Quantum phase transitions of correlated electrons and atoms

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Why study quantum phase transitions?

- Theory for a quantum system with strong correlations: describe phases on either side of $g_c$ by expanding in deviation from the quantum critical point.
- Critical point is a novel state of matter without quasiparticle excitations.
- Critical excitations control dynamics in the wide quantum-critical region at non-zero temperatures.

Important property of ground state at $g = g_c$:
- temporal and spatial scale invariance;
- characteristic energy scale at other values of $g$: $\Delta \sim |g - g_c|^{\nu}$
Outline

I. The Quantum Ising chain

II. The superfluid-Mott insulator quantum phase transition

III. The cuprate superconductors
   *Superfluids proximate to finite doping Mott insulators with VBS order?*

IV. Vortices in the superfluid

V. Vortices in superfluids near the superfluid-insulator quantum phase transition
   *The “quantum order” of the superconducting state: evidence for vortex flavors*
I. Quantum Ising Chain
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Degrees of freedom: $j = 1 \ldots N$ qubits, $N$ "large"

$$\left| \uparrow \right>_j, \left| \downarrow \right>_j$$

or

$$\left| \rightarrow \right>_j = \frac{1}{\sqrt{2}} \left( \left| \uparrow \right>_j + \left| \downarrow \right>_j \right), \quad \left| \leftarrow \right>_j = \frac{1}{\sqrt{2}} \left( \left| \uparrow \right>_j - \left| \downarrow \right>_j \right)$$

Hamiltonian of decoupled qubits:

$$H_0 = -Jg \sum_j \sigma_j^x$$
Coupling between qubits:

\[ H_1 = -J \sum_j \sigma_j^z \sigma_{j+1}^z \]

\[
\left( |\rightarrow\rangle_j \langle\leftarrow| + |\leftarrow\rangle_j \langle\rightarrow| \right) \left( |\rightarrow\rangle_{j+1} \langle\leftarrow| + |\leftarrow\rangle_{j+1} \langle\rightarrow| \right)
\]

Prefers neighboring qubits are either \( |\uparrow\rangle_j \uparrow\rangle_{j+1} \) or \( |\downarrow\rangle_j \downarrow\rangle_{j+1} \) (not entangled)

Full Hamiltonian

\[ H = H_0 + H_1 = -J \sum_j \left( g \sigma_j^x + \sigma_j^z \sigma_{j+1}^z \right) \]

leads to entangled states at \( g \) of order unity
Experimental realization

LiHoF$_4$
Weakly-coupled qubits ($g \gg 1$)

Ground state:

$$|G\rangle = \cdots \rightarrow \rightarrow \rightarrow \rightarrow \cdots$$

$$-\frac{1}{2g} |\cdots \rightarrow \rightarrow \rightarrow \leftarrow \rightarrow \rightarrow \cdots \rangle - \cdots$$

Lowest excited states:

$$|\ell_j\rangle = \cdots \rightarrow \rightarrow \rightarrow \leftarrow_j \rightarrow \rightarrow \rightarrow \rightarrow \cdots + \cdots$$

Coupling between qubits creates "flipped-spin" quasiparticle states at momentum $p$

$$|p\rangle = \sum_j e^{ipx_j/\hbar} |\ell_j\rangle$$

Excitation energy $\varepsilon(p) = \Delta + 4J \sin^2 \left(\frac{pa}{2\hbar}\right) + O\left(g^{-1}\right)$

Excitation gap $\Delta = 2gJ - 2J + O\left(g^{-1}\right)$

Entire spectrum can be constructed out of multi-quasiparticle states
Dynamic Structure Factor $S(p,\omega)$:

- Cross-section to flip a $|\rightarrow\rangle$ to a $|\leftarrow\rangle$ (or vice versa)
- While transferring energy $\hbar\omega$ and momentum $p$

$$Z\delta(\omega - \varepsilon(p))$$

Structure holds to all orders in $1/g$

At $T > 0$, collisions between quasiparticles broaden pole to a Lorentzian of width $1/\tau_\varphi$ where the phase coherence time $\tau_\varphi$ is given by

$$\frac{1}{\tau_\varphi} = \frac{2k_B T}{\pi \hbar} e^{-\Delta/k_B T}$$

Ground states:

\[ |G \uparrow\rangle = |\cdots \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \rangle \]

\[ -\frac{g}{2} |\cdots \uparrow \uparrow \uparrow \uparrow \downarrow \uparrow \uparrow \uparrow \uparrow \cdots \rangle - \cdots \]

Second state \[ |G \downarrow\rangle \] obtained by \[ \uparrow \Leftrightarrow \downarrow \]

\[ |G \downarrow\rangle \text{ and } |G \uparrow\rangle \text{ mix only at order } g^N \]

Lowest excited states: domain walls

\[ |d_j\rangle = |\cdots \uparrow \uparrow \uparrow \uparrow \uparrow \downarrow \downarrow \downarrow \downarrow \cdots \rangle + \cdots \]

Coupling between qubits creates new “domain-wall” quasiparticle states at momentum \( p \)

\[ |p\rangle = \sum_j e^{ipx_j/\hbar} |d_j\rangle \]

Excitation energy \( \epsilon(p) = \Delta + 4Jg \sin^2 \left( \frac{pa}{2\hbar} \right) + O(g^2) \)

Excitation gap \( \Delta = 2J - 2gJ + O(g^2) \)
Dynamic Structure Factor $S(p, \omega)$: Strongly-coupled qubits ($g \ll 1$)

Cross-section to flip a $|\rightarrow\rangle$ to a $|\leftarrow\rangle$ (or vice versa)
while transferring energy $\hbar \omega$ and momentum $p$

Structure holds to all orders in $g$

At $T > 0$, motion of domain walls leads to a finite phase coherence time $\tau_\varphi$, and broadens coherent peak to a width $1/\tau_\varphi$ where

$$\frac{1}{\tau_\varphi} = \frac{2k_B T}{\pi \hbar} e^{-\Delta/k_B T}$$

Entangled states at $g$ of order unity

"Flipped-spin" Quasiparticle weight $Z$

$Z \sim (g - g_c)^{1/4}$

Ferromagnetic moment $N_0$

$N_0 \sim (g_c - g)^{1/8}$

Excitation energy gap $\Delta$

$\Delta \sim |g - g_c|$
Dynamic Structure Factor $S(p, \omega)$:

Cross-section to flip a $|\rightarrow\rangle$ to a $|\leftarrow\rangle$ (or vice versa) while transferring energy $\hbar \omega$ and momentum $p$.

Critical coupling ($g = g_c$)

$$\sim (\omega^2 - c^2 p^2)^{-7/8}$$

No quasiparticles --- dissipative critical continuum
\[ H_I = -J \sum_i \left( g \sigma_i^x + \sigma_i^z \sigma_{i+1}^z \right) \]

\[ \chi(\omega) = \frac{i}{\hbar} \sum_k \int_0^\infty dt \left[ \sigma_j^z(t), \sigma_k^z(0) \right] e^{i\omega t} \]

\[ = \frac{A}{T^{7/4} \left( 1 - i\omega / \Gamma_R + \ldots \right)} \]

\[ \Gamma_R = \left( 2 \tan \frac{\pi}{16} \right) \frac{k_B T}{\hbar} \]

\[ \langle \sigma_j^z \sigma_k^z \rangle \sim \frac{1}{|j - k|^{1/4}} \]


II. The superfluid-Mott insulator quantum phase transition
Bose condensation
Velocity distribution function of ultracold $^{87}\text{Rb}$ atoms

Apply a periodic potential (standing laser beams) to trapped ultracold bosons ($^{87}\text{Rb}$)
Momentum distribution function of bosons

Bragg reflections of condensate at reciprocal lattice vectors

Superfluid-insulator quantum phase transition at $T=0$
Bosons at filling fraction $f = 1$

Weak interactions: superfluidity

Strong interactions: Mott insulator which preserves all lattice symmetries

Bosons at filling fraction $f = 1$

$\langle \Psi \rangle \neq 0$

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Strong interactions: insulator
Bosons at filling fraction $f = 1/2$

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Strong interactions: insulator

**Insulating phases of bosons at filling fraction** $f = 1/2$

- **Charge density wave (CDW) order**
- **Valence bond solid (VBS) order**
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Can define a common CDW/VBS order using a generalized "density" $\rho(r) = \sum Q \rho_Q e^{iQ.r}$

All insulators have $\langle \Psi \rangle = 0$ and $\langle \rho_Q \rangle \neq 0$ for certain $Q$

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Insulating phases of bosons at filling fraction \( f = 1/2 \)

\[
\frac{1}{\sqrt{2}} \left( + \right) = \text{Valence bond solid (VBS) order}
\]

Charge density wave (CDW) order

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Superfluid-insulator transition of bosons at generic filling fraction \( f \)

The transition is characterized by multiple distinct order parameters (boson condensate, VBS/CDW order)

*Traditional* (Landau-Ginzburg-Wilson) *view:* Such a transition is first order, and there are no precursor fluctuations of the order of the insulator in the superfluid.
Superfluid-insulator transition of bosons at generic filling fraction $f$

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**Traditional (Landau-Ginzburg-Wilson) view:**
Such a transition is first order, and there are no precursor fluctuations of the order of the insulator in the superfluid.

**Recent theories:**
Quantum interference effects can render such transitions second order, and the superfluid does contain precursor VBS/CDW fluctuations.

III. The cuprate superconductors

Superfluids proximate to finite doping
Mott insulators with VBS order?
La$_2$CuO$_4$
La$_2$CuO$_4$

Mott insulator: square lattice antiferromagnet

\[ H = \sum_{<ij>} J_{ij} \vec{S}_i \cdot \vec{S}_j \]
La$_{2-\delta}$Sr$_\delta$CuO$_4$

Superfluid: condensate of paired holes

$\langle \vec{S} \rangle = 0$
Many experiments on the cuprate superconductors show:

- Tendency to produce modulations in spin singlet observables at wavevectors \((2\pi/a)(1/4,0)\) and \((2\pi/a)(0,1/4)\).
- Proximity to a Mott insulator at hole density \(\delta = 1/8\) with long-range charge modulations at wavevectors \((2\pi/a)(1/4,0)\) and \((2\pi/a)(0,1/4)\).
The cuprate superconductor $\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2$

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Superfluids proximate to finite doping Mott insulators with VBS order?
Experiments on the cuprate superconductors also show strong vortex fluctuations above $T_c$.

Measurements of Nernst effect are well explained by a model of a liquid of vortices and anti-vortices.


Main claims:

• There are precursor fluctuations of VBS order in the superfluid.

• There fluctuations are intimately tied to the quantum theory of vortices in the superfluid
IV. Vortices in the superfluid

*Magnus forces, duality, and point vortices as dual “electric” charges*
Excitations of the superfluid: Vortices

Central question:
In two dimensions, we can view the vortices as point particle excitations of the superfluid. What is the quantum mechanics of these “particles”?
In ordinary fluids, vortices experience the Magnus Force

\[ F_M = (\text{mass density of air}) \cdot (\text{velocity of ball}) \cdot (\text{circulation}) \]
For a vortex in a superfluid, this is

\[
F_M = (m \rho) \left( \left( v_s - \frac{dr_v}{dt} \right) \times \hat{z} \right) \left( \oint v_s \cdot dr \right)
\]

\[
= n h \rho \left( v_s - \frac{dr_v}{dt} \right) \times \hat{z}
\]

where \( \rho \) = number density of bosons
\( v_s \) = local velocity of superfluid
\( r_v \) = position of vortex
For a vortex in a superfluid, this is

\[ F_M = (m\rho) \left( \left( \mathbf{v}_s - \frac{d\mathbf{r}_v}{dt} \right) \times \mathbf{\hat{z}} \right) \left( \oint \mathbf{v}_s \cdot d\mathbf{r} \right) \]

\[ = n\hbar \rho \left( \mathbf{v}_s - \frac{d\mathbf{r}_v}{dt} \right) \times \mathbf{\hat{z}} \]

\[ = n \left( \mathbf{E} + \frac{d\mathbf{r}_v}{dt} \times \mathbf{B} \right) \]

where \( \mathbf{E} = \rho \mathbf{v}_s \times \mathbf{\hat{z}} \) and \( \mathbf{B} = -\hbar \rho \mathbf{\hat{z}} \)

**Dual picture:**
The vortex is a quantum particle with dual “electric” charge \( n \), moving in a dual “magnetic” field of strength = \( \hbar \times \) (number density of Bose particles)
V. Vortices in superfluids near the superfluid-insulator quantum phase transition

The “quantum order” of the superconducting state: evidence for vortex flavors
- The vortices are quantum particles moving in a periodic potential with the symmetry of the square lattice, and in the presence of a dual “magnetic” field of strength $= h \rho$, where $\rho$ is the number density of bosons per unit cell.

- The vortex motion can be described by the effective Hofstadter Hamiltonian:

$$\mathcal{H}_v = -t \sum_{\langle ij \rangle} (e^{iA_{ij}} \varphi_i^* \varphi_j + \text{c.c.})$$

where $\varphi_i$ is an operator which annihilates a vortex particle at site $i$ of a square lattice.

![Diagram](image)

$$A_1 + A_2 + A_3 + A_4 = 2\pi f$$

where $f$ is the boson filling fraction.
Bosons at filling fraction $f = 1$

- At $f=1$, the “magnetic” flux per unit cell is $2\pi$, and the vortex does not pick up any phase from the boson density.

- The effective dual “magnetic” field acting on the vortex is zero, and the corresponding component of the Magnus force vanishes.
Bosons at rational filling fraction $f=p/q$

Quantum mechanics of the vortex “particle” in a periodic potential with $f$ flux quanta per unit cell

**Space group symmetries of Hofstadter Hamiltonian:**

$T_x, T_y$ : Translations by a lattice spacing in the $x, y$ directions

$R$ : Rotation by 90 degrees.

**Magnetic space group:**

$$T_x T_y = e^{2\pi i f} T_y T_x$$

$$R^{-1} T_y R = T_x$$

$$R^{-1} T_x R = T_y^{-1}$$

$$R^4 = 1$$

The low energy vortex states must form a representation of this algebra
Vortices in a superfluid near a Mott insulator at filling $f=p/q$

Hofstadter spectrum of the quantum vortex “particle” with field operator $\phi$

At filling $f=p/q$, there are $q$ species of vortices, $\phi_\ell$ (with $\ell=1\ldots q$), associated with $q$ degenerate minima in the vortex spectrum. These vortices realize the smallest, $q$-dimensional, representation of the magnetic algebra.

$$T_x : \phi_\ell \to \phi_{\ell+1} \quad ; \quad T_y : \phi_\ell \to e^{2\pi i \ell f} \phi_\ell$$

$$R : \phi_\ell \to \frac{1}{\sqrt{q}} \sum_{m=1}^{q} \phi_m e^{2\pi i \ell m f}$$
Vortices in a superfluid near a Mott insulator at filling $f=p/q$

The $q\varphi_\ell$ vortices characterize both superconducting and VBS/CDW orders

VBS order:
Status of space group symmetry determined by
density operators $\rho_Q$ at wavevectors $Q_{mn} = \frac{2\pi p}{q}(m,n)$

$$\rho_{mn} = e^{i\pi mnf} \sum_{\ell=1}^{q} \varphi_\ell^* \varphi_{\ell+n} e^{2\pi i\ell mf}$$

$T_x : \rho_Q \rightarrow \rho_Q e^{iQ \cdot \hat{x}}$ ; $T_y : \rho_Q \rightarrow \rho_Q e^{iQ \cdot \hat{y}}$

$R : \rho(Q) \rightarrow \rho(RQ)$
Vortices in a superfluid near a Mott insulator at filling $f=p/q$

- The excitations of the superfluid are described by the quantum mechanics of $q$ flavors of low energy vortices moving in zero dual "magnetic" field.

- The orientation of the vortex in flavor space implies a particular configuration of VBS order in its vicinity.
Mott insulators obtained by “condensing” vortices

Spatial structure of insulators for $q=2$ ($f=1/2$)
Field theory with projective symmetry
Spatial structure of insulators for $q=4$ ($f=1/4$ or $3/4$)

$a \times b$ unit cells; $q/a', q/b', ab/q'$
all integers
Vortices in a superfluid near a Mott insulator at filling $f=p/q$

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- The orientation of the vortex in flavor space implies a particular configuration of VBS order in its vicinity.

- Any pinned vortex must pick an orientation in flavor space: this induces a halo of VBS order in its vicinity.
Vortex-induced LDOS of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ integrated from 1meV to 12meV at 4K

Vortices have halos with LDOS modulations at a period $\approx 4$ lattice spacings


Measuring the inertial mass of a vortex

The spatial extent of the LDOS modulations measures the region over which the vortex executes its zero-point motion. The size of this region can be determined by solving the equations of motion

$$m_v \frac{d^2 \mathbf{r}}{dt^2} = F_M$$

and so is determined by the inertial vortex mass $m_v$. 
Measuring the inertial mass of a vortex

_Preliminary_ estimates for the BSCCO experiment:

Inertial vortex mass \( m_v \approx 10m_e \)

Vortex magnetoplasmon frequency \( \nu_p \approx 1 \text{ THz} = 4 \text{ meV} \)

Future experiments can directly detect vortex zero point motion by looking for resonant absorption at this frequency.

Vortex oscillations can also modify the electronic density of states.
Superfluids near Mott insulators

The Mott insulator has average Cooper pair density, \( f = p/q \) per site, while the density of the superfluid is close (but need not be identical) to this value.

- Vortices with flux \( \hbar/(2e) \) come in multiple (usually \( q \)) “flavors”
- The lattice space group acts in a projective representation on the vortex flavor space.
- These flavor quantum numbers provide a distinction between superfluids: they constitute a “quantum order”
- Any pinned vortex must chose an orientation in flavor space. This necessarily leads to modulations in the local density of states over the spatial region where the vortex executes its quantum zero point motion.