

Title: Amplitude mode of the d-density wave state and its relevance to high-Tc cuprates

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Abstract: We study the spectrum of the amplitude mode, the analog of the Higgs mode in high energy physics, for the d-density wave (DDW) state proposed to describe the anomalous phenomenology of the pseudogap phase of the high Tc cuprates. Even though the state breaks translational symmetry by a lattice spacing and is described by a particle-hole singlet order parameter at the wave vector $q = Q = (\pi, \pi)$, remarkably, we find that the amplitude mode spectrum can have peaks at both $q = (0, 0)$ and $q = Q = (\pi, \pi)$. In general, the spectra is non-universal, and, depending on the microscopic parameters, can have one or two peaks in the Brillouin zone, signifying confluence of two kinds of magnetic excitations. In light of the recent unexpected observations of multiple magnetic excitations in the pseudogap phase our theory sheds important light on how multiple inelastic neutron peaks at different wave vectors can arise even with an order parameter that condenses at $Q = (\pi, \pi)$.

[Reference: arXiv:1207.6834]

Amplitude mode of the d -density wave state and its relevance to high- T_c cuprates

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Collaborators: **Sudip Chakravarty, Jay D. Sau and Sumanta Tewari**



Participants

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Introduction

- Even after more than 25 years of intensive efforts, normal state properties of the cuprate high- T_c superconductors in the intermediate range of hole doping continue to pose theoretical challenges.
- In this underdoped regime, the system evinces a gap in the spectrum of unidentified origin (pseudogap) below a temperature $T^* > T_c$.
- An understanding of the pseudogap phase is believed to hold the key to the high T_c in cuprates.

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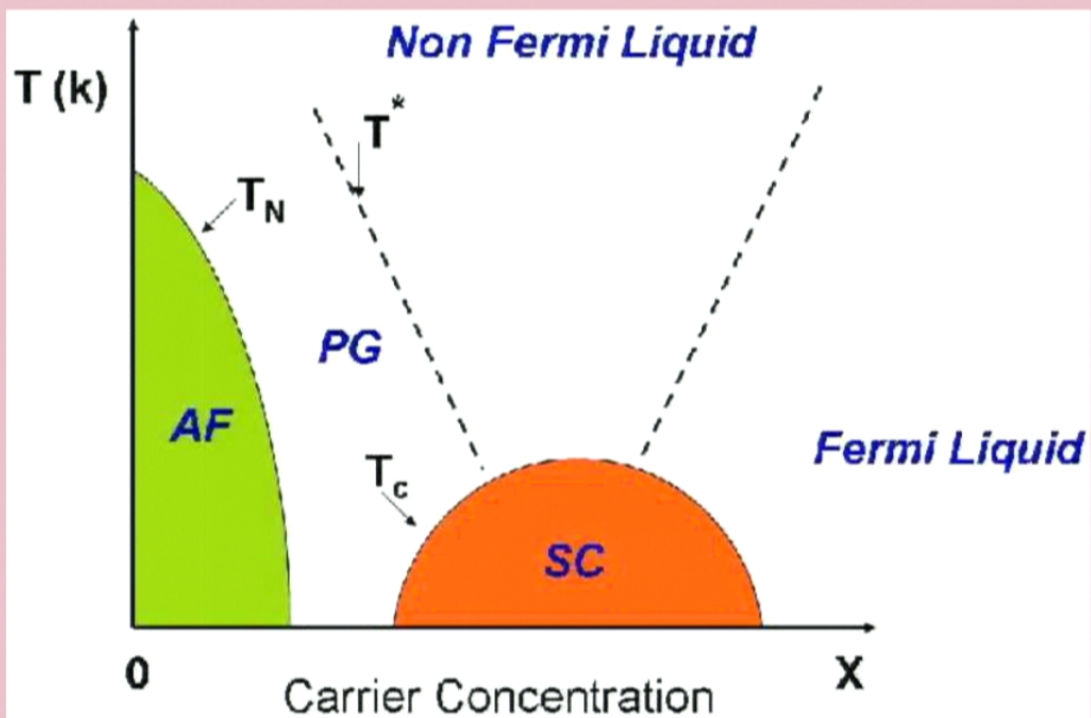
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Hole-doped Cuprate



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Pseudogap Region

- Ever since the discovery of pseudogap in high- T_c SC, it has been a profound mystery. To this day, its origin is vigorously debated.
- In one view, pseudogap is a remnant of the d -wave superconducting gap that defines a crossover temperature T^* in the phase diagram.
- The other view argues for a broken symmetry at T^* .
- Here, we assume much of the associated phenomenology can be described in a unified manner by the single assumption of a spin singlet $d_{x^2-y^2}$ density wave (DDW).

S. Chakravarty, R. B. Laughlin, D. K. Morr and C. Nayak (2001)

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Results and Implications

- We have calculated the spectrum of the amplitude mode for the DDW state and deduced important experimental consequences for the inelastic scattering experiments in the pseudogap phase.
- Although the DDW state order parameter condenses at the wave vector $q = Q = (\pi, \pi)$, the spectrum can be peaked at both $q = (0, 0)$ and $q = Q = (\pi, \pi)$.
- These turn out to be very unusual and were missed in an earlier work.

S. Tiwari and S. Chakravarty (2002)

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Results and Implications ...

- These results shed important light on recent exp on cuprates, which quite unexpectedly find multiple magnetic excitation modes at different wave vectors, the origin of which remains mysterious.

Y. Li *et al* (2012); H.A. Mook *et al* (unpublished)

- As to the elastic signature of singlet DDW, two neutron scattering measurements provide some evidence for it.

H.A. Mook *et al* (2002, 2004)

- The identification of the DDW state can be considerably strengthened by careful experimentation of the predictions of the inelastic amplitude spectrum that we offer.

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d-Density Wave Order Parameter

- The DDW state has circulating plaquette currents alternating between clockwise and anticlockwise directions in the neighboring plaquettes of an underlying square lattice, which can be taken as the lattice of the Cu atoms on the 2D CuO₂ planes.
- Thus it gives rise to tiny anti-ferromagnetically ordered orbital moments in the CuO₂ planes.
- The ordered state breaks time reversal, rotation by $\pi/2$, parity, and translational symmetry by one lattice spacing, but the product of any two of these symmetries is preserved.

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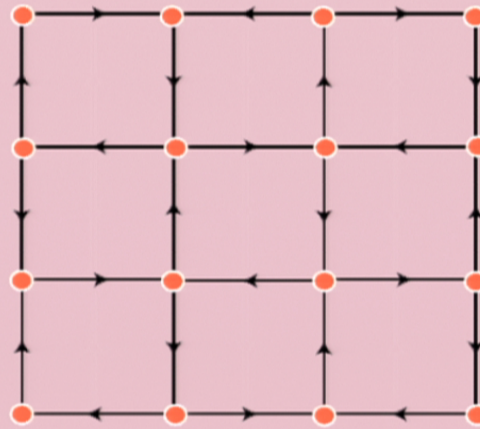
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d-Density Wave Order Parameter



The relevant order parameter characterizing the DDW state is a particle-hole spin-singlet pair condensing at wavevector $\mathbf{Q} = (\pi, \pi)$:

$$\langle c_{\mathbf{k},\alpha}^\dagger c_{\mathbf{k}+\mathbf{Q},\beta} \rangle = i \Delta_{\mathbf{Q}} f_{\mathbf{k}} \delta_{\alpha\beta},$$

where $f_{\mathbf{k}} = (\cos k_x - \cos k_y)$.

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Nature of the Spectrum

- The principal result is that the spectra are *not* confined to only the ordering wave vector \mathbf{Q} , but can have finite-frequency peaks at both $\mathbf{q} = (0, 0)$ and $\mathbf{q} = \mathbf{Q}$, as well as considerable spectral weight over a substantial region of the momentum space.
- The emergence of a $\mathbf{q} = \mathbf{0}$ peak, even with a mean field state that breaks lattice translation symmetry, indicates $\mathbf{q} = \mathbf{0}$ fluctuations hidden within the DDW state.
- In its phase diagram, one finds *orbital ferromagnetic* (OF) as well as orbital antiferromagnetic (DDW) phases. The model then belongs to the universality class of the classical six-vertex model.

S. Chakravarty (2002)

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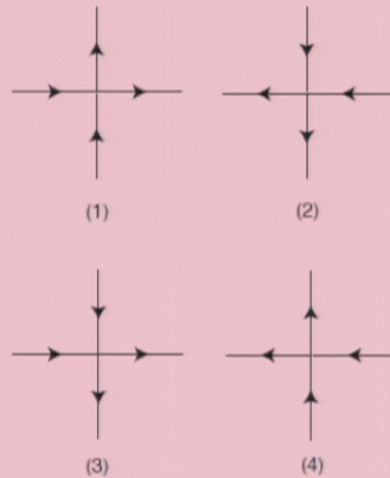
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The 6-vertex Model

For no source or sink, that is, $\nabla \cdot \mathbf{j} = 0$, there are 2 incoming and 2 outgoing currents at a vertex of a square lattice \rightarrow altogether $\frac{4!}{2!2!} = 6$ possible vertices.



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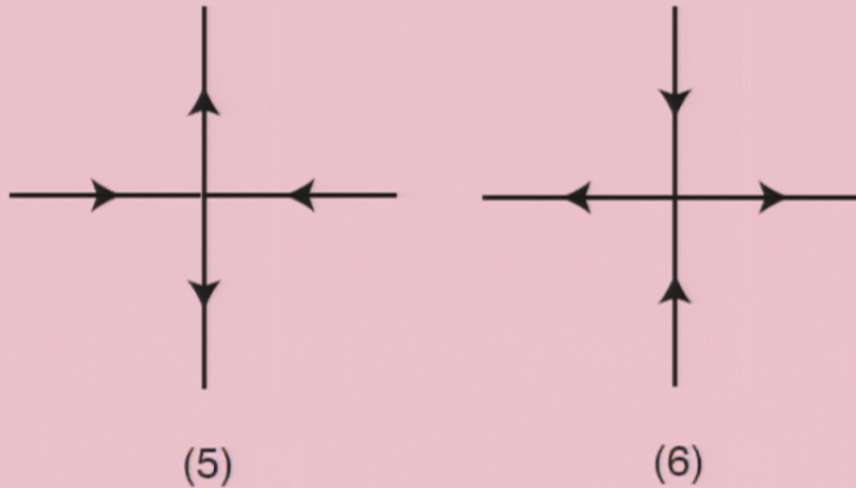
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Vertices for Staggered Circulating Currents

The configuration of the ordered singlet DDW state is a result of juxtaposing the following 2 of the 6 possible vertices:



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Hamiltonian

$$H = \sum_{\mathbf{k}, \sigma} (\epsilon_{\mathbf{k}} + \varepsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}, \sigma}^{\dagger} c_{\mathbf{k}, \sigma} + g^{-1} \sum_{\mathbf{q}} \hat{\Delta}_{\mathbf{q}}^{\dagger} \hat{\Delta}_{\mathbf{q}},$$

where

$$\hat{\Delta}_{\mathbf{q}} = \frac{g}{2} \sum_{\mathbf{k}} f_{\mathbf{k} + \frac{\mathbf{q} - \mathbf{q}}{2}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k} + \mathbf{q}},$$

$\epsilon_{\mathbf{k}} = -2t (\cos k_x + \cos k_y)$, $\varepsilon_{\mathbf{k}} = 4t' \cos k_x \cos k_y$, and $f_{\mathbf{k}} = (\cos k_x - \cos k_y)$ in the full 2D Brillouin-zone (FBZ).

Anticipating a commensurate DDW order, we fold the FBZ to the reduced Brillouin-zone (RBZ), which can be defined in terms of the rotated coordinates:

$$\frac{k_x + k_y}{\sqrt{2}} \rightarrow k'_x, \quad \frac{k_x - k_y}{\sqrt{2}} \rightarrow k'_y, \quad (k'_x, k'_y) \in \left[-\frac{\pi}{\sqrt{2}}, \frac{\pi}{\sqrt{2}}\right]$$

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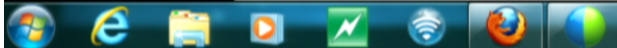


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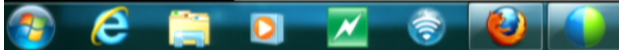


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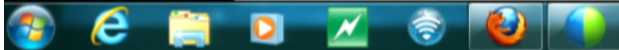


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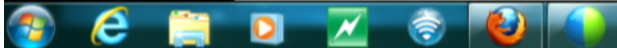


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The Various Gap Parameters

- At $\mathbf{q} = \mathbf{Q}$, $\hat{\Delta}_{\mathbf{Q}}$ represents the conventional DDW gap parameter.
- At $\mathbf{q} = \mathbf{0}$, $f_{\mathbf{k}-\mathbf{Q}/2} = (\sin k_x - \sin k_y)$ leads to uniform current flows along $+x$ and $+y$ dirns.
- At $\mathbf{q} = \mathbf{Q} = \mathbf{Q} + \bar{\mathbf{Q}}$, where $\bar{\mathbf{Q}} = (\pi, -\pi)$, $f_{\mathbf{k}+\bar{\mathbf{Q}}/2} = (\sin k_x + \sin k_y)$ leads to current flows along $+x$ and $-y$ dirns.
- At $\mathbf{q} = \bar{\mathbf{Q}}$, $f_{\mathbf{k}+(\bar{\mathbf{Q}}-\mathbf{Q})/2} = (\cos k_x + \cos k_y)$ leads to alternate current sources and sinks. But we will choose their fugacity to vanish.

Thus $\hat{\Delta}_{\mathbf{q}}$ represents the full six-vertex model. We will find that only $\hat{\Delta}_{\mathbf{Q}}$ develops a mean-field expectation value in the saddle-point soln, though there are fluctuations from the others.

Participants



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Action

Using the Hubbard-Stratonovich transformation and replacing $\{\hat{\Delta}_{\mathbf{q}+\mathbf{Q}}, \hat{\Delta}_{\mathbf{q}+\mathbf{Q}+\mathbf{Q}}\} \rightarrow \{i\hat{\Delta}_{\mathbf{q}+\mathbf{Q}}, i\hat{\Delta}_{\mathbf{q}+\mathbf{Q}+\mathbf{Q}}\}$, we get:

$$S = \sum_{\mathbf{k}, \omega} \Psi_{\mathbf{k}, \omega}^{\dagger} \{(-i\omega - \mu + \varepsilon_{\mathbf{k}})\sigma_0 + \epsilon_{\mathbf{k}}\sigma_3\} \Psi_{\mathbf{k}, \omega} \\ - 2g^{-1} \sum_{\mathbf{q}, \omega, a, b} \hat{\Delta}_{b, \mathbf{q}, \omega}^{(a)\dagger} \Delta_{b, \mathbf{q}, \omega}^{(a)} + g^{-1} \sum_{\mathbf{q}, \omega, a, b} \Delta_{b, \mathbf{q}, \omega}^{*(a)} \Delta_{b, \mathbf{q}, \omega}^{(a)},$$

where

$$\hat{\Psi}_{\mathbf{k}, \omega}^{\dagger} = \begin{pmatrix} c_{\mathbf{k}, \omega}^{\dagger} & c_{\mathbf{k}+\mathbf{Q}, \omega}^{\dagger} \end{pmatrix}$$

Here, $\hat{\Delta}_{b, \mathbf{q}}^{(a)} = \hat{\Delta}_{\mathbf{q}+b+a\mathbf{Q}}$, with $a = \{0, 1\}$ and $b = \{0, \mathbf{Q}\}$; $f_{\mathbf{k}+\mathbf{q}/2}^{(a, b)}$ are the corresponding structure factors. We also define $\rho_{b=0, \mathbf{k}+\mathbf{q}/2}^{(a)} = f_{\mathbf{k}+\mathbf{q}/2}^{(a, 0)} \sigma_3$, $\rho_{b=\mathbf{Q}, \mathbf{k}+\mathbf{q}/2}^{(a)} = f_{\mathbf{k}+\mathbf{q}/2}^{(a, \mathbf{Q})} \sigma_2$.

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Response

The measurement of dissipation from any probe that couples to $\hat{\Delta}_{b,\mathbf{q},\omega}^{(a)}$ will be of the form:

$$\text{Im}\langle \Delta_{b,\mathbf{q},\omega}^{(a)} \Delta_{b',-\mathbf{q},-\omega}^{(a')} \rangle = \text{Im}[V_{b,b'}^{(a,a')}(\mathbf{q},\omega)],$$

where

$$V(\mathbf{q},\omega) = U(q,\omega)^{-1}$$

Peaks in the response function thus correspond to poles of $V(\mathbf{q},\omega)$.

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Numerical Results

Given a choice for the mean-field parameter $\Delta_{\mathbf{Q}}$, the hole-doping x , and the band-structure parameters t, t' , we first solve the mean-field eqns. These are then used to calculate the correlators, which may possibly be measured in inelastic neutron scattering measurements.

There are no static saddle point solutions corresponding to $\langle \hat{\Delta}_{\mathbf{q}} \rangle$ and $\langle \hat{\Delta}_{\mathbf{q}+\mathbf{Q}} \rangle$ for the range of parameters considered. But the spectrum contains a component also near $\mathbf{q} \sim \mathbf{0}$, which can be interpreted as OF fluctuations of the bond currents.

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Plots

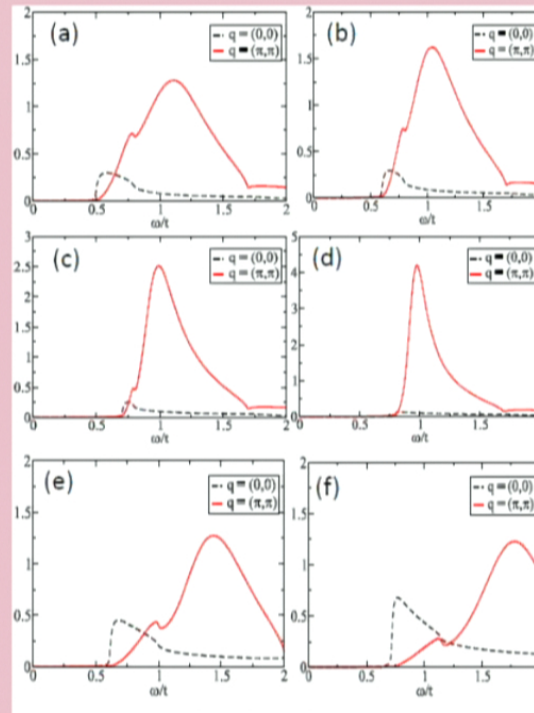


Figure: Response as a function of ω/t for $\mathbf{q} = \mathbf{Q}$ (solid curve) and $\mathbf{q} = \mathbf{0}$ (dashed curve). Panels (a)-(c): $\Delta_{\mathbf{Q}} = 0.3t$, and $x = 0.06$ (a), $x = 0.1$ (b), $x = 0.14$ (c), $x = 0.18$ (d). Panels (e)-(f): $x = 0.06$, and $\Delta_{\mathbf{Q}} = 0.4t$ (e) and $\Delta_{\mathbf{Q}} = 0.5t$ (f).

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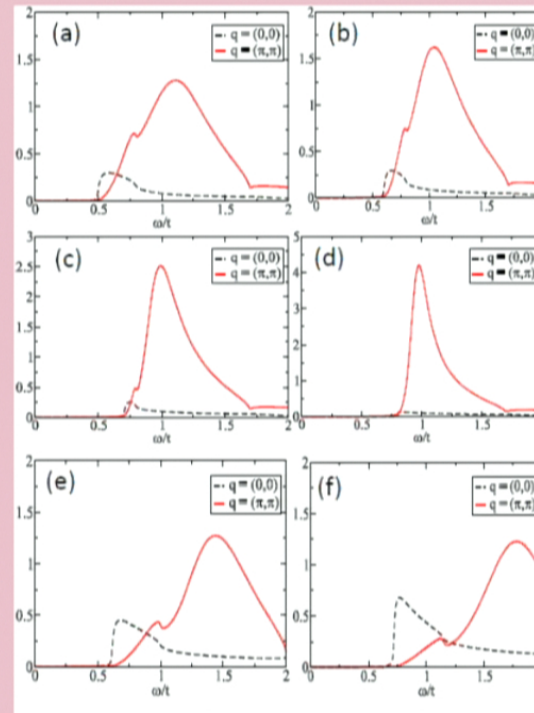


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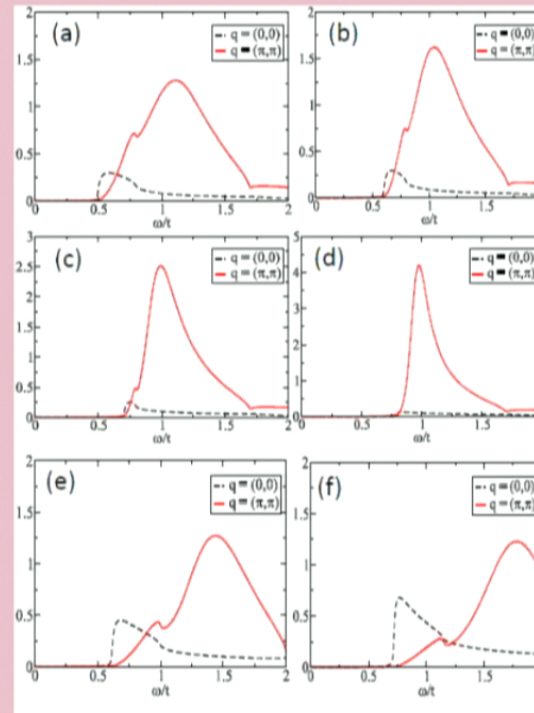


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Analysis of the Plots

- In the plots, the underdoped regime shows a noticeable finite-frequency peak at $\mathbf{q} = \mathbf{0}$ coexisting with a finite frequency peak at \mathbf{Q} .
- The intensity at $\mathbf{q} = \mathbf{0}$ goes down with increasing x , but the amplitudes strongly depend on the microscopic parameters. This implies that the amplitude fluctuation spectra can have finite frequency peaks at both $\mathbf{q} = \mathbf{0}$ and $\mathbf{q} = \mathbf{Q}$, or only a single peak.
- Such non-universality indicates that different families of cuprates, or even samples at different hole dopings within same family, may have different fluctuation spectra. These may have important consequences for inelastic neutron scattering experiments.

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Conclusion

- Using the functional integral formalism, we calculate the collective mode spectrum of the DDW state.
- Since the ordered state breaks only discrete symmetries, there is no gapless phase mode.
- Our central result is that the amplitude mode spectrum of the DDW state can be peaked at both $\mathbf{q} = (0, 0)$ and $\mathbf{q} = \mathbf{Q} = (\pi, \pi)$, even though the ordered state condenses only at the wave vector \mathbf{Q} .

Thank you for your attention!

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