Collective modes in the d-density wave state of the cuprates

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Using a functional integral formulation, we analyze the collective modes in the d-density wave state. Since only discrete symmetries are broken, no massless phase mode is present. The only relevant fluctuation is the amplitude fluctuation of the order parameter, which is treated at the gaussian level above the long range order. These fluctuations give rise to a massive mode, the analog of the $U(1)$ Higgs, or amplitude mode at wave-vector $(\pi, \pi)$. Neutrons in inelastic neutron scattering experiments couple to this mode via the orbital currents and are likely to produce direct measurements of this amplitude boson.

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Much attention has recently been paid to a discrete symmetry broken state, the d-density wave (DDW), as a possible candidate for the anomalous normal state of the underdoped cuprate superconductors. Below the pseudogap temperature scale, $T^*$, the system is conjectured to condense into the DDW state, which is responsible for much of the observed physics of the pseudogap phase. Further down in temperature, below the superconducting transition temperature $T_c$, the DDW and the d-wave superconductor (DSC) are expected to coexist and compete for the same regions on the Fermi surface. In a range of the hole-doping concentration, $x$, suitable for making up the underdoped systems, the competition between the two orders consistently explains the unique variation of the superconducting order parameter with doping.

The DDW state, under various names and guises, appeared in the literature on many occasions. More elaborate treatments of some of the properties of the system, most relevant to experiments on the high-$T_c$ superconductors, were discussed recently. However, these authors, for the most part, treated the system in the framework of Hartree-Fock mean field theory, one consequence of which was that, all information about the collective modes - and experimental implications thereof - remained uninvestigated. In this paper, we intend to fill this gap by elucidating the structure of the collective modes and pointing out how they can actually be detected in experiments.

The DDW state has plaquette-currents, alternating clockwise-anticlockwise in the neighboring plaquettes of an underlying square lattice. Thus, it gives rise to tiny orbital moments. The relevant order-parameter characterizing the d-density wave is a particle-hole spin-singlet pair, condensing at an wavevector $Q = (\pi, \pi)$. The bipartite square lattice band-structure is equivalent under the transformation $Q \rightarrow -Q$ and this forces the order parameter to be imaginary, a fact which is ultimately responsible for the breaking of the time-reversal symmetry and the resulting spontaneous bond-currents. The phase of the order parameter being fixed by the specific symmetries it breaks, the only natural collective excitation one expects is the amplitude fluctuation of the order-parameter, which will give rise to a finite frequency mode, the amplitude mode, centered at $Q$. We will explicitly calculate the frequency to be $2\Delta_{DDW}$, where $\Delta_{DDW}$ is the DDW single particle gap at $(\pi, 0)$, which can be estimated from photo-emission experiments above $T_c$. We will also show how inelastic neutron scattering, coupling to the bond-currents, should directly reveal this mode. In fact, well-defined, but damped features at wave-vector $Q$ and energy comparable to $2\Delta_{DDW}$ have indeed been seen above $T_c$ in inelastic neutron scattering of the cuprates. These damped peaks are in sharp contrast to the resonant peak below $T_c$, which occurs at the same wave-vector and comparable energy, but is resolution-limited in frequency. This opens up a tantalizing possibility that the amplitude mode of the DDW state, which is the analog of the Higgs mode of $U(1)$ gauge theory, may actually have already been observed in experiments. Clearly, the issue needs further investigation.

In order to analyze the collective modes, let us start with the Hamiltonian in momentum space,

$$H = \sum_{k, \sigma} (\epsilon_k - \mu) c_{k, \sigma}^\dagger c_{k, \sigma} - \sum_{k, k', q, \alpha, \beta} g_{kk'}^q c_{k+q, \alpha} c_{k, \beta} c_{k', \beta} c_{k', q+\beta},$$

where $c_{k, \sigma}^\dagger$ creates a particle with momentum $k$ and spin $\sigma$, $c_k$ is the free electron band structure $-2t(\cos k_x + \cos k_y)$, $\mu$ is the chemical potential, and $g_{kk'}^q$ is the interaction matrix element. A more realistic band structure would include the effect of a next-neighbor hopping $t'$. A small $t'$ does not change our results qualitatively, so we ignore it for simplicity. In the half filled limit, $\mu = 0$; it takes non-zero negative values when holes are doped into the system. In this paper we will work in units where the lattice constant is unity and will also set $\hbar = c = k_B = 1$.

The particle-hole spin-singlet d-density wave order parameter is anisotropic in $k$-space,

$$\langle c_{k, \alpha}^\dagger c_{k+q, \beta} \rangle = \frac{\Phi_Q}{2} f_k \delta_{\alpha\beta},$$

where $\Phi_Q$ is the magnitude of the order parameter, and $f_k = (\cos k_x - \cos k_y)$. So, we will take the effective part of the full interaction factorizable as

$$g_{kk'}^q = f_k f_{k'} g.$$
This would enable us to always maintain the $d_{x^2-y^2}$-wave symmetry of the order parameter and discuss long wavelength fluctuations around it. For a discussion of the DDW state, we will ignore the other parts of the interaction and the fluctuations of other symmetries.

The Hamiltonian now takes the form

$$ H = \sum_{k,\sigma}(\epsilon_k - \mu)c_k^\dagger c_k - g^{-1} \sum_q \hat{\Delta}(q) \hat{\Delta}(q), \quad (4) $$

where,

$$ \hat{\Delta}(q) = g \sum_{k,\alpha} f_k c_{k\alpha} c_{k+q\alpha}. \quad (5) $$

Note, for $q = Q$, a commensurate wave-vector, $\hat{\Delta}(Q)$ is antihermitian and is, in operator form, the DDW gap parameter.

In functional integral form, the partition function is

$$ Z = N \int Dc^+ Dc e^{-S}, \quad (6) $$

where

$$ S = \int_0^\beta d\tau \left( \sum_{k,\sigma}(\partial_\tau + \epsilon_k - \mu)c_k^\dagger c_k - g^{-1} \sum_q \hat{\Delta}(q) \hat{\Delta}(q) \right), \quad (7) $$

and $N$ is a normalization constant. By introducing an auxiliary boson field $\Delta_k$ through the Hubbard-Stratonovich transformation, the interaction term is made quadratic in the Fermion fields. In frequency space, the new action is given by

$$ S_0 = \sum_{k,\omega} \frac{\beta}{g} \Delta(k,\omega) \Delta(k,\omega) + \sum_{k_1,k_2,\omega_1,\omega_2} \Psi_{k_1,\omega_1}^\dagger M_{\omega_1,\omega_2}^k \Psi_{k_2,\omega_2}, \quad (8) $$

where the $\sigma$’s are the Pauli matrices acting in the space of $\Psi_{k,\sigma}$, and, $\sigma^z = \sigma_1 \pm i\sigma_2$.

In Eq. 3 the full Brillouin zone has been folded to the magnetic, or reduced Brillouin zone (RBZ), to facilitate the discussion of the DDW state; the momentum integrations are restricted to the RBZ, and a spin-sum over the Fermionic variables is implied. After integrating out the Fermion fields, the partition function is given by

$$ Z = N' \int \prod_{k,\omega} d\Delta_{k,\omega}^\dagger d\Delta_{k,\omega} e^{-S}, \quad (10) $$

where,

$$ S = \sum_{k,\omega} \frac{\beta}{g} \Delta^\dagger(k,\omega) \Delta(k,\omega) - 2 \ln \det M, \quad (11) $$

and $N'$ is now a different normalization constant. The factor of two in the second term of $S$ comes from the spin-summation. By taking $\partial S/\partial \Delta^\dagger(k,\omega) = 0$ and $\partial S/\partial \Delta(k,\omega) = 0$, we find the saddle point,

$$ \Delta(k,\omega) = 0, \text{ for } k \neq Q, \text{ or } \omega \neq 0, \quad (12) $$

and,

$$ \Delta(Q,0) = \Delta_Q = g \sum_k f_k^2 \left( \Delta_Q \right) \Theta(\mu + E_k). \quad (13) $$

Here, $E_k \equiv \sqrt{\epsilon_k^2 + f_k^2 |\Delta_Q|^2}$ and $\Theta(x)$ is a unit step function. Equation 13 is the $d$-density wave mean-field gap equation. Notice, with this definition of $E_k$, the DDW single-particle gap at $(\pi,0)$, $\Delta_{DDW} = 2|\Delta_Q|$. As $\hat{\Delta}(Q)$ is antihermitian, the gap parameter $\Delta(Q,0)$ must be pure imaginary. Hence, though $\hat{\Delta}(Q,0) = \Delta_Q e^{i\theta}$ satisfies the gap equation equally well, the phase of the order parameter is locked to $\pm \frac{\pi}{4}$. Thus, there are no massless phase modes in the long-wavelength
collective fluctuations of the order parameter. Put another way, since the order parameter breaks only discrete symmetries, there are no Goldstone modes in the system. For an incommensurate version of the DDW state, where the ordering wave-vector is not commensurate with the lattice, there is a collective massless mode, the sliding density wave mode. But this mode will be pinned by the impurities as well, in second order of the impurity potential.

\[
\delta S = \sum_{k, \omega} (A_{k+Q, \omega} \Delta_k^{\dagger} \Delta_{k+Q, \omega} + A_{-k-Q, \omega} \Delta_{-k+Q, \omega} - \Delta_{-k-Q, \omega}) + B_{k+Q, \omega} (\Delta_{k+Q, \omega}^{\dagger} \Delta_{k+Q, \omega} + \Delta_{-k-Q, \omega}^{\dagger} \Delta_{-k-Q, \omega}) + \frac{\beta}{2g} + \sum_{k, \omega'} f_k^2 \frac{(i \omega' - \mu - \epsilon_{k}) [i(\omega' + \omega) - \mu - \epsilon_{k+Q}]}{([i(\omega' + \mu)]^2 - E_k^2) [([i(\omega' + \omega) + \mu)]^2 - E_{k+Q}^2])}
\]

where the prime over the summation indicates exclusion of the points \((k = 0)\) and \((\omega = 0)\). \(A\) and \(B\) are given by,

\[
A_{k+Q, \omega} = \frac{\beta}{2g} + \sum_{k', \omega'} f_{k'}^2 \frac{(i \omega' - \mu - \epsilon_{k}) [i(\omega' + \omega) - \mu - \epsilon_{k+Q}]}{([i(\omega' + \mu)]^2 - E_k^2) [([i(\omega' + \omega) + \mu)]^2 - E_{k+Q}^2])}
\]

\[
B_{k+Q, \omega} = \sum_{k', \omega'} f_{k'}^2 f_{k+Q, \omega} \Delta_k^{\dagger} \Delta_{k+Q, \omega}
\]

Noting that \(\Delta_{k+Q, \omega}^{\dagger} = -|\Delta_Q|^2\) in the definition of \(B_{k+Q, \omega}\), we collapse Eq. [14] onto,

\[
\delta S = \sum_{k, \omega} (A_{k+Q, \omega} + A_{-k-Q, \omega} + 2 \tilde{B}_{k+Q, \omega}) \times \Delta_{k+Q, \omega}^{\dagger} \Delta_{k+Q, \omega}
\]

where \(\tilde{B}_{k+Q, \omega}\) is \(B_{k+Q, \omega}\) with \(\Delta_Q\) replaced by \(|\Delta_Q|\) in the numerator.

The dispersion for the collective mode can be read off by equating the fluctuation kernel to zero \([14]\).

\[
A_{k+Q, \omega} + A_{-k-Q, \omega} + 2 \tilde{B}_{k+Q, \omega} = 0
\]

In the case of a superconductor, there is no symmetry property, such as Eq. [13], for the fluctuation fields. Gaussian fluctuations around the superconducting saddle point has a form very similar to Eq. [14] and the collective modes are given by the determinantal equation, \(A'_{k, \omega} A'_{-k, -\omega} - B'_{k, \omega} B'_{-k, -\omega} = 0\). Using the properties, \(A'_{k, \omega} = A'_{-k, -\omega}\) and \(B'_{k, \omega} = B'_{-k, -\omega}\) \([14]\) which are specific to a superconductor, this splits up into two equations, \(A'(k, \omega) - B'(k, \omega) = 0\), and \(A'(k, \omega) + B'(k, \omega) = 0\). These are precisely the two equations giving the phase and the amplitude mode dispersions, respectively. The phase mode is massless, and the massive amplitude mode is centered at \(q = (0, 0)\). In the case of DDW, because of the symmetry property of the fluctuation fields which leaves the order parameter purely imaginary, one of the equations drops out, and, we are left with just one equation, that for the amplitude mode.

\[
\frac{\beta}{g} = -2 \sum_{k, \omega} \frac{f_k^2}{(i \omega' + \mu - E_k^2)} \frac{\mu}{2} \frac{\omega' + \mu}{E_k^2} - 8 i \omega' \mu
\]

following the gap equation, in the limit \(k = 0\), the frequency \(\omega\) for the amplitude mode is given by,

\[
\sum_{k', \omega'} \frac{f_{k'}^2}{(i \omega' + \mu - E_{k'}^2)} \frac{\mu}{2} \frac{\omega' + \mu}{E_k^2} - 8 i \omega' \mu = 0
\]

After the internal frequency summation, the last equation, at zero temperature, reduces to,

\[
\sum_{k'} \frac{f_{k'}^2}{E_{k'}} \Theta(\mu + E_{k'}) \frac{\omega^2}{(\omega^2 + 4 E_{k'}^2)} = 0
\]
Let us first analyze the mode-frequencies for the simpler case of an \( s \)-wave density wave, the charge density wave (CDW). In this case, \( f_k = 1 \), and \( \Delta_Q = \Delta \), a real quantity. Even if the order parameter is real, the last equation, with the substitution of \( f_k \) by 1, still gives the frequencies of the amplitude mode. This is because, for a real order parameter, Eq. 1\(^2\) holds with a + sign, and, \( B_k + Q \omega \) and \( B_k + Q \omega \) are same. Consequently, one can still collapse Eq. 1\(^4\) on to Eq. 1\(^3\) and get the same equation for the amplitude mode. Considering, then, Eq. 2\(^2\) for CDW, we note that, for \( \mu = 0 \), the roots are at \( \omega = \pm 2\Delta \). This implies the mode-frequencies at \( E = i\omega = \pm 2\Delta \). The modes come in pair, for the absorptive and emissive responses, respectively. For increasing values of \(|\mu|\), the modes are shifted, finally, for large values of \(|\mu|\), the frequencies scale with \( \pm 2\sqrt{2/|\mu|} \).

Returning to the case of DDW, where \( f_k \) is nontrivial, we have to perform the internal momentum integral numerically. First, after some simple manipulations, Eq. 2\(^2\) is brought to the dimensionless form,

\[
I(z) = \sum_{k'} \frac{f^2_{k'}}{(e^2_{k'} + f^2_{k'})^{1\over2}} \Theta(\mu + E_{k'}) \frac{z^2 + f^2_{k'} + 2(\mu - |\Delta_Q|)^2}{z^2 + e^2_{k'} + f^2_{k'}} = 0, \tag{23}
\]

where, \( z = \frac{\omega}{2|\Delta_Q|} \), and \( e_{k'} = \frac{\omega}{|\Delta_Q|} \).

In analogy with the \( s \)-wave case, one can easily see from here that, at large \( \mu/|\Delta_Q| \), where the \( f^2_{k'} \) term in the numerator can be neglected in comparison, the roots of the last equation are at \( z \approx \pm i\sqrt{2/|\Delta_Q|} \), i.e., at real frequencies \( E = i\omega \simeq \pm 2\sqrt{2}\mu \). If \( \mu \) behaves with doping of holes in the system in a manner similar to a Fermi liquid, then it can be quite large, and eventually scales with \( t \), the largest scale in the problem. In such a case, the amplitude mode in the DDW system is at very high energy and is virtually inaccessible in thermal neutron scattering. Also, a mode so high up in energy is expected to be heavily damped, since there is a large phase-space of excitations it can decay into. Consequently, one can not in the case of large \(|\mu|\) meaningfully talk about the amplitude mode in connection with experiments. But a large value of the chemical potential may not be the case in the underdoped regime of the cuprates\(^4\) where various kinds of charge inhomogeneities and impurities may actually pin the doped holes. Indeed, there are some indications\(^4\) that \( \mu \) remains pinned close to zero in these systems. Under such a scenario, the shift of the mode-frequencies due to chemical potential is small, and the results are qualitatively similar to the case of half-filling, \( \mu = 0 \). Thus, in order to make contact with experiments, we will only discuss the case of chemical potential pinned to zero, assuming it does not shift appreciably with doping in the underdoped regime of the cuprates.

Assuming \( \mu = 0 \), and replacing \( z \) by \( iu \) in the left hand side of Eq. 2\(^2\), we have numerically performed the momentum integral over the RBZ. The reason for replacing \( z \) by \( iu \) is that, we will eventually look for roots of the equation on the imaginary axis such that the mode-frequencies after analytic continuation become real. In figure 1, we show the results of the integration plotted as a function of \( u \).

![FIG. 1: Results of the integral given in Eq. 2\(^2\), \( I(u) \), plotted as a function of \( u \), where \( u = -iz \). The parameters used are \( t = 0.25 \) eV, \( |\Delta_Q| = 0.01 \) eV, and \( \mu = 0 \). \( I(u) \) has a root at \( u = 2 \). Since it is an even function of \( u \), the other root, not shown here, occurs at \( u = -2 \).](image-url)

Calling the dimensionless function of \( u \) in Eq. 2\(^2\) \( I(u) \), we note that it has a root at \( u = 2 \). Since \( I(u) \) is an even function of \( u \), there is another root at \( u = -2 \). Tracing back the transformations, we find the amplitude mode frequencies at

\[
E = i\omega = i2|\Delta_Q| |z = -2|\Delta_Q| |u = \pm 4|\Delta_Q| = \pm 2|\Delta_{DDW}|. \tag{24}
\]

The last equality follows by recalling the DDW single-particle gap at \((\pi,0), \Delta_{DDW} = 2|\Delta_Q| \). So, we conclude that the amplitude modes for the DDW state lie at frequencies \( \pm 2\Delta_{DDW} \).

At the level of our computation, the mode is undamped, i.e., an exact eigenstate of the system. But, since the ordered state is a particle-hole condensate in contrast to a superconductor, it can easily couple to other degrees of freedom in the cuprates. The mode can, for example, couple to the optical phonons, which are abundant in the system. These other degrees of freedom will act as an external bath to the system of the amplitude boson, and provide it with some frequency width. We can meaningfully talk about the mode - and its manifestations in experiments - only as long as this width is not too big.

In order to make contact with the neutron scattering experiments, let us start with the interaction potential between the incoming neutron and the electrons carrying the orbital current, \( V_{int} \).\(^4\)
\[ V_{\text{int}} = \sum_{(ij)} \text{i} e_{\sigma \tau} c_{i \sigma} \exp(i \int_{i}^{j} \mathbf{A} \cdot \mathrm{d}l) + \text{h.c.} \] (24)

Here, \( \mathbf{A} \) is the electromagnetic gauge potential generated by the neutron magnetic moment \( \mu_{n} \), \( \mathbf{A} = \mu_{n} \times (\mathbf{r}_{e} - \mathbf{r}_{n})/(|\mathbf{r}_{e} - \mathbf{r}_{n}|) \), \( \mu_{n} = -1.91 \mu_{N} \mathbf{S} \), and \( \mathbf{r}_{e} \) and \( \mathbf{r}_{n} \) are the electron and neutron coordinates, respectively. Because the gauge field generated by the neutron is weak, we can approximate \( V_{\text{int}} \) by \( V_{\text{int}} = i e t \sum_{(ij)} (\int_{i}^{j} \mathbf{A} \cdot \mathrm{d}l)(c_{i \sigma}^{\dagger} c_{j \sigma} - c_{j \sigma}^{\dagger} c_{i \sigma}) \).

To find the cross section, we first have to evaluate the matrix element of the interaction potential between the initial and final states of the neutron, \( \langle \mathbf{k}_{f} | \int_{n}^{n} | \mathbf{k}_{i} \rangle = \int d^{3}r_{n} V_{\text{int}} \exp(iq \cdot r_{n}) \), where \( q = k_{f} - k_{i} \). After doing the integral over the neutron coordinates \( \mathbf{r}_{n} \), summing over the initial and final states in the scattering process, and then, putting \( q = Q = (\pi, \pi) \), we find,

\[ \langle \mathbf{k}_{f} | V_{\text{int}} | \mathbf{k}_{i} \rangle = \frac{8ie \mu_{e}}{\pi} \sum_{k, \sigma} (\cos k_{x} - \cos k_{y})_{k+Q, \sigma} c_{k+Q, \sigma}^{\dagger} c_{k, \sigma}. \] (25)

Apart from some coefficients, the expression on the right hand side of the last equation is precisely the DDW gap in the operator form. In other words, the coupling of the neutron with the system at \((\pi, \pi)\) is, as expected, through the orbital currents.

Finally, averaging over the neutron spin states using \( \sum_{\sigma, \sigma'} \rho_{\sigma, \sigma'} \langle \sigma_{i} | \mu_{n} | \sigma_{f} \rangle \langle \sigma_{f} | \mu_{n} | \sigma_{i} \rangle = \mu^{2} \delta_{\sigma, \sigma'} \), and, following standard steps\[5\] we derive,

\[ \frac{d^{2} \sigma}{d \Omega d\omega_{f}} = \frac{8ie \mu_{e}}{\pi g} (\Delta_{Q, \omega}^{2} - \Delta_{-Q, -\omega}^{2}). \] (26)

Here, \( \Delta_{Q, \omega} \) is the frequency transform of the gap parameter, \( \Delta_{Q} \), given, in operator form for a general \( q \), in Eq.\[5\].

The expression on the right hand side of the last equation is precisely the quantity we evaluated in the analysis of the DDW amplitude mode. The quantity \( \langle \Delta_{Q, \omega} \Delta_{-Q, -\omega} \rangle \), in imaginary time ordered form, can be directly taken over from Eq.\[13\].

\[ \langle T_{\tau} \Delta_{Q, \omega} \Delta_{-Q, -\omega} \rangle = \frac{1}{A_{Q, \omega} + A_{-Q, -\omega} + 2B_{Q, \omega}} \] (27)

As we found earlier, this function has poles at \( \omega = \pm i2\Delta_{\text{DDW}} \). These are the dissipative and the absorptive responses of the system, respectively. At zero temperature, the relevant pole is that for the dissipative response only. After analytically continuing the frequency, the corresponding retarded function will have a pole at \( \omega = 2\Delta_{\text{DDW}}, \) implying a sharp peak at that frequency. This peak captures the amplitude boson for the DDW state in inelastic neutron scattering. As we emphasized before, the sharpness of the response is really an artifact of our calculation, which excludes the coupling of the boson to other degrees of freedom, such as the optic phonons. A fuller treatment should bring in some damping to the mode. Indeed, the peaks above \( T_{\tau} \) in the neutron scattering of the cuprates are broad.\[3\] Clearly, more work is needed in this direction to establish this. To establish the correct momentum dispersion will require a more microscopic model than that considered. From translational invariance one can argue that the square of the mode frequency is an analytic function of the momentum, that is, it must begin quadratically. However, the coefficient of the leading momentum dependence is expected\[4\] to be complex implying damping of the collective mode at a finite wavevector away from \( Q = (\pi, \pi) \).

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