Collective excitations in competing phases in two and three dimensions

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Introduction

- Study of collective behavior of many particles rather than individual ones
- Complex interplay of various degrees of freedom
- Governs many structural, magnetic, and electronic phenomena

Phases of interest

- s-wave superconductivity (SC), charge-density wave (CDW), and antiferromagnetism (AFM)
- Nesting vectors (lattice constant = 1): $\vec{Q} = (\pi, \pi)$ (square lattice), $\vec{Q} = (\pi, \pi, \pi)$ (sc lattice)

Observables of excitations of interest

- (CDW) Exciton: $1/N \sum_k \left(g_{\vec{k}\uparrow} + g_{\vec{k}\downarrow}\right)$
- (AFM) Longitudinal magnon: $1/N \sum_k \left(g_{\vec{k}\uparrow} - g_{\vec{k}\downarrow}\right)$
- (AFM) Transversal magnon: $1/N \sum_k \left(\tau_{\vec{k}} + \tau_{\vec{k}}^\dagger\right)$
- (SC) Amplitude (Higgs) mode: $1/N \sum_k \left(f_{\vec{k}} + f_{\vec{k}}^\dagger\right)$
- (SC) Phase (Anderson-Bogoliubov) mode: $\mathrm{i}/N \sum_k \left(f_{\vec{k}} - f_{\vec{k}}^\dagger\right)$

Abbreviations

$$n_{k\sigma} := c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma}$$
$$f_k := c_{-\vec{k}\downarrow} c_{\vec{k}\uparrow}$$
$$g_{k\sigma} := c_{\vec{k}\sigma}^\dagger c_{\vec{k}+\vec{Q}\sigma}$$
$$\tau_k := c_{\vec{k}\uparrow}^\dagger c_{\vec{k}\downarrow}$$

Model

Hamiltonian: Extended Hubbard model

$$H = -t \sum_{\langle i,j\rangle,\sigma} \left(c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}\right) + \mu \sum_{i,\sigma} n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \frac{V}{2} \sum_{\langle i,j\rangle,\sigma} n_{i\sigma} n_{j\sigma}\,,$$

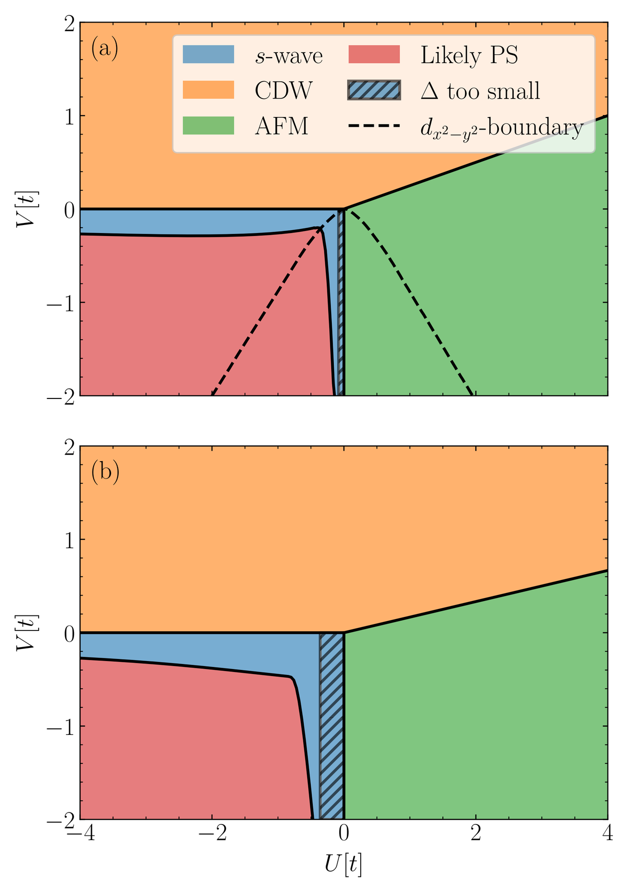
- Half-filling, on both a square and a simple cubic lattice, temperature $T = 0$
- A simple model exhibiting a rich phase diagram

Static mean-field theory

- Used to deal with the interaction terms and to obtain expectation values for iEoM
- Terms depend on $\hat{\gamma}(\vec{k}) := \frac{1}{D} \sum_{\alpha=1}^{D} \cos(k_\alpha)$
  $\Rightarrow$ density of states $\rho(\gamma) := \frac{1}{N} \sum_{\vec{k}} \delta(\gamma - \hat{\gamma}(\vec{k}))$

$$\Delta_{\text{CDW}} = \left(\frac{U}{2N} - \frac{zV}{N}\right) \sum_\sigma \int \rho(\gamma) \langle g_\sigma(\gamma) \rangle \mathrm{d}\gamma$$
$$\Delta_{\text{SC}} = \frac{U}{N} \int \rho(\gamma) \langle f(\gamma) \rangle \mathrm{d}\gamma$$
$$\Delta_{\text{AFM}} = \frac{U}{2N} \int \rho(\gamma) \left(\langle g_\uparrow(\gamma) \rangle - \langle g_\downarrow(\gamma) \rangle\right) \mathrm{d}\gamma$$
$$\Delta_n = \frac{V}{N} \sum_\sigma \int \rho(\gamma) \gamma \langle n_\sigma(\gamma) \rangle \mathrm{d}\gamma$$

- Allows us to tackle both 2D and 3D systems



Mean-field phase diagram of the extended Hubbard model at $T = 0$. (a) Square lattice (b) simple cubic lattice. $d_{x^2-y^2}$ from Ref. [3].

Phase diagram

- Mostly the same for both lattices, $d_{x^2-y^2}$-wave SC for $V < 0$ on the square lattice is inaccessible to us
- Red region: Mean-field self-consistency converges to s-wave SC, but $\mathcal{M}$ is not nonnegative $\Rightarrow$ not the true groundstate. Literature suggests a phase-separated state. [4]
- Striped region: Inaccuracies due to finite discretization dominate; here the gap is of the same order of magnitude as our gap

Method: Iterated equations of motion (iEoM)

Key ideas [1, 2]

- Objective: capture collective excitations
- Consider a time-dependent operator $\hat{a}(t) = \sum_j c_j(t) \hat{A}_j$ and the symplectic product $(\hat{A}|\hat{B}) := \langle [\hat{A}^\dagger, \hat{B}] \rangle$
- Write the Heisenberg EoM as matrix-vector EoM (w.r.t. to full interaction Hamiltonian)

$$\frac{\mathrm{d}}{\mathrm{d}t} \hat{a}(t) = \sum_j \frac{\mathrm{d}}{\mathrm{d}t} c_j(t) \hat{A}_j = \mathrm{i} \sum_j c_j(t) [H, \hat{A}_j]$$
$$\Rightarrow \sum_j \underbrace{(\hat{A}_i|\hat{A}_j)}_{:=\mathcal{N}_{ij}} \frac{\mathrm{d}}{\mathrm{d}t} c_j(t) = \mathrm{i} \sum_j \underbrace{(\hat{A}_i|[\hat{H}, \hat{A}_j])}_{:=\mathcal{M}_{ij}} c_j(t)$$
$$\Rightarrow \mathcal{N} \frac{\mathrm{d}}{\mathrm{d}t} \vec{c}(t) = \mathrm{i} \mathcal{M} \vec{c}(t)\,.$$

- Generalized eigenvalue problem $\omega \mathcal{N} \vec{v} = \mathcal{M} \vec{v}$, real solutions if either $\mathcal{M}$ or $\mathcal{N}$ is nonnegative.
  $\to \mathcal{M}$ is nonnegative is thermal equilibrium

Green's functions

- Elements of the matrix $\mathcal{G}(\omega) := \mathcal{N}[-(\omega + \mathrm{i}0^+)\mathcal{N} - \mathcal{M}]^{-1} \mathcal{N}$ are Fourier-transformed Green's functions
- Specifically

$$\mathcal{G}_{ij}(\omega) = G_{\hat{A}_i \hat{A}_j^\dagger}(\omega) = -\mathrm{i} \int_0^\infty \langle [A_i(t), A_j^\dagger(0)] \rangle e^{\mathrm{i}(\omega + \mathrm{i}0^+)t} \mathrm{d}t$$

- The matrices $\mathcal{N}$ and $\mathcal{M}$, and therefore also $\mathcal{G}(\omega)$, exhibit a block structure
- Lengthy calculations yield a quadratic form for the two blocks, denoted $|_X$ and $|_P$

$$\mathcal{G}(z = \omega + \mathrm{i}0^+) = \mathcal{N} \frac{1}{-z\mathcal{N} - \mathcal{M}} \mathcal{N}$$
$$\to \mathcal{G}|_X(z) = -\mathcal{L}^\dagger \tilde{N}_X^{-1/2} \frac{1}{z^2 - \tilde{M}_X} \tilde{N}_X^{-1/2} \mathcal{L}, \qquad \mathcal{G}|_P(z) = -\mathcal{L} \tilde{N}_P^{-1/2} \frac{1}{z^2 - \tilde{M}_P} \tilde{N}_P^{-1/2} \mathcal{L}^\dagger$$

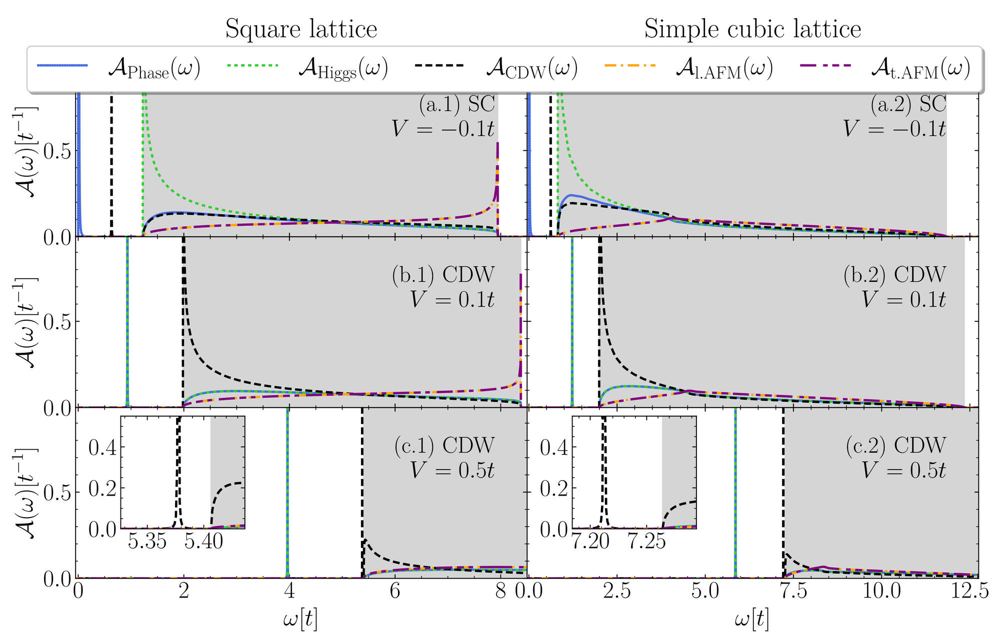
- Matrix inverse by tridiagonalization and subsequent continued fraction expansion with square-root terminator

Possible outlook

- Incorporating phase-separated states into the mean-field theory
  - thereby providing deeper analysis of the negative V regime of phase diagrams and collective excitations
- Coupling the electronic system to the electromagnetic field to include the Anderson-Higgs mechanism for superconductors
- Incorporating different fillings
- Describing multi-band systems with even richer phases and collective excitations

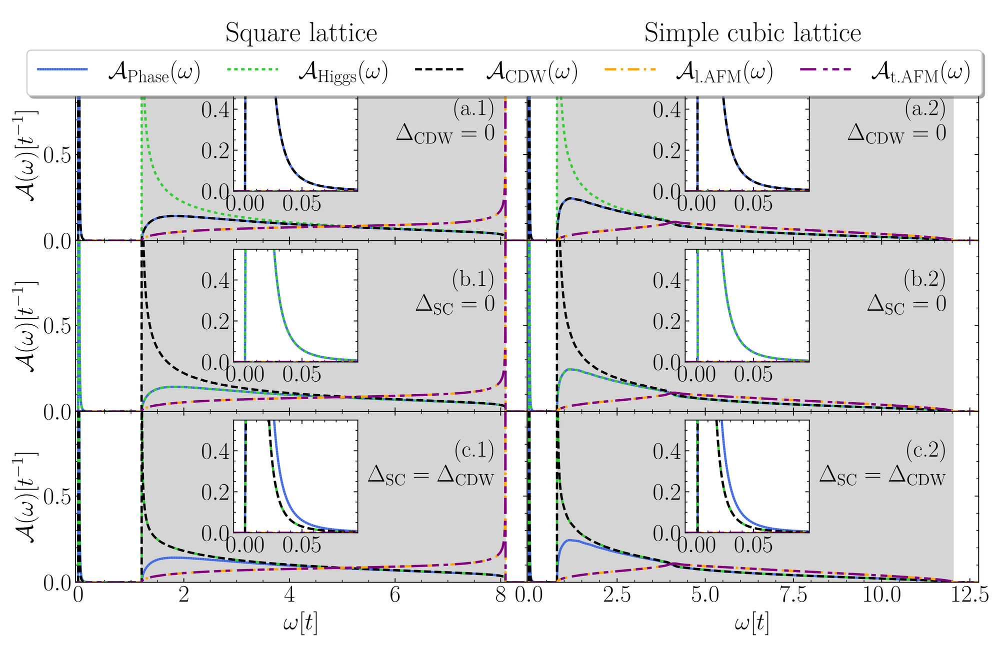
Spectral functions

Close to SC-CDW phase transition



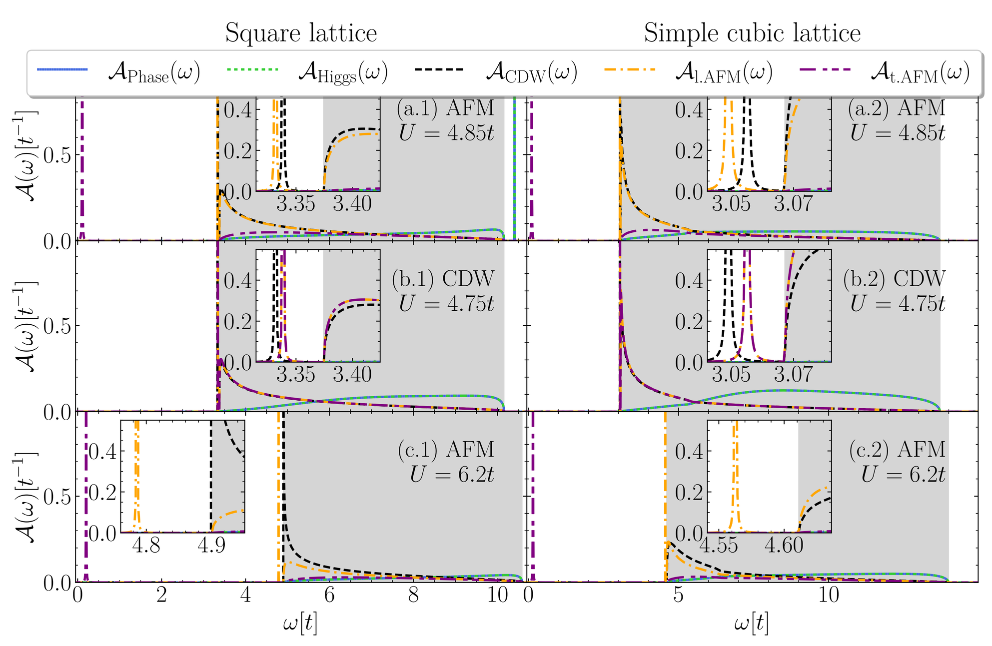
- $U = -2.5t$
- SC phase:
  - Peak at 0: Anderson-Bogoliubov mode, $\propto \delta'(\omega)$
  - Singularity at 2Δ: Higgs mode, $\propto 1/\sqrt{\omega - 2\Delta}$
  - CDW spectral function has a peak below the two-particle continuum
- CDW phase:
  - Phase and amplitude SC spectral functions are identical
  - Both have a peak below the two-particle continuum
  - For moderate V: singularity in the CDW spectral function, $\propto 1/\sqrt{\omega - 2\Delta}$
  - For larger V: peak below the continuum

CDW-SC coexistence at $V = 0$



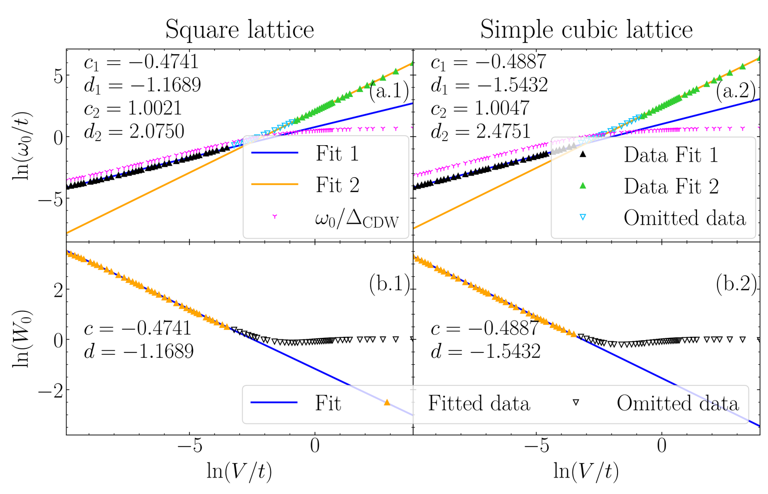
- Coexistence is the result of an SO(4) symmetry of the Hubbard model at half-filling [5]
- The ratio $\Delta_{\text{CDW}}/\Delta_{\text{SC}}$ may be chosen arbitrarily as long as $\Delta_{\text{tot}} := \sqrt{\Delta_{\text{CDW}}^2 + \Delta_{\text{SC}}^2} = \text{const}$
- Anderson-Bogoliubov mode always exits
- For $\Delta_{\text{CDW}} = 0$, the Higgs mode exists at $\omega = 2\Delta_{\text{tot}}$, while the CDW spectral function has a peak at $\omega = 0$
- The reverse applies for $\Delta_{\text{SC}} = 0$
- $\Delta_{\text{CDW}} = \Delta_{\text{SC}}$ yields a mixture of the two

Close to AFM-CDW phase transition

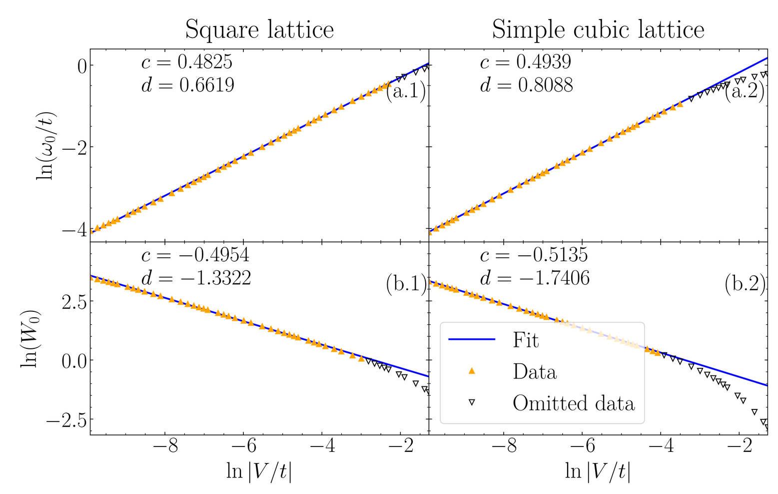


- $V = 1.2t$ (square lattice) and $V = 0.8t$ (simple cubic lattice) $\Rightarrow$ phase transition at $U = 4.8t$
- AFM phase: Transversal AFM spectral function has a peak at 0
- Longitudinal AFM spectral function behaves just like the CDW spectral function
- Close to the phase transition: Both have a peak below the continuum
- Further away: Only the spectral function corresponding to the phase has a peak below the continuum

Behavior of the peaks

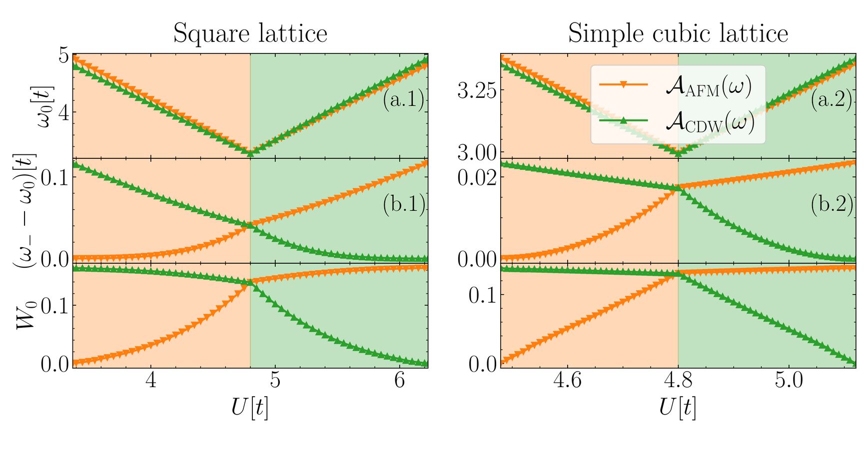


Weight and position of the peak in the SC spectral functions in the CDW phase.



Weight and position of the peak in the CDW spectral functions in the SC phase.

- Double-logarithmic plots $\Rightarrow y(V) = e^d |V|^c$
- The weights diverge as $1/\sqrt{|V|}$ while the peak positions move to 0 as $\sqrt{|V|}$
- For $V \gg t$, the weights become constant. The position grows linearly and the position in units of the gap becomes constant.



Weight and position of the peak in the AFM and CDW spectral functions close to the phase transition.

- Orange shading: System is in the CDW phase, green shading: System is in the AFM phase
- Peak position grows linearly with U as the system moves away from the phase transition
- But it moves into the continuum (b) quadratically
- At the same time, the weights also vanish

References

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