Collective modes at a disordered quantum phase transition

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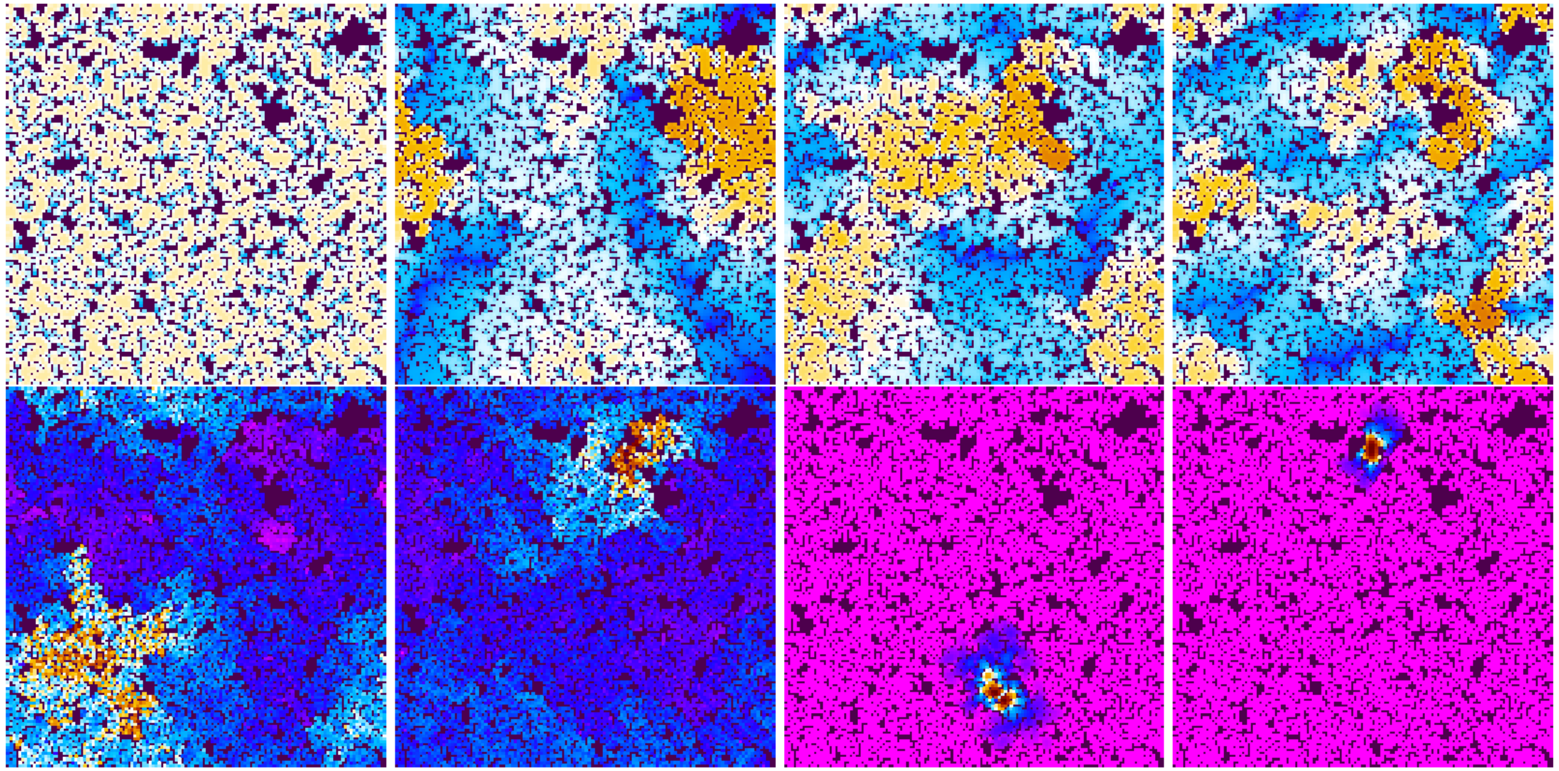

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Outline

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

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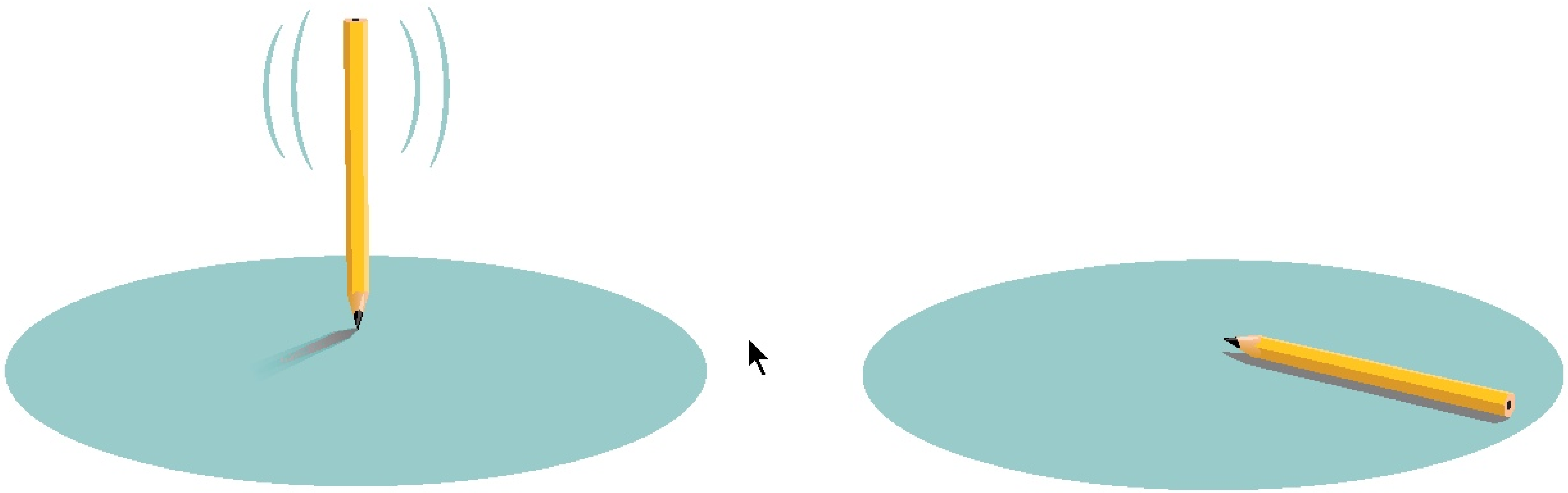
Spontaneous symmetry breaking

Does a symmetric Hamiltonian imply a symmetric equilibrium state?

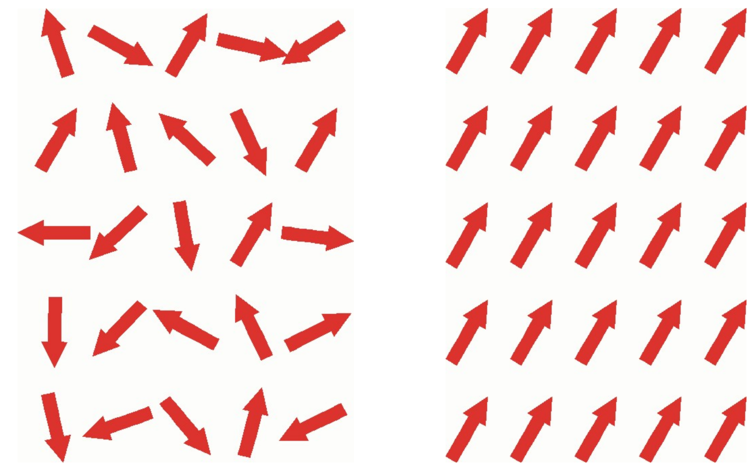


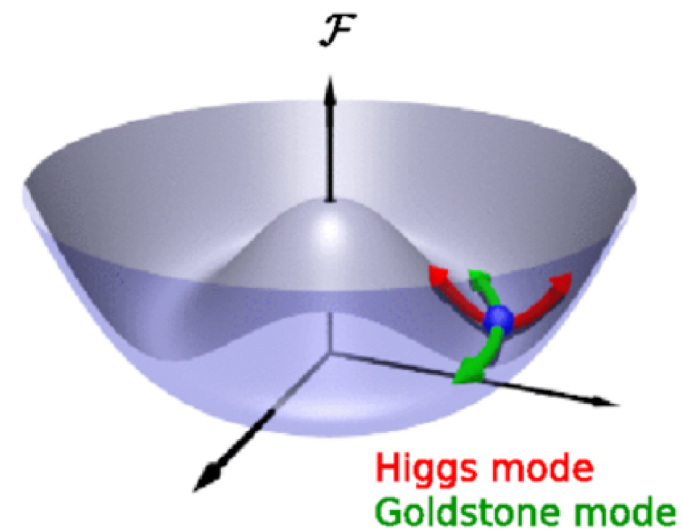
- world of this pencil is completely isotropic, all directions are equal
- symmetry is lost when pencil falls over, now only one direction holds
- state of lowest energy has **lower** symmetry than system

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**





"Mexican hat" potential for order parameter in symmetry-broken phase, $F = t\,\mathbf{m}^2 + u\,\mathbf{m}^4$

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

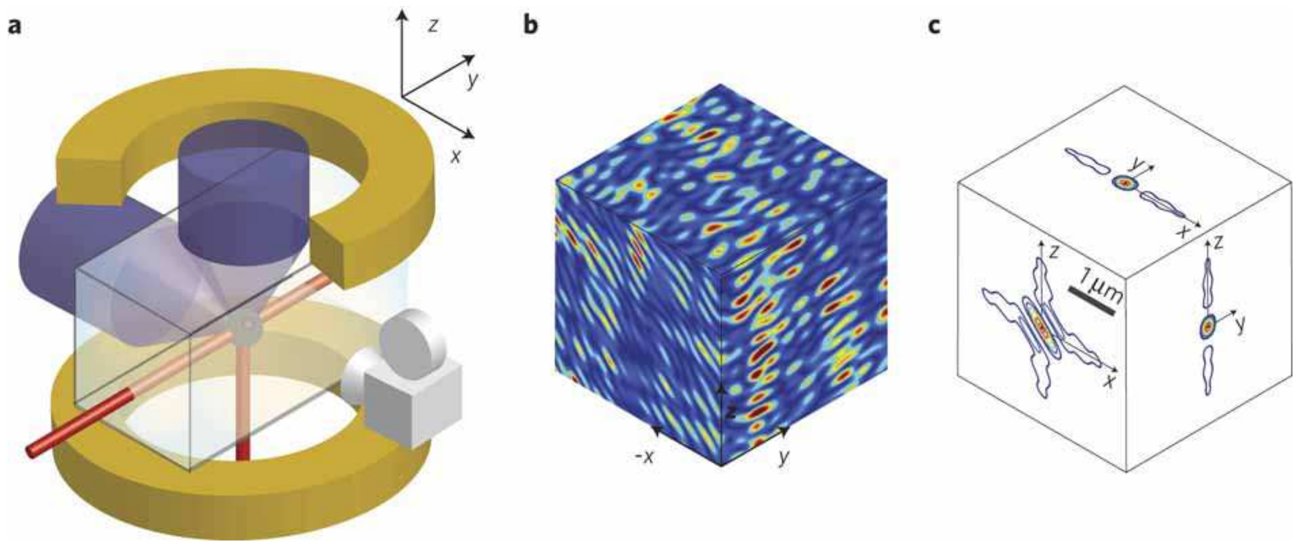
What is the fate of the Goldstone and Higgs modes near a disordered quantum phase transition?

- Collective modes: Goldstone and Higgs
- **Superfluid-Mott glass quantum phase transition**
- Fate of the collective modes at the superfluid-Mott glass transition
- Conclusions

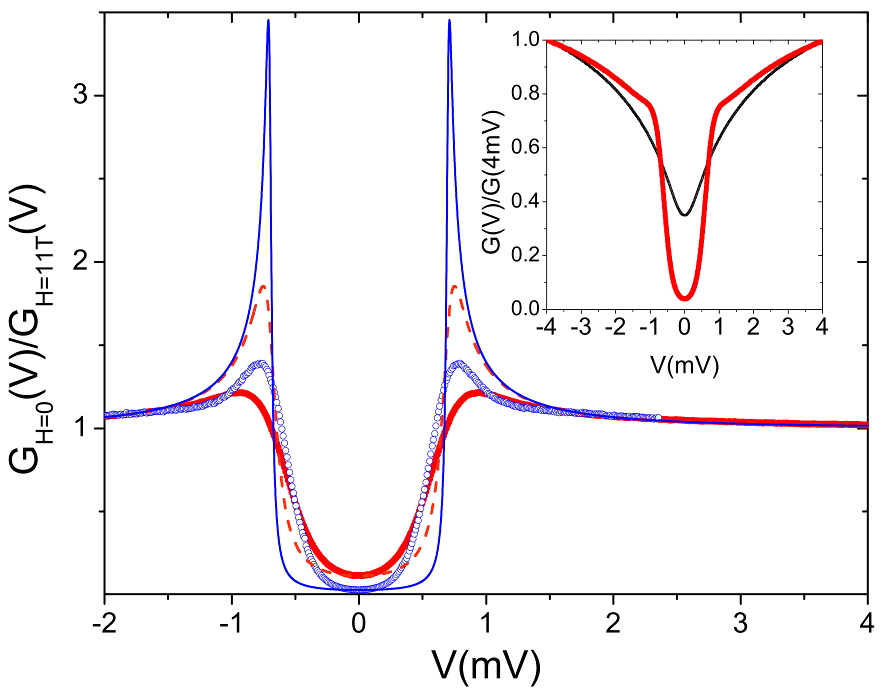
Disordered interacting bosons

Ultracold atoms in optical potentials:

- disorder: speckle laser field
- interactions: tuned by Feshbach resonance and/or density



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



Sherman et al., Phys. Rev. Lett. 108, 177006 (2012)

Disordered superconducting films:

- energy gap in **insulating** as well as **superconducting** phase
- preformed Cooper pairs ⇒ superconducting transition is bosonic

Bose-Hubbard model

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

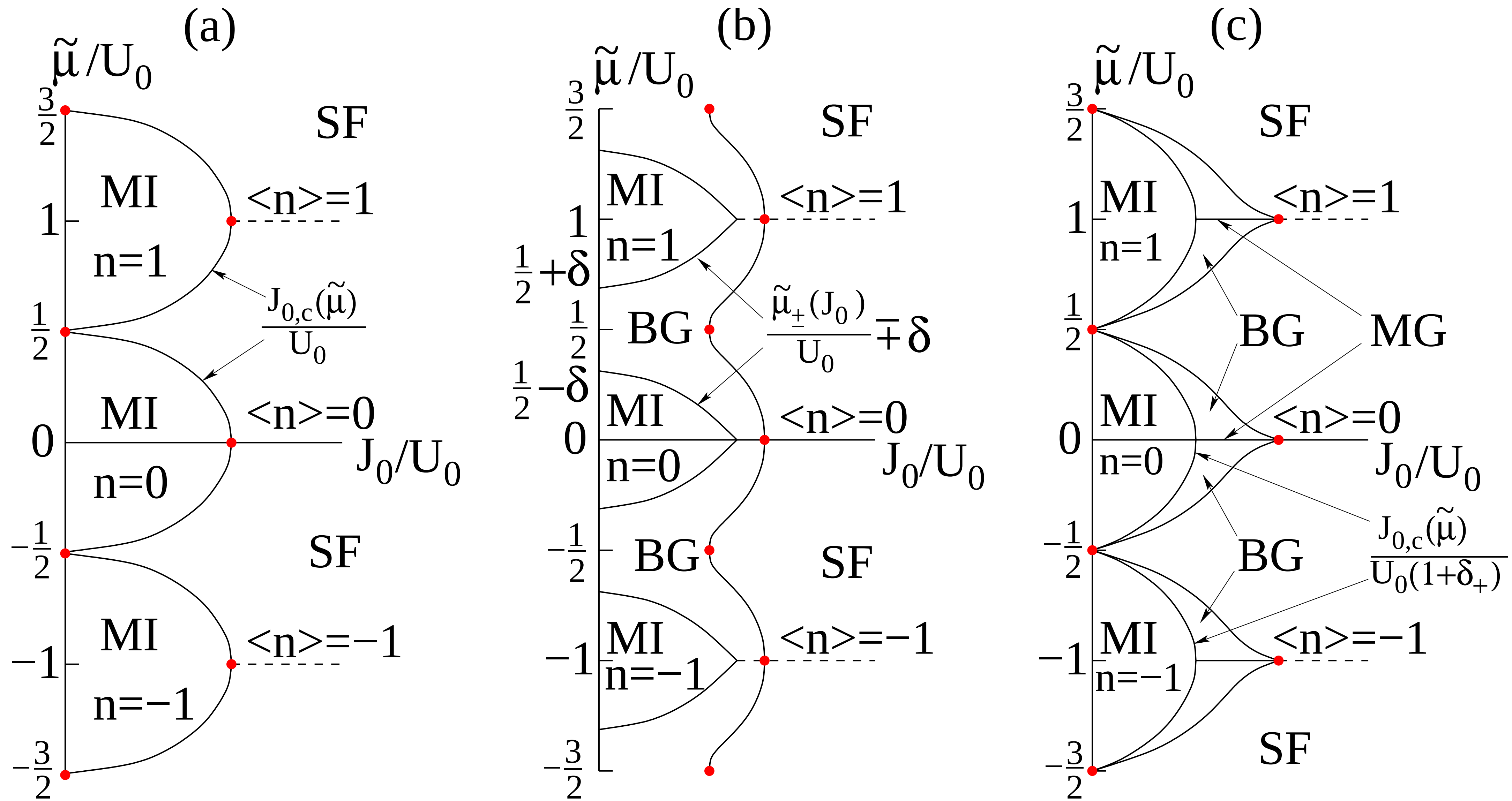
$$H = \frac{U}{2}\sum_i (\hat{n}_i - \bar{n}_i)^2 - \sum_{\langle i,j \rangle} J_{ij}(a_i^\dagger a_j + h.c.)$$

- 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 $k \gg 1$
  $\Rightarrow$ Hamiltonian **invariant** under $(\hat{n}_i - \bar{n}_i) \to -(\hat{n}_i - \bar{n}_i)$

Phase diagrams



clean **random potentials** **random couplings**

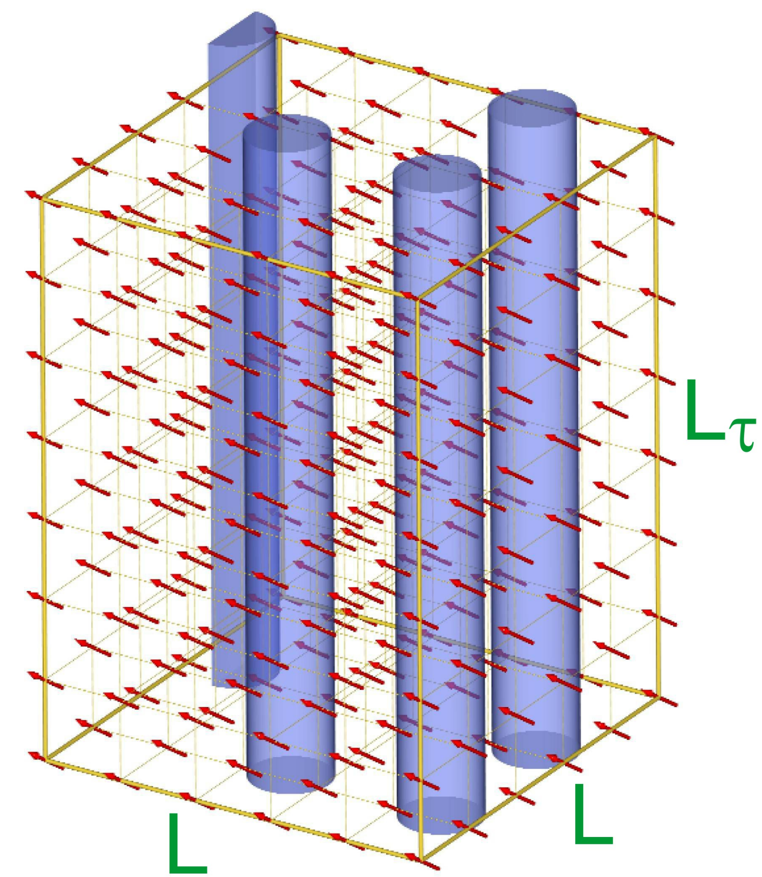
Weichman et al., Phys. Rev. B 7, 214516 (2008)

Monte Carlo simulations

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

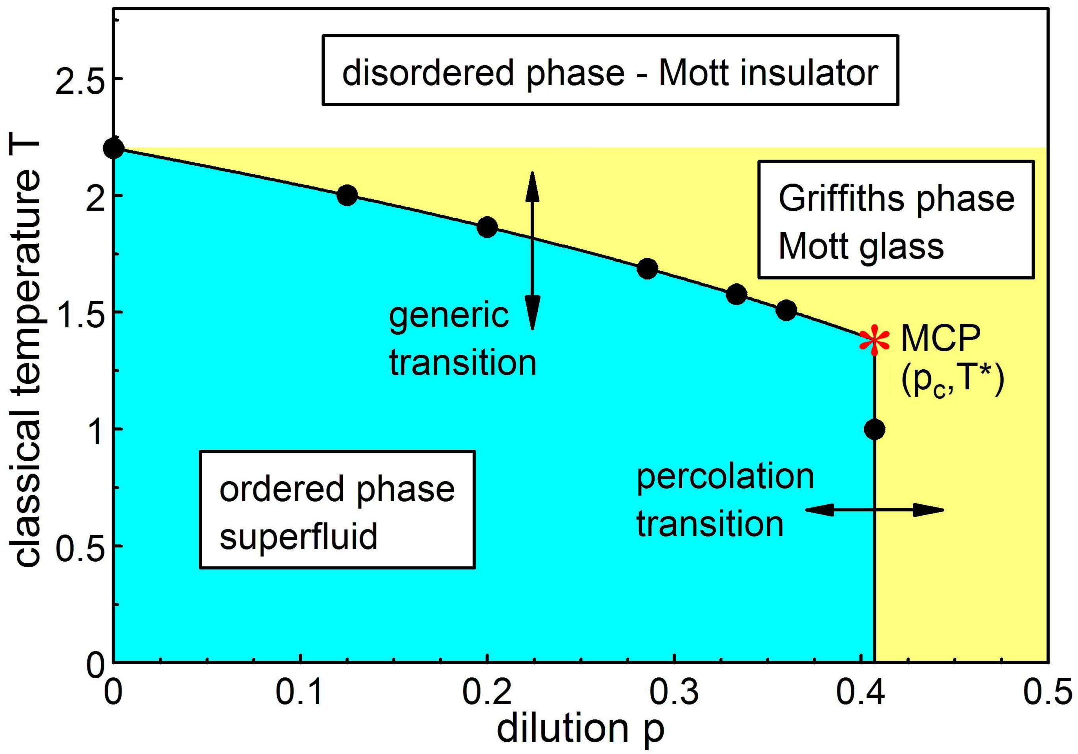
$$H_{\rm cl} = -J_\tau \sum_{i,t} \epsilon_i \mathbf{S}_{i,t} \cdot \mathbf{S}_{i,t+1} - J_s \sum_{\langle i,j \rangle, t} \epsilon_i \epsilon_j \mathbf{S}_{i,t} \cdot \mathbf{S}_{j,t}$$

- 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
- **ansiotropic** 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 ν exponents **fulfill** $d\nu > 2$
- Griffiths singularities **exponentially weak**
  (see J. Phys. A **39**, R143 (2006), PRL **112**, 075702 (2014))

(2+1)D exponents

exponent	clean	disordered
z	1	1.52
ν	0.6717	1.16
β/ν	0.518	0.48
γ/ν	1.96	2.52

PRB **94**, 134501 (2016)

(3+1)D exponents

exponent	clean	disordered
z	1	1.67
ν	0.5	0.90
β/ν	1	1.09
γ/ν	2	2.50

PRB **98**, 054514 (2018)

- Collective modes: Goldstone and amplitude (Higgs)
- Superfluid-Mott glass quantum phase transition
- **Fate of the collective modes at the superfluid-Mott glass transition**
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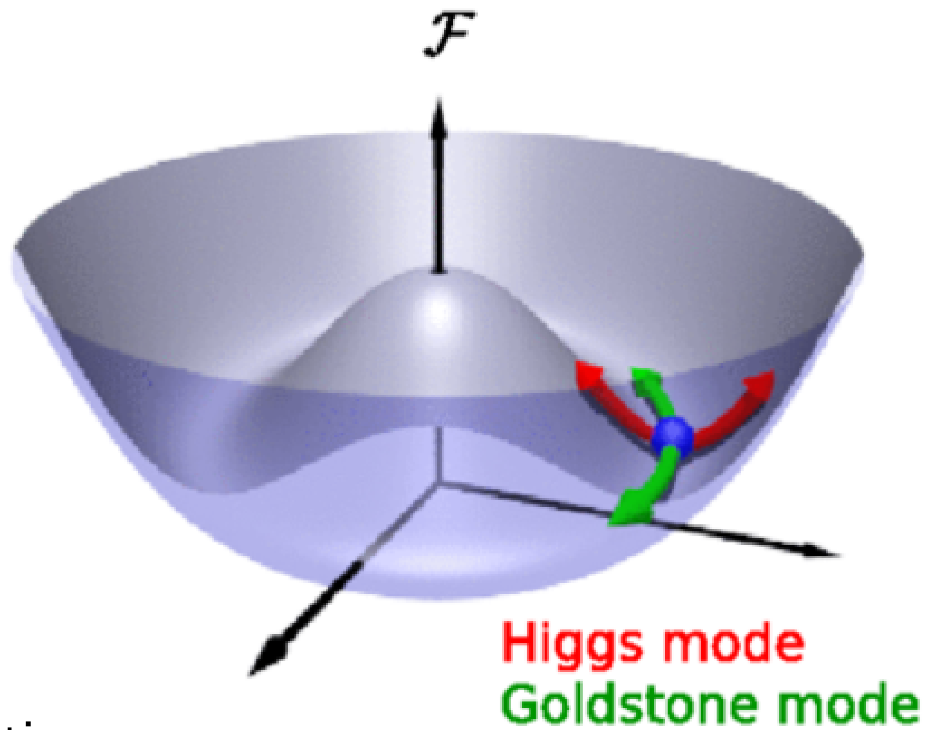
Amplitude mode: scalar susceptibility

- parameterize order parameter fluctuations into **amplitude** and **direction**

$$\vec{\phi} = \phi_0(1+\rho)\hat{\mathbf{n}}$$



- 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

$$\chi_{\rho\rho}(\vec{x},\tau) = \langle\rho(\vec{x},\tau)\rho(0,0)\rangle$$

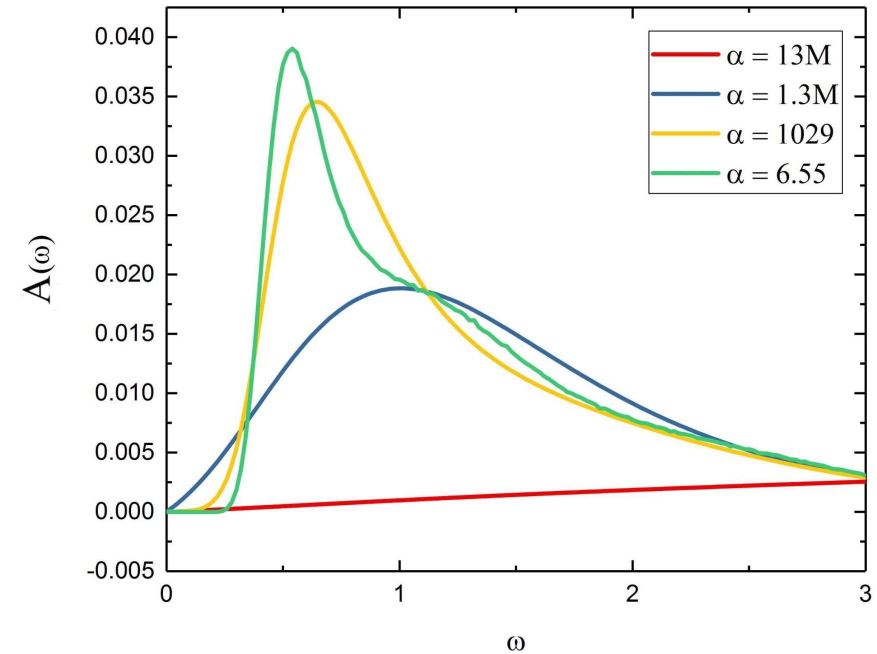
- **Wick rotation** required: analytical continuation from imaginary to real times/frequencies

  $\Rightarrow$ **maximum entropy method** to compute spectral function $A(\vec{q},\omega) = \chi''_{\rho\rho}(\vec{q},\omega)/\pi$

Analytic continuation - maximum entropy method

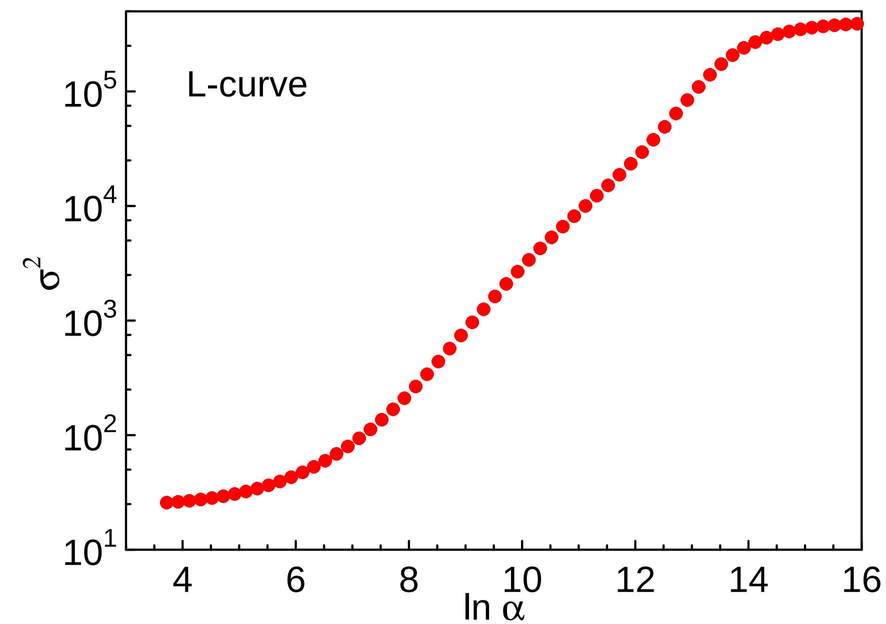
- **Matsubara susceptibility** vs. **spectral function**

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



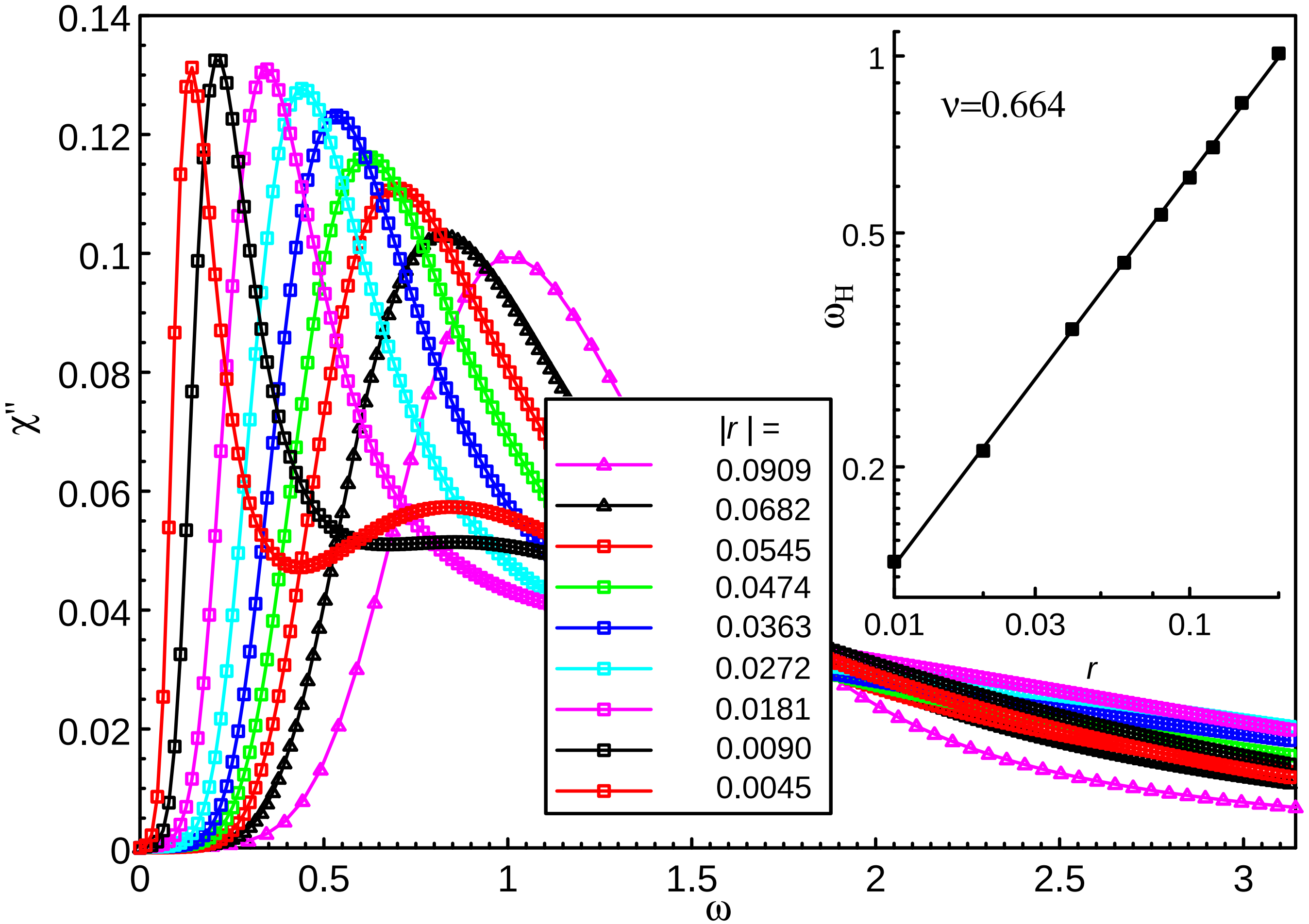
Maximum entropy method:

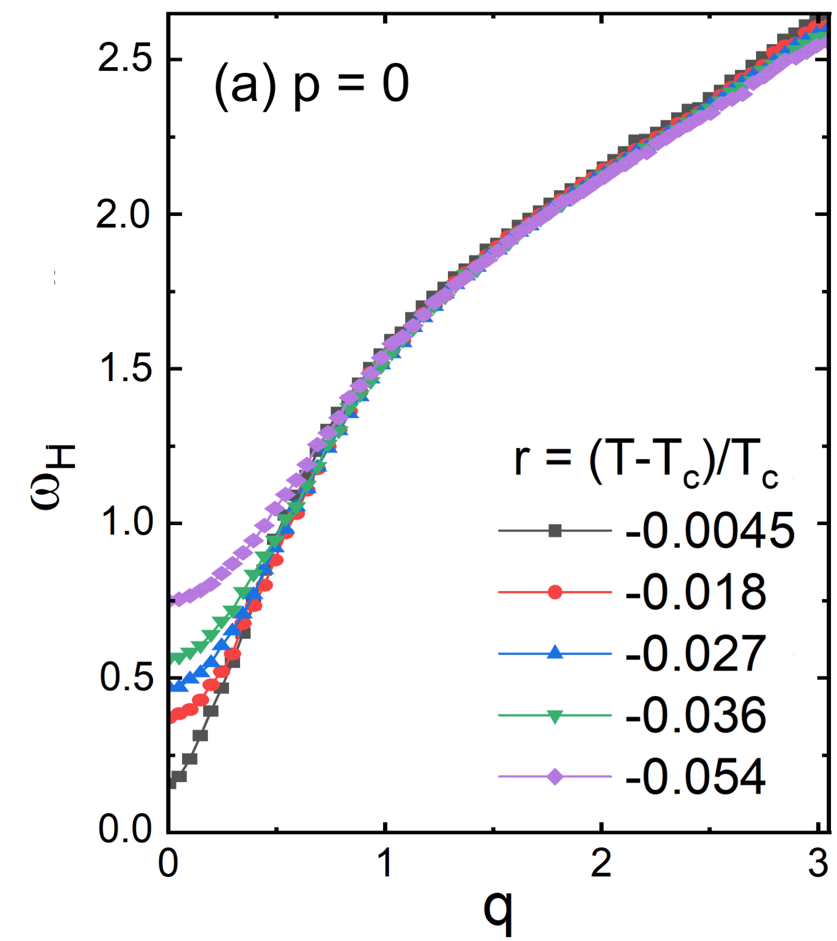
- inversion is ill-posed problem, highly sensitive to noise
- fit $A(\vec{q}, \omega)$ to $\chi_{\rho\rho}(\vec{q}, i\omega_m)$ MC data by minimizing
  $Q = \frac{1}{2}\sigma^2 - \alpha S$
- parameter α balances between fit error σ^2 and entropy S of $A(\vec{q}, \omega)$, i.e., between fitting information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



Amplitude mode in clean undiluted system

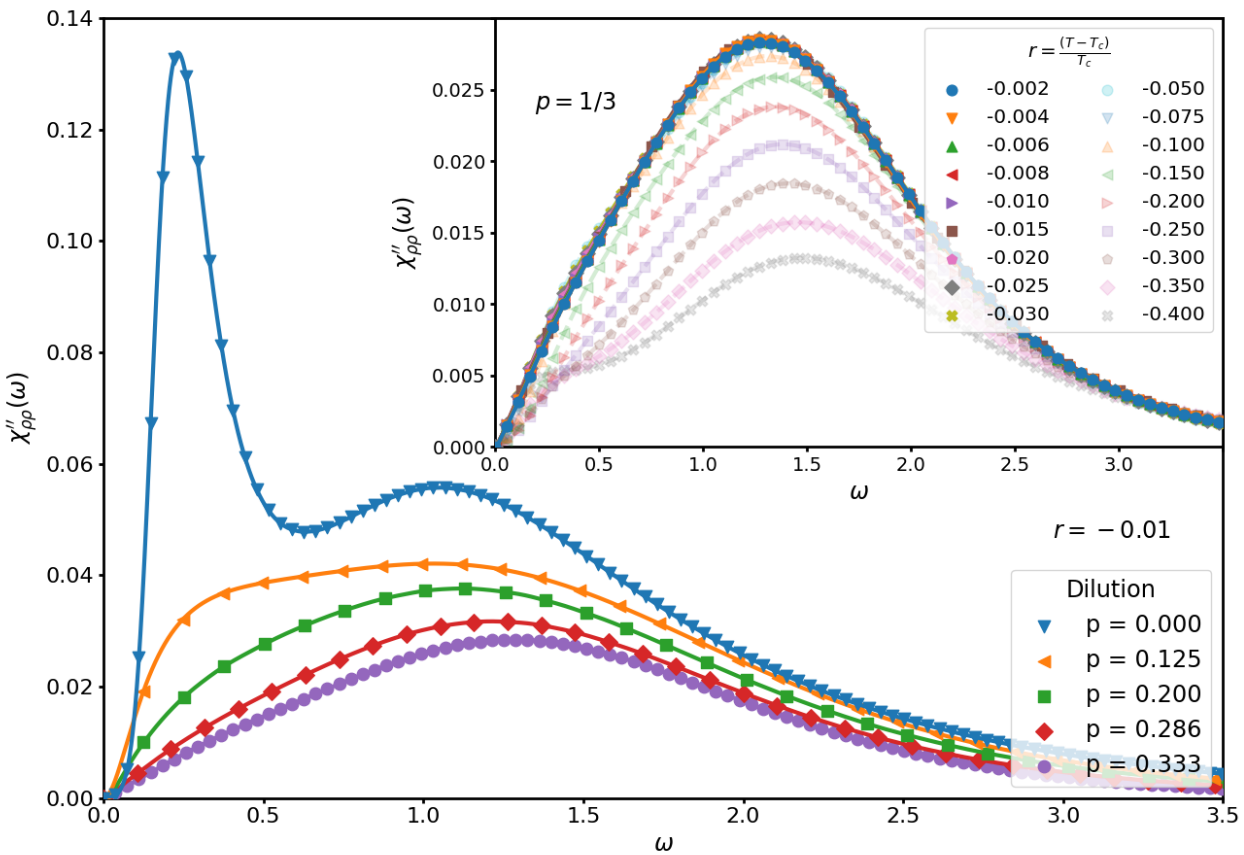
Scaling form (in 2d): $\chi_{\rho\rho}(0, \omega) = |r|^{3\nu-2} X(\omega |r|^{-\nu})$ [Podolsky + Sachdev, PRB 86, 054508 (2012)]

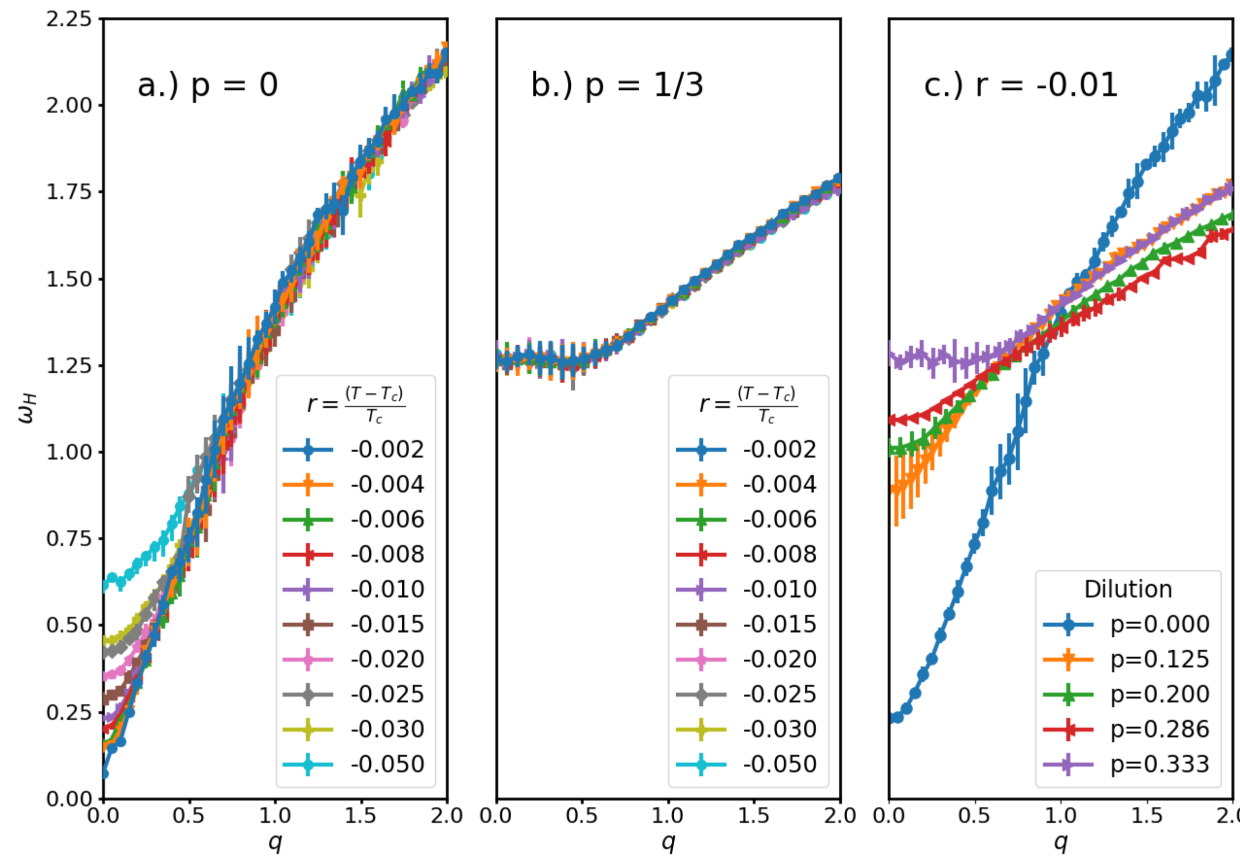




- sharp Higgs peak in spectral function
- Higgs energy (mass) ω_H scales as expected with distance from criticality r

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 $|\bar{n}-1\rangle$, $|\bar{n}\rangle$, and $|\bar{n}+1\rangle$ on each site

Variational wave function:

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

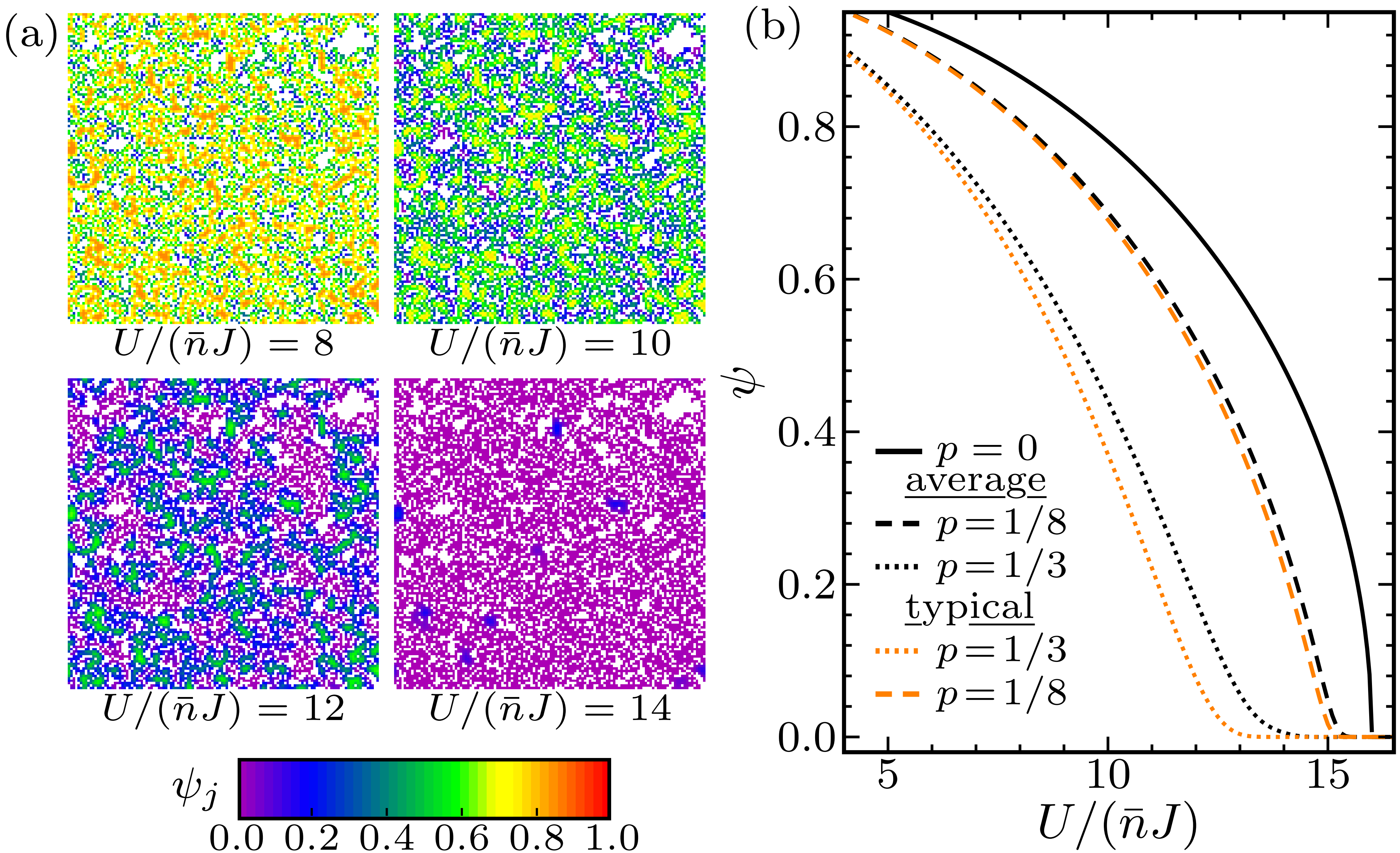
- locally interpolates between **Mott insulator,** $\theta = 0$, and **superfluid limit,** $\theta = \pi/2$

Mean-field energy:

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

- 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)

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

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

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

H_ϕ has similar structure but different coefficients

H_ϕ and H_θ can be solved by **Bogoliubov transformation**

Excitations in clean system

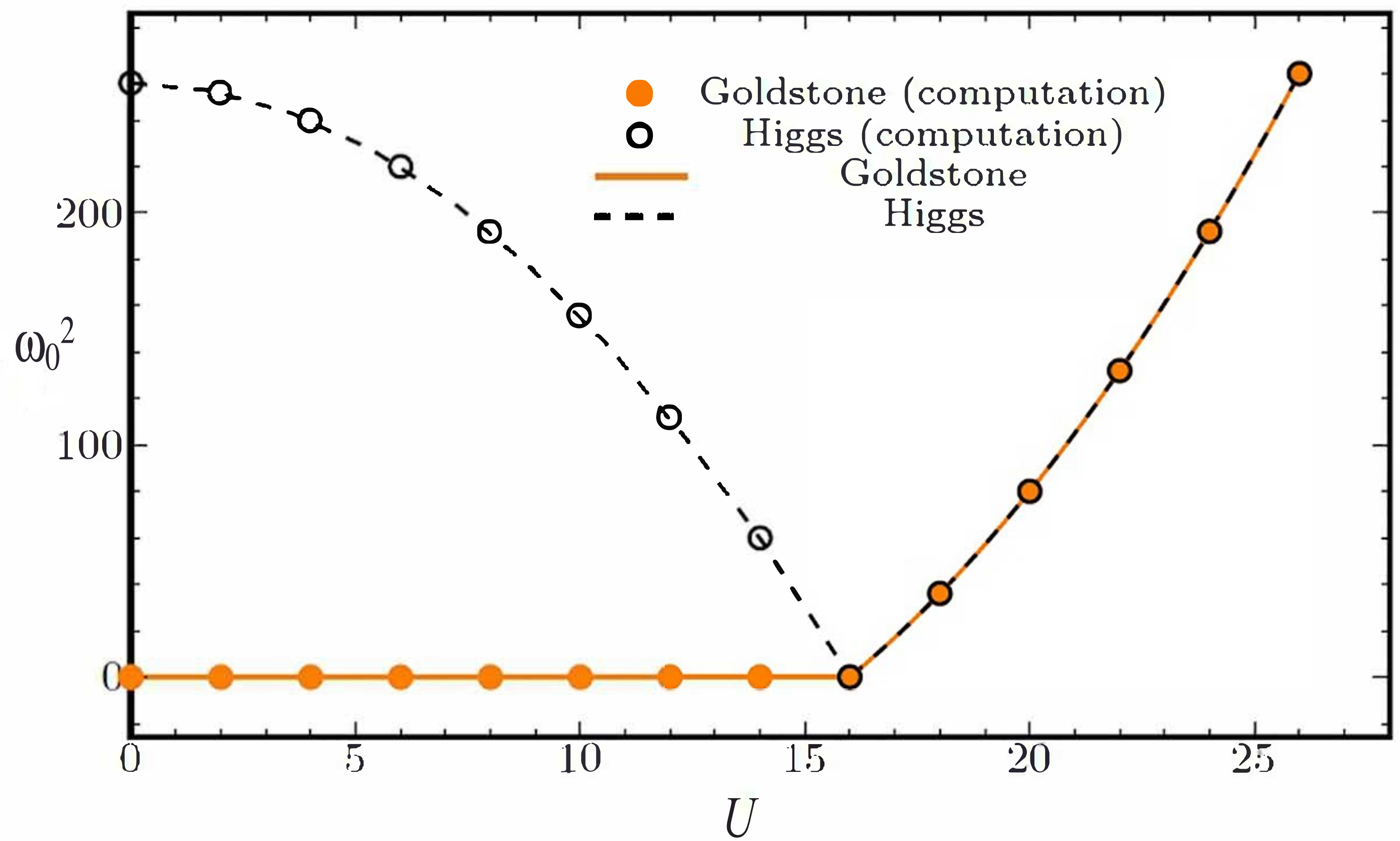
- mean-field quantum phase transition at $U = 16J$
- all excitations are spatially extended (plane waves)

Mott insulator

- all excitations are gapped

Superfluid

- Goldstone mode is gapless
- amplitude (Higgs) modes is gapped, gap vanishes at QCP



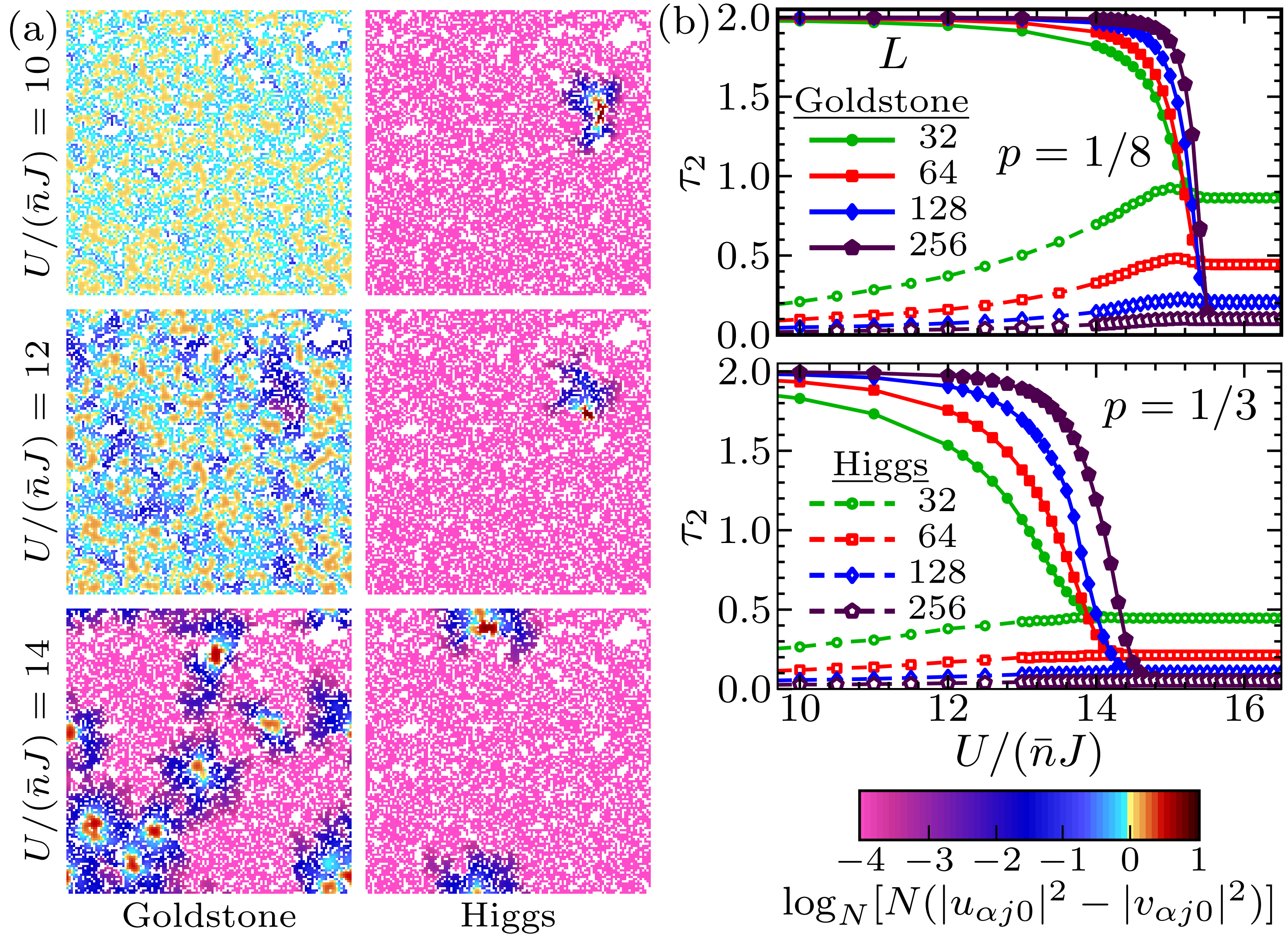
Excitations in diluted system

- 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

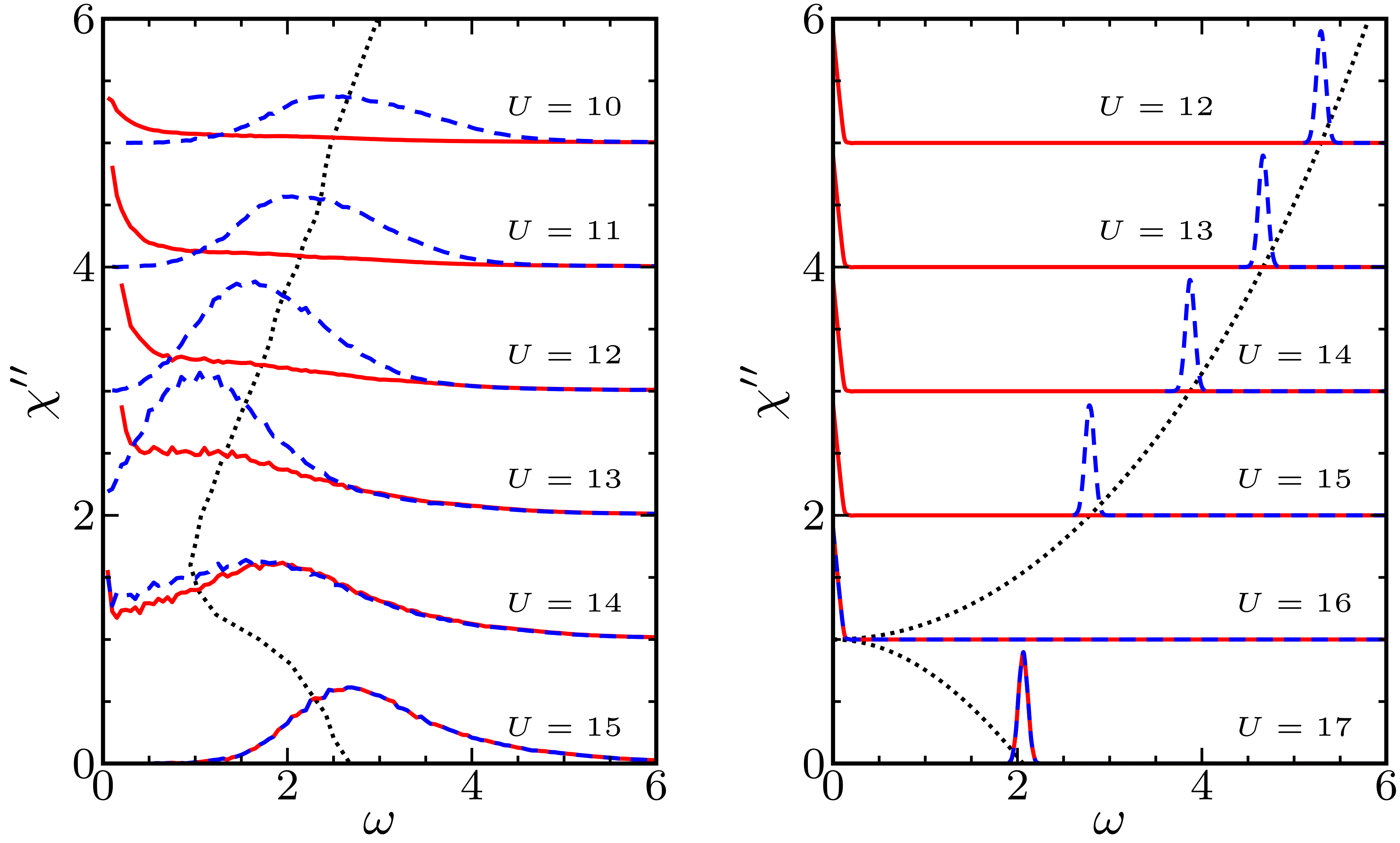
$$P^{-1}(0) = \sum_j (|u_{\alpha j0}|^2 - |v_{\alpha j0}|^2)^2$$

- generalized fractal dimension

$$\tau_2(0) = \ln P(0) / \ln L$$



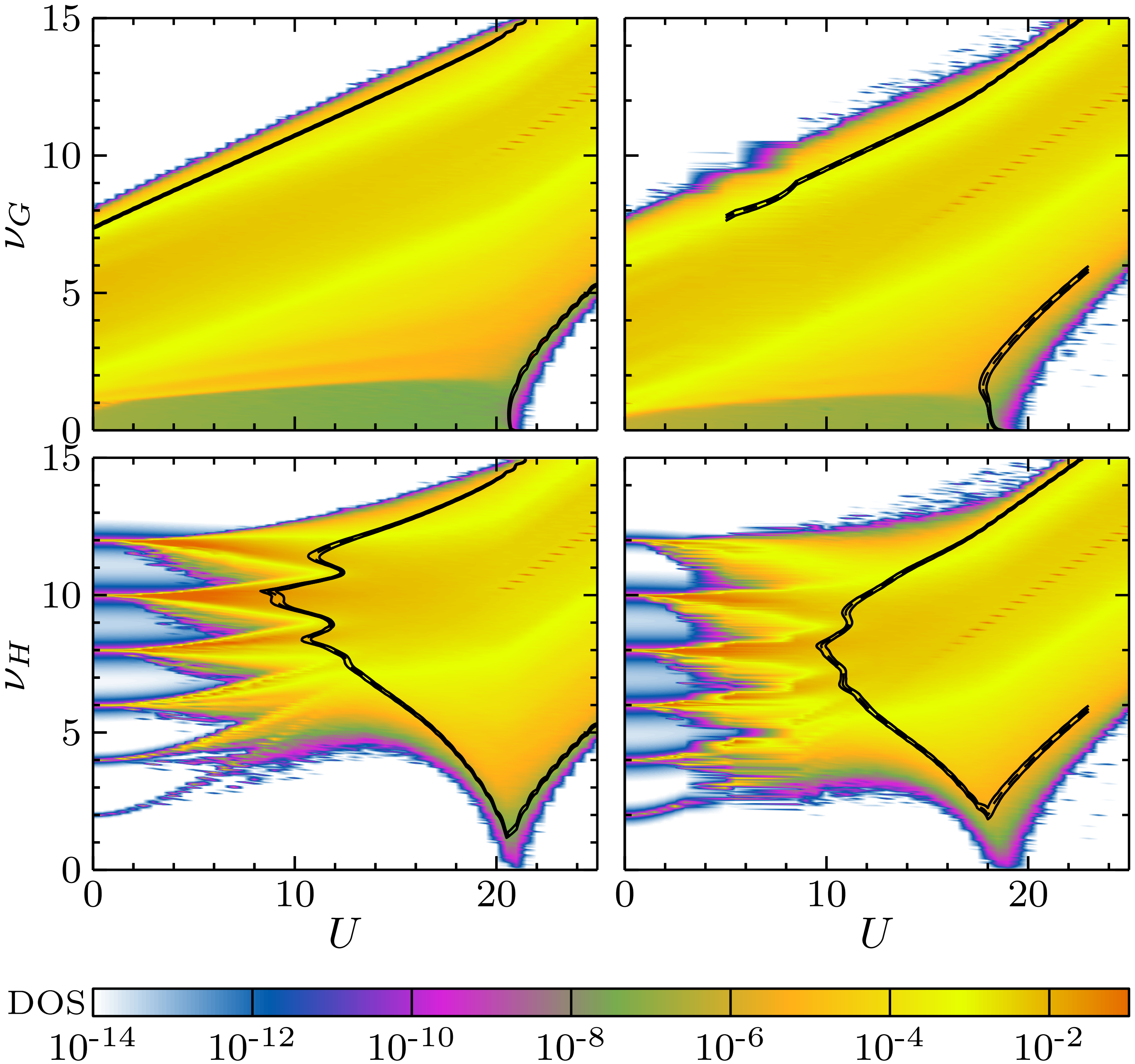
Longitudinal and transverse susceptibilities ($q = 0$)



diluted, $p = 1/3$

clean

Preview: Collective modes in $(3+1)$ dimensions



- inhomogeneous mean-field theory for 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

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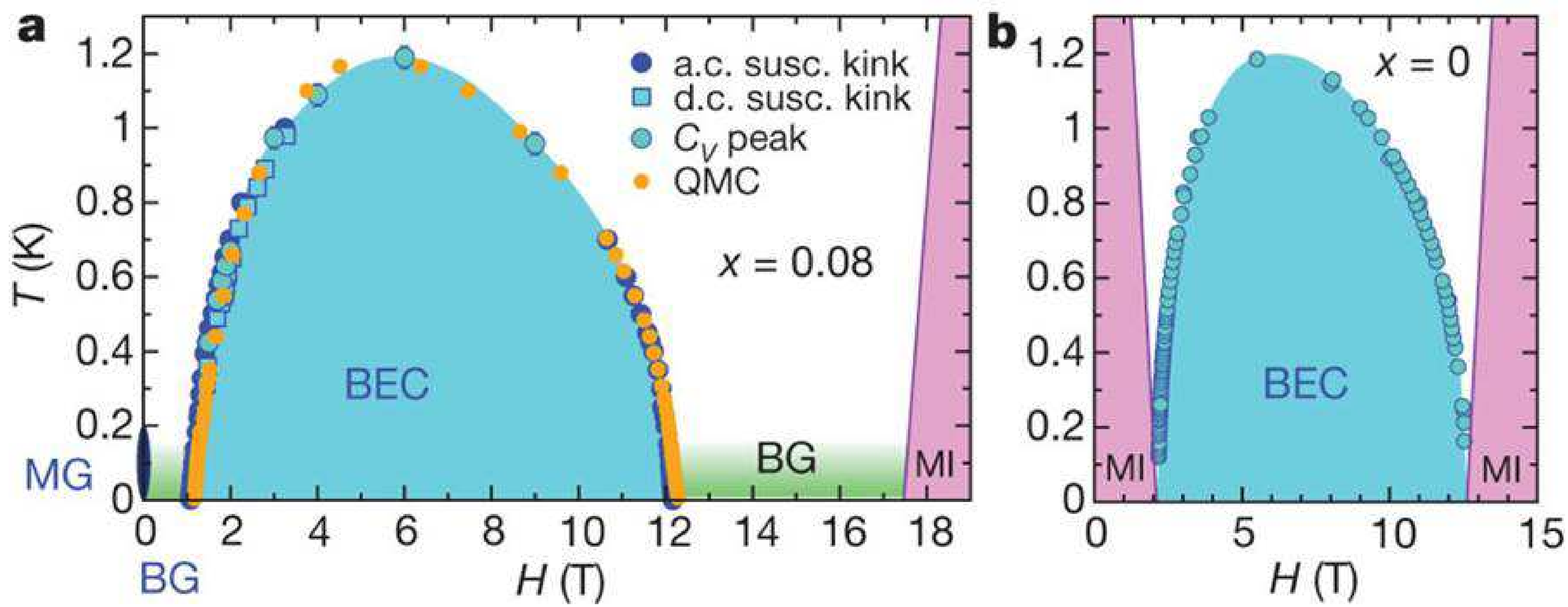
Thermodynamics: Phys. Rev. B **94**, 134501 (2016), Phys. Rev. B **98**, 054514 (2018)

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:



Yu et al., Nature 489, 379 (2012)

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

Stability of clean quantum critical point against dilution

Harris criterion:

A clean critical point is (perturbatively) stable against weak disorder if its correlation length exponent ν 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 ν **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

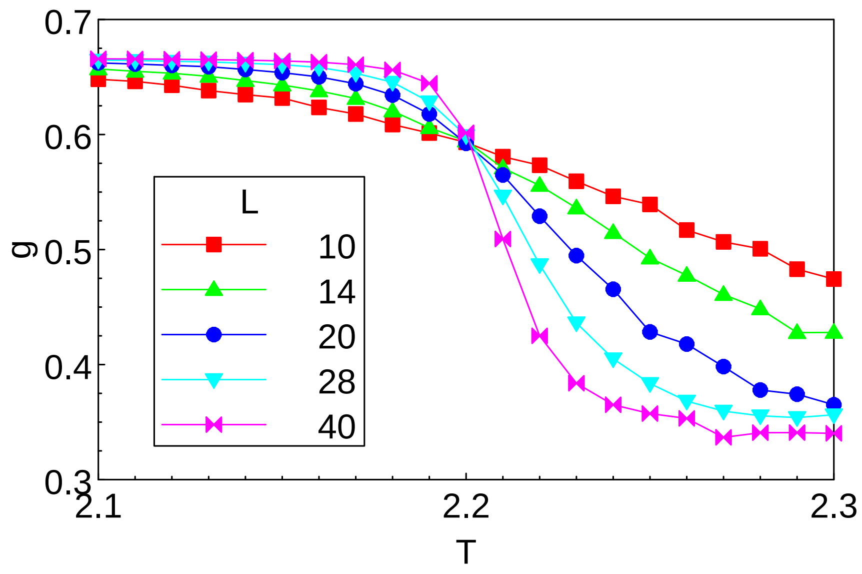
Finite-size scaling

Binder cumulant:

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

Isotropic systems:

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

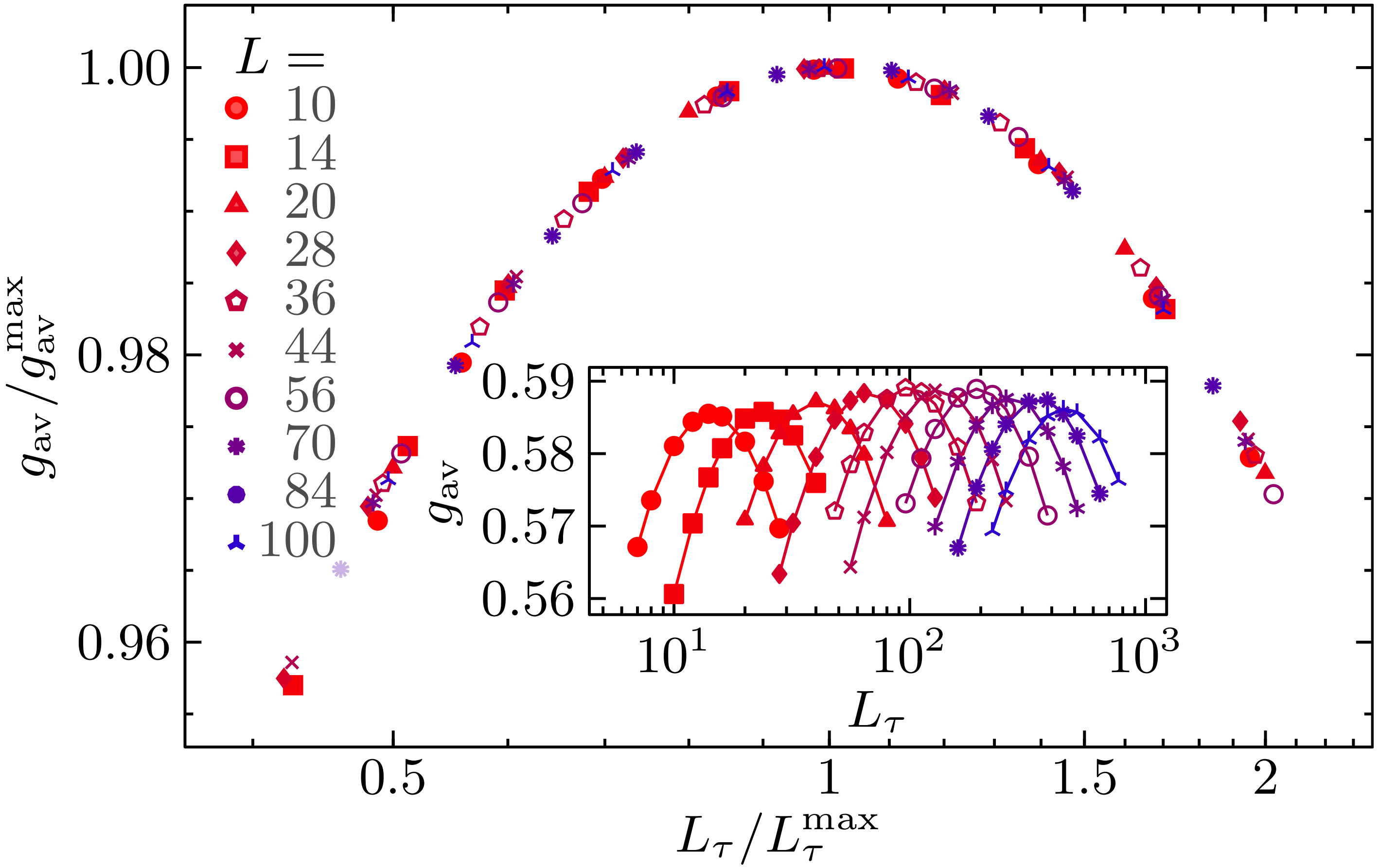


Anisotropic systems:

- L and L_τ are not equivalent, L_τ scales like $L_\tau \sim L^z$ (or even as $\ln L_\tau \sim L^\psi$)
- conventional scaling: $g_{\rm av}(r,L,L_\tau) = X(rL^{1/\nu}, L_\tau/L^z)$

  activated scaling: $g_{\rm av}(r,L,L_\tau) = X(rL^{1/\nu}, \ln(L_\tau)/L^\psi)$
- How to choose correct sample shapes if dynamical exponent z (or tunneling exponent ψ) is not known?

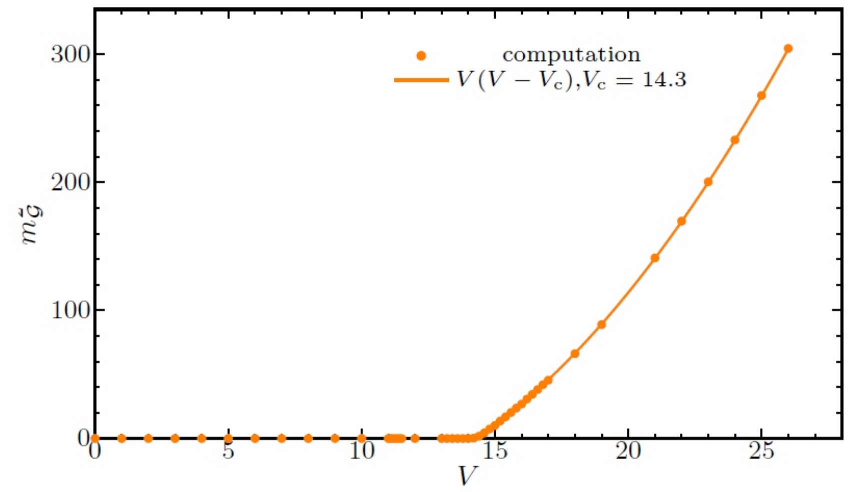
Anisotropic finite-size scaling



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

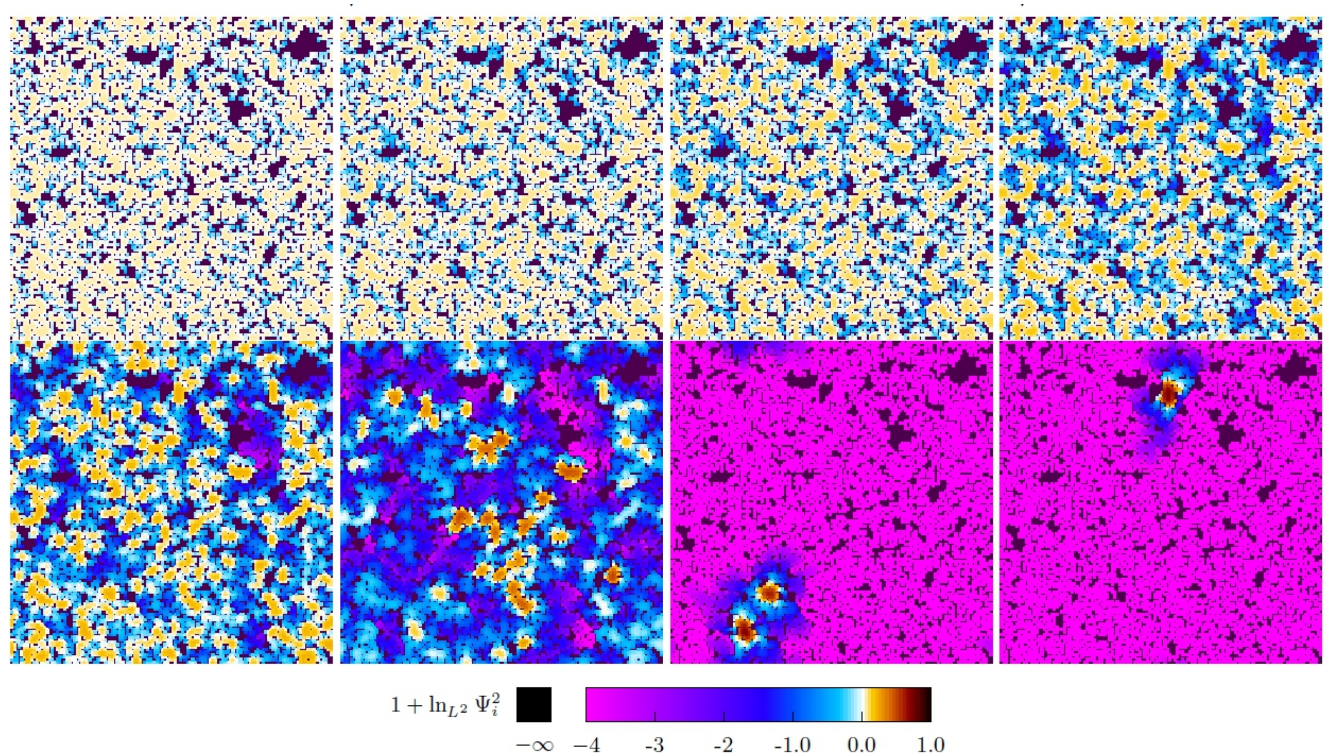
Diluted lattice: Goldstone mode

- 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

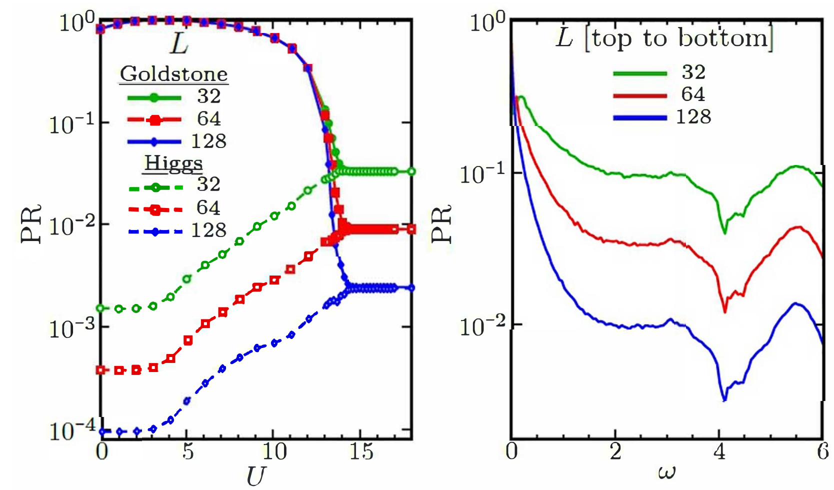


Goldstone mode: localization properties

- inverse participation ratio:

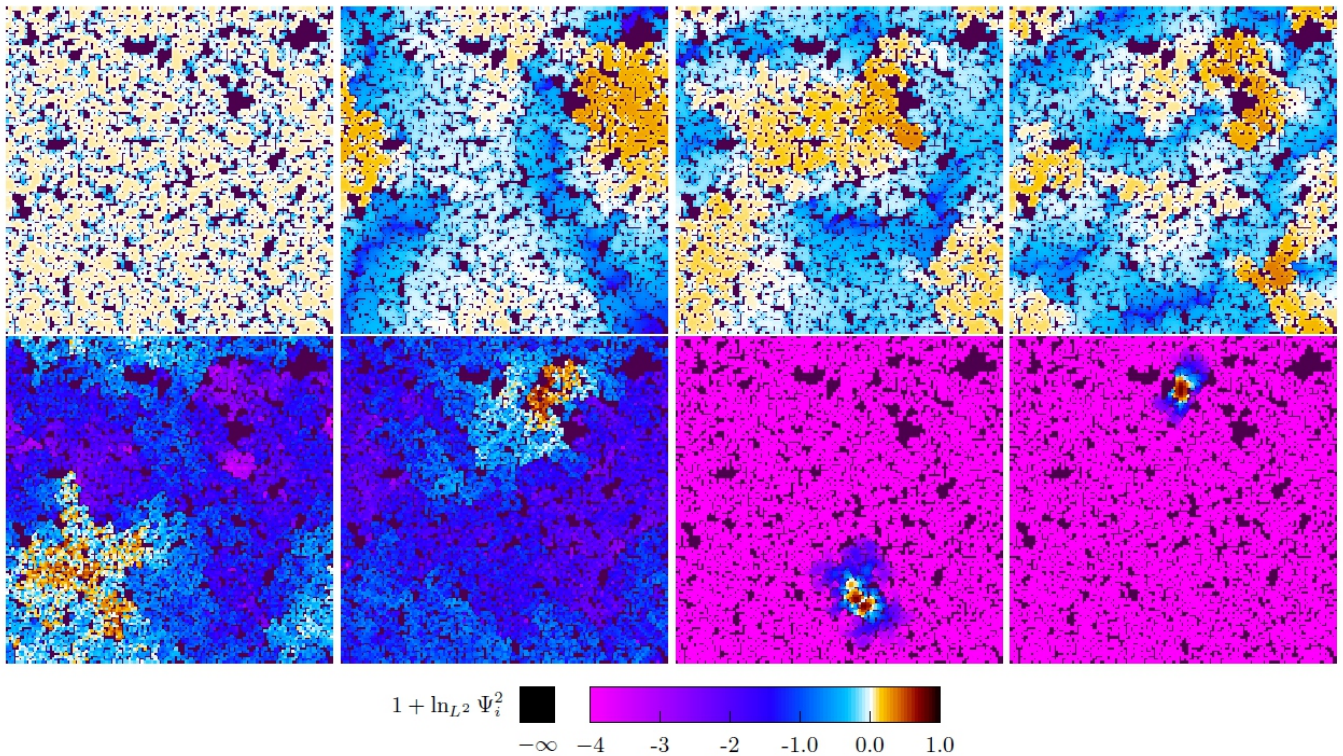
$$P^{-1} = N \sum_i |\psi_i|^4$$

$P \to 1$ for delocalized states
$P \to 0$ for localized states



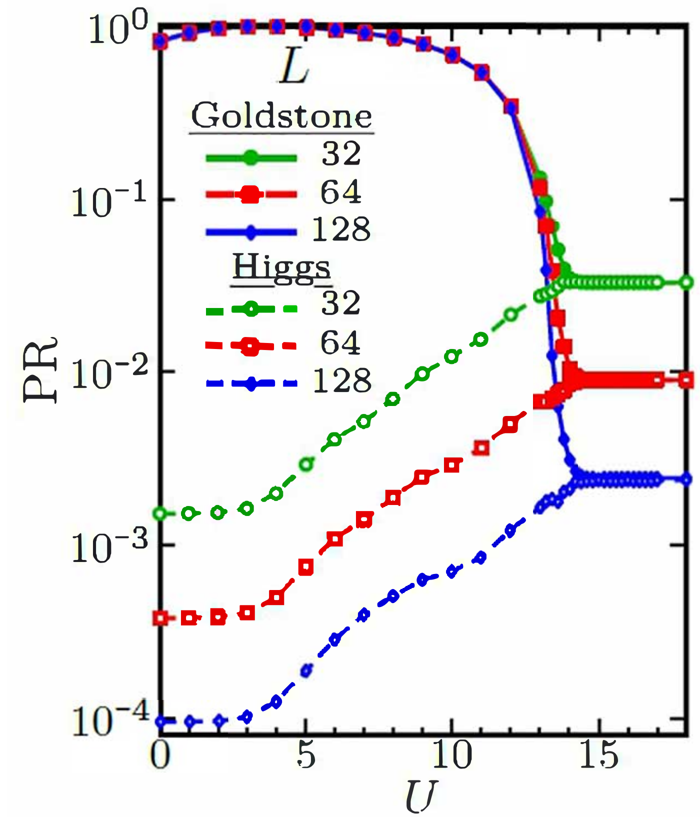
- wave function at $U = 8$ as function of excitation energy

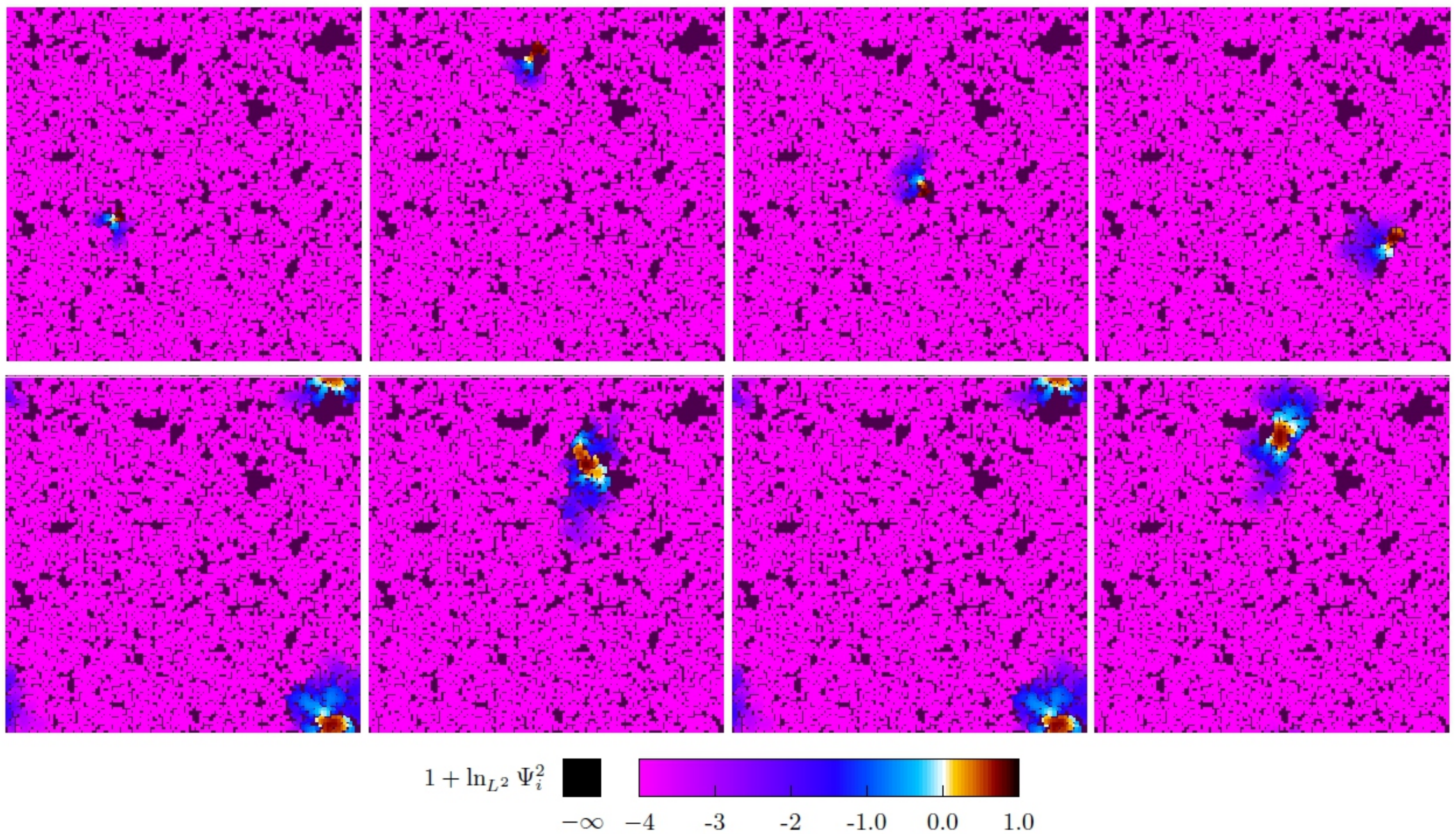
- delocalized at $\omega = 0$, localized for higher energies



Amplitude (Higgs) mode

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





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