r(\boldsymbol{\nabla}\theta_v)^2, && (172)\\ &= \frac{1}{2}K\int d^2r\frac{1}{r^2}, && (173)\\ &= \pi K\ln L/a, && (174) \end{aligned}$$

where $a$ is the UV cutoff set by the vortex core and $L$ the system size.

Although energetically vortices seem to be forbidden, at finite temperature they carry significant amount of translational entropy that for sufficiently high temperature can indeed out-compete the energy, lowering the overall free energy. To see this, we note that a single vortex entropy contribution is a logarithm of the number of states, in this case positions $\sim L^2/a^2$ available to it, giving total free-energy vortex contribution

$$\begin{aligned} F_v &= E_v - TS_v = \pi K\ln L/a - k_B\ln L^2/a^2, && (175)\\ &= (\pi K - 2k_BT)\ln L/a. && (176) \end{aligned}$$

This thus indicates (ignoring the aformentioned effects of dipole screening) that vortex free-energy is positive for $k_BT < \frac{\pi}{2}K$ and negative for $k_BT > \frac{\pi}{2}K$. Thus we expect a vortex unbinding KT phase transition at $T_{KT} = \frac{\pi}{2}K/k_B$ from a superfluid state with quasi-long-range order to a normal state with short-range (exponential) order.

3. *duality and Magnus force*

## IX. SUPERFLUID AND MOTT INSULATOR ON THE LATTICE

So far we have only studied bosons in a continuum. We learned above that while they do exhibit a finite $T$ transition, at $T = 0$ and finite density, bosons in a *continuum* always form a superfluid ground state. Thus, at $T = 0$ the transition driven by $\mu$ is a trivial vacuum-to-superfluid transition. Now we ask whether it is possible to prevent bosons from forming a superfluid ground state at $T = 0$. Indeed it is, but (setting aside some more exotic models) only in the presence of a lattice or quenched disorder that break Galilean invariance. While there are a number of realizations of such lattice bosons in a solid state context (e.g., $He^4$ on a substrate and variety of magnetic systems), it was explicitly demonstrated in bosonic $Rb^{87}$ atoms confined in an optical lattice by Greiner, et al.[15]. The physics of this

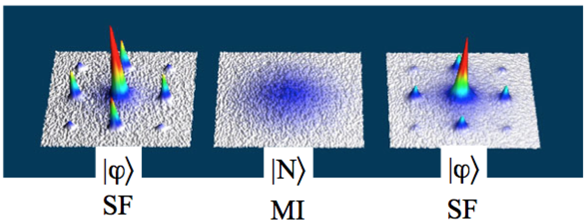


FIG. 8: False-color time-of-flight images illustrating superfluid-to-Mott insulator transition in $Rb^{87}$ bosonic atoms confined to an optical lattice, as a function of lattice depth controlled by laser intensity[15].

Superfluid-to-Mott Insulator (SF-MI) quantum (occuring at $T = 0$) phase transition[19] has been studied extensively dating back to the early work by Efetov '79 and by Doniach '81[16], and most extensively explored by Fisher, et al.[17]. In the context of cold atoms in an optical lattice, the system was analyzed in detail by Jaksch, et al[18] who stimulated experiments by Greiner, et al.

To capture the physics beyond the continuum, incorporating the lattice one can first diagonalize the noninteracting Hamiltonian of bosons moving in a periodic potential and use the corresponding Wannier (single site $i$) $\phi_i(r) = \langle r|i\rangle$ basis to construct a lattice model representing dynamics of bosons on a lattice. In the simplest single-band approximation this is the so-called Bose-Hubbard model described by a lattice Hamiltonian

$$H_{BH} = -\sum_{ij} t_{ij} a_i^\dagger a_j + U \sum_i a_i^\dagger a_i^\dagger a_i a_i, \tag{177}$$

where $t_{ij}$ is the single-particle hopping matrix element and on site energy that in the simplest case can be taken to vanish for all but nearest neighbors $ij$ pair. $U$ is the "Hubbard U" interaction parameter that controls boson on-site interaction. These parameters can be derived from the continuum Hamiltonian of bosons in a periodic potential[18].

We will not analyze this model in detail, but will only make qualitative remarks. It is quite clear that for low lattice filling fraction $n = N_{bosons}/N_{latticesites}$, the model reduces to that in the continuum, analyzed above and a superfluid ground state emerges at $T = 0$, minimizing the kinetic energy by small phase fluctuations and large number fluctuations characteristic of a superfluid. In contrast, at high *commensurate* filling fraction $n = 0, 1, 2, \ldots$, and for large $U$ the on-cite energy $U$ dominates and the ground state is the so-called "Mott insulator" (after Nevin Mott, who first proposed and studied insulators driven by interactions rather than by single-particle band gap of fermionic "band insulator" or by disorder in "Anderson insulator") in which on-site number fluctuations are small, thereby minimizing the on-site boson interactions $U$. At lowest order at large $U/tgg1$ the resulting Mott insulator is well-described by a Fock state on each site $i$, with the many-body ground state, $|MI\rangle \approx \sum_i (a_i^\dagger)^n |0\rangle$.

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