Collective modes at a disordered quantum phase transition

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Outline

- Collective modes: Goldstone and amplitude (Higgs)
- Superfluid-Mott glass quantum phase transition
- Fate of the collective modes at the superfluid-Mott glass transition
- Conclusions
Spontaneous symmetry breaking

Does a symmetric Hamiltonian imply a symmetric equilibrium state?

- world of this pencil is completely isotropic, all directions are equal
- symmetry is lost when pencil falls over, now only one direction holds
- state of lowest energy has lower symmetry than system

Rotational symmetry has been broken spontaneously!
Broken symmetries and collective modes

- systems with **broken continuous symmetry**:
  - planar magnet breaks $O(2)$ rotation symmetry
  - superfluid wave function breaks $U(1)$ symmetry

- **Amplitude mode**: corresponds to fluctuations of order parameter amplitude

- **Goldstone (phase) mode**: corresponds to fluctuations of order parameter phase

- **Amplitude mode** can be considered condensed matter analogue of **Higgs boson**

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**Goldstone theorem:**
When a continuous symmetry is spontaneously broken, massless Goldstone modes appear.

"Mexican hat" potential for order parameter in symmetry-broken phase, $F = t m^2 + u m^4$
What is the fate of the Goldstone and Higgs modes near a disordered quantum phase transition?
• Collective modes: Goldstone and Higgs
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Disordered interacting bosons

Ultracold atoms in optical potentials:
- disorder: speckle laser field
- interactions: tuned by Feshbach resonance and/or density

Disordered superconducting films:
- energy gap in insulating as well as superconducting phase
- preformed Cooper pairs \( \Rightarrow \) superconducting transition is bosonic

F. Jendrzejewski et al., Nature Physics 8, 398 (2012)

Sherman et al., Phys. Rev. Lett. 108, 177006 (2012)
Bose-Hubbard model

Bose-Hubbard (quantum rotor) Hamiltonian in two (and three) space dimensions:

\[ H = \frac{U}{2} \sum_i (\hat{n}_i - \bar{n}_i)^2 - \sum_{\langle i,j \rangle} J_{ij} (a_i^\dagger a_j + h.c.) \]

- superfluid ground state if **Josephson couplings** \( J_{ij} \) dominate
- insulating ground state if **charging energy** \( U \) dominates
- chemical potential \( \mu_i = U \bar{n}_i \)

**Particle-hole symmetry:**

- large integer filling \( \bar{n}_i = k \) with integer \( k \gg 1 \)
  \[ \Rightarrow \text{Hamiltonian invariant under} \ (\hat{n}_i - \bar{n}_i) \to -(\hat{n}_i - \bar{n}_i) \]
Phase diagrams

Weichman et al., Phys. Rev. B 7, 214516 (2008)
Monte Carlo simulations

- map Hamiltonian onto classical \((d + 1)\)-dimensional XY model for particle-hole symmetric case

\[
H_{cl} = -J_{\tau} \sum_{i,t} \epsilon_i S_{i,t} \cdot S_{i,t+1} - J_s \sum_{\langle i,j \rangle,t} \epsilon_i \epsilon_j S_{i,t} \cdot S_{j,t}
\]

- disorder: site dilution (fraction \(p\) of lattice sites randomly removed)

- combine Wolff cluster algorithm and conventional Metropolis updates

- system sizes up to \(L = 150, \ L_\tau = 1792\) in \((2+1)d\) and \(L = 80, \ L_\tau = 320\) in \((3+1)d\)

- several dilutions from \(p = 0\) to lattice percolation threshold \(p_c\)

- averages over 10 000 to 50 000 disorder configurations

- anisotropic finite-size scaling analysis

columnar disorder in classical XY model, correlated in imaginary time
Thermodynamic critical behavior

- clean system violates Harris criterion $d\nu > 2$
- disordered system in new universality class
- conventional power-law critical behavior
- universal critical exponents for dilutions $0 < p < p_c$
- disordered $\nu$ exponents fulfill $d\nu > 2$
- Griffiths singularities exponentially weak (see J. Phys. A 39, R143 (2006), PRL 112, 075702 (2014))

| Exponent | Clean | Disordered |
|----------|-------|------------|
| $z$     | 1     | 1.52       |
| $\nu$   | 0.6717| 1.16       |
| $\beta/\nu$ | 0.518 | 0.48       |
| $\gamma/\nu$ | 1.96  | 2.52       |

**Text from the graph:**
- ordered phase - superfluid
- disordered phase - Mott insulator
- Griffiths phase - Mott glass
- generic transition
- percolation transition
- MCP ($p_c, T^*$)

| Exponent | Clean | Disordered |
|----------|-------|------------|
| $z$     | 1     | 1.67       |
| $\nu$   | 0.5   | 0.90       |
| $\beta/\nu$ | 1     | 1.09       |
| $\gamma/\nu$ | 2     | 2.50       |

PRB 94, 134501 (2016)

PRB 98, 054514 (2018)
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**Amplitude mode: scalar susceptibility**

- Parameterize order parameter fluctuations into **amplitude** and **direction**
  \[ \vec{\phi} = \phi_0 (1 + \rho) \hat{n} \]

- Amplitude mode is associated with **scalar** susceptibility
  \[ \chi_{\rho\rho}(\vec{x}, t) = i \Theta(t) \langle [\rho(\vec{x}, t), \rho(0, 0)] \rangle \]

- Monte-Carlo simulations compute **imaginary time** correlation function
  \[ \chi_{\rho\rho}(\vec{x}, \tau) = \langle \rho(\vec{x}, \tau) \rho(0, 0) \rangle \]

- **Wick rotation** required: analytical continuation from imaginary to real times/frequencies
  \[ \Rightarrow \text{maximum entropy method} \] to compute spectral function
  \[ A(q, \omega) = \chi''_{\rho\rho}(q, \omega) / \pi \]
Analytic continuation - maximum entropy method

- Matsubara susceptibility vs. spectral function

\[ \chi_{\rho\rho}(\vec{q}, i\omega_m) = \int_0^\infty d\omega A(\vec{q}, \omega) \frac{2\omega}{\omega_m^2 + \omega^2} \]

**Maximum entropy method:**

- inversion is ill-posed problem, highly sensitive to noise
- fit \( A(\vec{q}, \omega) \) to \( \chi_{\rho\rho}(\vec{q}, i\omega_m) \) MC data by minimizing
  \[ Q = \frac{1}{2} \sigma^2 - \alpha S \]
- parameter \( \alpha \) balances between fit error \( \sigma^2 \) and entropy \( S \) of \( A(\vec{q}, \omega) \), i.e., between fitting information and noise
- best \( \alpha \) value chosen by L-curve method [see Bergeron et al., PRE 94, 023303 (2016)]
Amplitude mode in clean undiluted system

Scaling form (in 2d):

$$\chi_{\rho \rho}(0, \omega) = |r|^{3\nu - 2} X(\omega |r|^{-\nu})$$  

[Podolsky + Sachdev, PRB 86, 054508 (2012)]

- sharp Higgs peak in spectral function
- Higgs energy (mass) $\omega_H$ scales as expected with distance from criticality $r$
Amplitude mode in disordered system

- spectral function shows broad peak near $\omega = 1$
- peak is noncritical: does not move as quantum critical point is approached
- amplitude fluctuations not soft at criticality
- violates expected scaling form $\chi_{\rho\rho}(0, \omega) = |r|^{(d+z)\nu-2} X(\omega |r|^{-z\nu})$

Note: $(d + z)\nu - 2 > 0$
What is the reason for the absence of a sharp amplitude mode at the superfluid-Mott glass transition?
Quantum mean-field theory

\[ H = \frac{U}{2} \sum_i \epsilon_i (\hat{n}_i - \bar{n}_i)^2 - J \sum_{\langle i,j \rangle} \epsilon_i \epsilon_j (a_i^\dagger a_j + h.c.) \]

- truncate Hilbert space: keep only states \(|\bar{n} - 1\rangle, |\bar{n}\rangle, \text{ and } |\bar{n} + 1\rangle\) on each site

Variational wave function:

\[ |\Psi_{MF}\rangle = \prod_i |g_i\rangle = \prod_i \left[ \cos \left( \frac{\theta_i}{2} \right) |\bar{n}\rangle_i + \sin \left( \frac{\theta_i}{2} \right) \frac{1}{\sqrt{2}} \left( e^{i\phi_i} |\bar{n} + 1\rangle_i + e^{-i\phi_i} |\bar{n} - 1\rangle_i \right) \right] \]

- locally interpolates between **Mott insulator**, \(\theta = 0\), and **superfluid limit**, \(\theta = \pi/2\)

Mean-field energy:

\[ E_0 = \langle \Psi_{MF} | H | \Psi_{MF} \rangle = \frac{U}{2} \sum_i \epsilon_i \sin^2 \left( \frac{\theta_i}{2} \right) - J \sum_{\langle i,j \rangle} \epsilon_i \epsilon_j \sin(\theta_i) \sin(\theta_j) \cos(\phi_i - \phi_j) \]

- solved by **minimizing** \(E_0\) w.r.t. \(\theta_i \Rightarrow\) coupled nonlinear equations
Mean-field theory: local order parameter \( m_i = \langle a_i \rangle = \sin(\theta_i) e^{i\phi_i} \)

Note: Mean-field theory fails close to critical point, creates smeared phase transition:
Mean-field theory: excitations

• **define local excitations** (orthogonal to $|g_i\rangle$, OP phase fixed at 0)

$$|g_i\rangle = \cos\left(\frac{\theta_i}{2}\right)|\bar{n}\rangle_i + \sin\left(\frac{\theta_i}{2}\right)\frac{1}{\sqrt{2}}(|\bar{n} + 1\rangle_i + |\bar{n} - 1\rangle_i)$$

$$|\theta_i\rangle = \sin\left(\frac{\theta_i}{2}\right)|\bar{n}\rangle_i - \cos\left(\frac{\theta_i}{2}\right)\frac{1}{\sqrt{2}}(|\bar{n} + 1\rangle_i + |\bar{n} - 1\rangle_i)$$

$$|\phi_i\rangle = \frac{1}{\sqrt{2}}(|\bar{n} + 1\rangle_i - |\bar{n} - 1\rangle_i)$$

• **expand H to quadratic order in excitations:** $H = E_0 + H_\theta + H_\phi$

$$H_\theta = \sum_i \left[ \frac{U}{2} + 2J \sum_{j'} \sin(\theta_i) \sin(\theta_j) \right] \epsilon_i b_{\theta i}^\dagger b_{\theta i} - J \sum_{\langle i,j \rangle} \cos(\theta_i) \cos(\theta_j) \epsilon_i \epsilon_j (b_{\theta j}^\dagger + b_{\theta i})(b_{\theta j}^\dagger + b_{\theta j})$$

$H_\phi$ has similar structure but different coefficients

$H_\phi$ and $H_\theta$ can be solved by **Bogoliubov transformation**
Excitations in clean system

- mean-field quantum phase transition at $U = 16J$
- all excitations are spatially extended (plane waves)

Mott insulator
- all excitations are gapped

Superfluid
- Goldstone mode is gapless
- amplitude (Higgs) modes is gapped, gap vanishes at QCP
Excitations in diluted system

- Goldstone mode **massless** in superfluid, as required by Goldstone’s theorem
- lowest Goldstone excitation undergoes **delocalization transition** upon entering superfluid
- Goldstone mode localized at higher energies
- Higgs mode **strongly localized** in both phases for all energies
- inverse participation number

\[ P^{-1}(0) = \sum_j (|u_{\alpha j 0}|^2 - |v_{\alpha j 0}|^2)^2 \]

- generalized fractal dimension

\[ \tau_2(0) = \ln P(0) / \ln L \]
Longitudinal and transverse susceptibilities \((q = 0)\)

\[\chi''(\omega)\]

\(U = 10, 11, 12, 13, 14, 15, 16, 17\)

\(\omega\) range: 0 to 6

Diluted, \(p = 1/3\)

Clean
Collective modes in \((3 + 1)\) dimensions

- inhomogeneous mean-field theory for 3d Bose-Hubbard model
- collective modes develop **mobility edges**

Goldstone (top) and amplitude (bottom) mode density of states and mobility edges for dilutions \(p = 1/5\) and \(1/3\)
Conclusions

- disordered interacting bosons undergo quantum phase transition from superfluid to insulating Mott glass
- conventional critical behavior with universal critical exponents, Griffiths effects exponentially weak
  [see classification in T.V., J. Phys. A 39, R143 (2006)]
- collective modes in superfluid phase show striking localization behavior
- Goldstone mode is delocalized at $\omega = 0$ but localizes with increasing energy
- amplitude (Higgs) mode is strongly localized for all energies
- broad incoherent scalar response at $q = 0$, violates naive scaling

Exotic collective mode dynamics even if critical behavior is conventional

Thermodynamics: Phys. Rev. B 94, 134501 (2016), Phys. Rev. B 98, 054514 (2018)
Collective modes: Phys. Rev. Lett. 125, 027002 (2020), Phys. Rev. B 104, 014511 (2021), Ann. Phys. 435 168526 (2021)
Disordered interacting bosons

Bosonic quasiparticles in doped quantum magnets:

- bromine-doped dichloro-tetrakis-thiourea-nickel (DTN)
- coupled antiferromagnetic chains of $S = 1 \text{ Ni}^{2+}$ ions
- $S = 1$ spin states can be mapped onto bosonic states with $n = m_s + 1$
Harris criterion:

A clean critical point is (perturbatively) stable against weak disorder if its correlation length exponent $\nu$ fulfills the inequality $d\nu > 2$.

Superfluid-Mott insulator transition:

- clean superfluid-Mott insulator quantum critical point is in $(d + 1)$-dimensional XY universality class
- correlation length critical exponent $\nu \approx 0.6717$ for $(2+1)$ dimensions and $\nu = 0.5$ for $(3+1)$ dimensions
- clean $\nu$ violates Harris criterion in both dimensions

$\Rightarrow$ clean critical behavior unstable against disorder (dilution)

Critical behavior of superfluid-Mott glass transition must be in new universality class
Finite-size scaling

Binder cumulant:

\[ g_{av} = \left[ 1 - \frac{\langle |m|^4 \rangle}{3\langle |m|^2 \rangle^2} \right]_{\text{dis}} \]

Isotropic systems:

- scaling form: \( g_{av}(r, L) = X(rL^{1/\nu}) \)
  \[ r = (T - T_c)/T_c \]
- \( g_{av} \) vs. \( T \) curves for different \( L \) cross at \( T_c \) with value \( g_{av}(0, L) = X(0) \)

Anisotropic systems:

- \( L \) and \( L_\tau \) are not equivalent, \( L_\tau \) scales like \( L_\tau \sim L^z \) (or even as \( \ln L_\tau \sim L^\psi \))
- conventional scaling: \( g_{av}(r, L, L_\tau) = X(rL^{1/\nu}, L_\tau/L^z) \)
- activated scaling: \( g_{av}(r, L, L_\tau) = X(rL^{1/\nu}, \ln(L_\tau)/L^\psi) \)
- How to choose correct sample shapes if dynamical exponent \( z \) (or tunneling exponent \( \psi \)) is not known?
Anisotropic finite-size scaling

- $g_{av}$ vs $L_\tau$ has maximum at "optimal" shape
- at criticality, $L_\tau^{\text{max}} \sim L^z$ (for activated scaling: $\ln(L_\tau^{\text{max}}) \sim L^\psi$)
- once optimal shapes are found, FSS works as usual
  optimal $g_{av}$ vs. $T$ curves cross at $T_c$: $g_{av}(0, L, L_\tau^{\text{max}}) = X(0, \text{const})$
Diluted lattice: Goldstone mode

- Goldstone mode becomes massless in superfluid phase, as required by Goldstone’s theorem

- Wave function of lowest excitation for $U = 8$ to 15

- Localized in insulator, delocalizes in superfluid phase
Goldstone mode: localization properties

- inverse participation ratio:
  \[ P^{-1} = N \sum_i |\psi_i|^4 \]
  \( P \to 1 \) for delocalized states
  \( P \to 0 \) for localized states

- wave function at \( U = 8 \) as function of excitation energy
- delocalized at \( \omega = 0 \), localized for higher energies
Amplitude (Higgs) mode

- amplitude mode strongly localized for all $U$ and all excitation energies

- wave function of lowest excitation for $U = 8$ to 15