About possible Phonon to Magnon alignment in 2 dimensions and theory of superconductivity in Copper-Oxide planes.

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We suggest that the phonon dispersion in cuprates becomes strongly anisotropic due to interaction with spin waves; moreover the phonon dispersion becomes singular along $|k_x| = |k_y|$ directions. This would allow more electrons to form Cooper pairs and increase temperature of the superconducting transition. The interaction of phonons with spin waves is more important than the interaction of phonons with free electrons, because spin waves do not have the Fermi surface constrain.

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The motivation for this work is to look for phonon-mediated mechanism of the high-temperature superconductivity which would give d-wave order parameter observed experimentally, particularly by scanning tunneling imaging of non-magnetic dopants. This letter will be focused on the dispersion of longitudinal acoustic phonons interacting with spin waves. This interaction has been introduced earlier to explain Raman spectra of high $T_c$ cuprates; it is similar to interaction of optical phonons with magnons seen possibly in midinfrared absorption of cuprates, Raman spectroscopy of Spin-Peierls systems, and reflectivity of CuO crystals. We basically undertake a search for new anisotropic phonon modes seen in photoemission.

The electron-phonon interaction in the Fermi-liquid theory does not lead to interaction between phonons and spin waves. The phonon propagator is renormalized by the polarization bubble of electron gas, the latter is proportional to the electron density in the same way as the polarization bubble of electron gas, the latter is proportional to the phase volume available for scattering.

Alternative description of spin waves - magnons can be derived from the Heisenberg Hamiltonian, just by attributing local spins to sites. In general the interaction energy $J \sim U^2/t$, where $U$ is the charging energy of local electron and $t$ is hopping matrix element. This matrix element depends exponentially on inter-atomic distance and so does the spin interaction $J$. We will show later that the spin-phonon interaction splits the dispersion of the longitudinal two-dimensional phonons and new branch becomes singular and anisotropic, namely it goes like

$$\omega \sim \frac{1}{dJ} \left( \frac{dJ}{da} \right)^2 \frac{1}{|\cos(k^x a) - \cos(k^y a)|}$$

(1)

and the divergence is cut off by the condition $\omega \ll J[\sin^2(k^x a/2) + \sin^2(k^y a/2)]$, where $a$ is the lattice constant of square lattice. The simple form Eq. (1) is valid for $\omega \gg \omega_0(k)$, where $\omega_0(k)$ is the dispersion law of longitudinal acoustic phonons.

The extra lattice stiffness comes out of zero-point energy of spin waves. The effect is similar to the nature of attraction between bodies (Van der Waals forces) due to zero-point oscillations of electromagnetic waves. By analogy, one can compute magnetostriction force due to polarization of magnon vacuum. However this force would compete with all other strains in solid state and would be hardly observable. In the same time dynamical $\omega > 0$ part of the magnon polarization operator has dramatic effect on phonon dispersion. The right way to integrate out all almost standing magnon waves aligned with phonon wave is to solve the Dyson equation as it is done below by making use of zero temperature diagrams.

Two main ingredients are necessary to conduct the calculation: the spin-spin correlation function and spin-phonon Hamiltonian (also known as magneto-elastic Hamiltonian). These two are not independent, for example taking into account next-neighbor exchange interaction would affect spin-spin correlation and spin-phonon interaction. The subject is even more complicated in our “target” systems - high $T_c$ cuprates; their spin-spin correlation function depends on doping and changes across the antiferromagnet to superconductor transition. Fortunately, the spin waves polarization operator contains $\omega$ integration which completely removes this dependence, so our result Eq. (1) is robust and should work even if the ground state does not have magnetic order at zero temperature.

According to the BCS theory the energy gap $\Delta_k$ is proportional to the phase volume available for scattering for two electrons with moments $\vec{k}$ and $-\vec{k}$ on the Fermi surface, when they lose energy $\omega$. The singular phonon dispersion leads to dramatic consequences for electron-electron pairing. The half-filled tight-binding model $E = t \cos(k^x a) + t \cos(k^y a)$ has rectangular Fermi surface $k^y = \pm \pi/a \pm \pi$. Assume that electron is on the line $k^x + k^y = \pi/a$. Then the interaction with dispersion Eq. (1) will keep electron on the same bond $k^x + k^y = \pi/a$, since it allows the process with $|k_{\uparrow}^x - k_{\downarrow}^x| = |k_{\uparrow}^y - k_{\downarrow}^y|$. Twice more scattering out phase volume is available from hot spots $(0, \pm \pi/a)$, $(\pm \pi/a, 0)$. For example from the point $\vec{k} = (0, \pi/a)$ the electron can be scattered out by new phonons to both $k_{\uparrow}^x + k_{\downarrow}^y = \pi/a$ and $k_{\uparrow}^x = k_{\downarrow}^y - \pi/a$ bonds. The order parameter becomes anisotropic $\Delta_{\vec{k},h.s.} = 2\Delta_{\vec{k},h.s.} \parallel k^x - k^y$. Phonons Eq. (1) allow deviations from the exact law $|k_{\uparrow}^x - k_{\downarrow}^x| = |k_{\uparrow}^y - k_{\downarrow}^y|$.
$\Delta_k$ is smooth function having maxima at hot spots.

The alignment of phonons to the crystalline lattice is suggestive solution to the HTSC problem. It allows to interacting electrons to go up $h\omega_{\text{max}}$ out of the Fermi surface (below $\hbar = 1$), increasing both the energy gap and transition temperature. Here $\omega_{\text{max}}$ is maximal (cutoff) frequency in Eq. (1). It sets up new energy scale between phonons and magnons; $\omega_{\text{max}}$ is much larger than the Debye frequency $\omega_D$ and much lower than the spin exchange energy $J$. The accurate calculation of $\Delta_k$ requires regularization of the singularity in Eq. (1) and it is not yet done.

Assume that the antiferromagnetic coupling constant $J > 0$ depends on distance

$$\mathcal{H} = \sum_{(ii')}(J + \frac{dJ}{da})\langle \vec{u}_i - \vec{u}_{i'}\rangle \vec{S}_i \vec{S}_{i'}$$

where each pair of adjacent sites $(ii')$ on square lattice is counted once, vector $\vec{u}_{i'}$ points from $i'$ to $i$, $\vec{u}_i$ is displacement of $i$th site, and $\vec{S}_i$ is the spin on $i$th site.

Consider the chain of sites counted along $x$ axis for fixed $y$, then the interaction term is

$$\mathcal{H} = \sum_i (u_i^x - u_{i-1}^x) \vec{S}_i \vec{S}_{i-1} = \sum_i u_i^x (\vec{S}_{i+1} - \vec{S}_{i-1})$$  \hspace{1cm} (3)

For the first glance this interaction vanishes because it is proportional to $\vec{S} \nabla_x \vec{S} = \nabla_x \vec{S}^2 = 0$. Extracting the following identity from the spin product

$$[\vec{S}_{i+1} + \vec{S}_{i-1}] [\vec{S}_{i+1} - \vec{S}_{i-1}] = 0$$

we will find interaction being proportional to higher power of derivatives. After some algebra

$$\mathcal{H} = -\frac{1}{2} \frac{dJ}{da} \sum_{(ii')} (\vec{u}_i - \vec{u}_{i'}) \vec{a}_{i'} \cdot (\vec{S}_{i'} - \vec{S}_i)^2$$

that can be verified by expansion of the square term. The magneto-elastic energy derived here is invariant under spin rotation as opposite to the so-called relativistic term$^{14}$. The relativistic part of the magneto-elastic energy is responsible for acoustic Faraday’s effect - rotation of phonon polarization around magnetization axis or Neél’s vector, observed recently in two dimensions$^{15}$. It will not be discussed here because i) the effect does not exist in disordered phase, ii) it is less important for large $\vec{k}$.

For each bond $j = (ii')$ we will introduce the time dependent phonon field $\phi(j) = (\vec{u}_i - \vec{u}_{i'}) \vec{a}_{i'} \sqrt{\rho}$, where $\rho$ is the material density. For longitudinal phonons the field is quantized as

$$\phi(\xi) = \frac{1}{\sqrt{\mathcal{N}^3}} \sum_{k} \frac{2\kappa_{k}^{x} k^{x}/k}{\sqrt{2\omega_{k}(k)}} \{ \sqrt{\rho} e^{i\vec{k}\rho - i\omega_{0}(k)t} + \text{c.c.} \}$$

for bond $j$ parallel to $x$-axis, and $y$-components of $\vec{k}$ should be taken if the bond $j$ is parallel to $y$ axis, besides $[b_{\vec{k}}, \sqrt{\rho}^{i}] = \delta_{\vec{k}\vec{0}}$, are boson operators, $\xi = (j, t)$, and

$$\kappa_{k}^{x} = (\sin(k^x a/2), \sin(k^y a/2)) \hspace{1cm} (6)$$

The propagator for this real field is

$$D(\xi, \xi') = -i\langle \phi(\xi) \phi(\xi') \rangle \hspace{1cm} D_{\omega, \vec{k}}^{(0)} = \frac{(\kappa_{\vec{k}})^2}{\omega - \omega_{k}(\vec{k}) + i\delta}$$

In further computations we will not need the explicit form of $\omega_{k}(\vec{k})$, and the only assumption is that $0 \leq \omega_{k}(\vec{k}) \leq \omega_{D}$, where $\omega_{D}$ is the Debye frequency. In other words we need $\omega_{k}(\vec{k})$ to be limited for all $\vec{k}$.

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and the propagator of spin waves

$$\chi(\xi, \xi') = -i\langle \phi(\xi) \phi^{\dagger}(\xi') \rangle \hspace{1cm} \chi_{\omega, \vec{k}} = \frac{1}{\omega - \omega_{\vec{k}} + i\delta}$$

Now we can put $z$ axis perpendicular to the plane of atomic lattice, as it was before spin wave quantization. The magnon dispersion for the Hamiltonian $J \vec{S}_i \vec{S}_{i'}$ is just $\omega_{\vec{k}}(\vec{k}) = 2J\kappa_{k}^{x}$, and we should preserve it since it should be consistent with interaction Hamiltonian.

The interaction Hamiltonian is the sum over $\alpha = x,y$

$$\mathcal{H} = \sum_{\omega, \vec{k}, \vec{q}} \sqrt{\rho}^{\omega} b_{\vec{k}, \vec{q}}^{\dagger} a_\alpha \kappa_{\vec{k} - \vec{q} + \vec{k}/2}^{\alpha} a_{\vec{q} + \vec{k}/2}^{\dagger} + \text{c.c.} \hspace{1cm} (10)$$
where
\[ g_{k,q}^2 = 4g_{k}^{2}k^{\alpha}q_{q}^{\alpha}k^{\alpha}/k \quad g_{k}^2 = \frac{dJ}{da} \frac{k^{2}k^{\alpha}/k}{\sqrt{2\omega_{k}(k)}} \] (11)

Then the Dyson equation for the phonon propagator becomes matrix,

\[ \left[ \frac{1}{D_{\omega,k}} \right]_{\alpha\beta} = \frac{1}{D_{\omega,k}^{(0)}} \delta_{\alpha\beta} - M_{\omega,k}^{\alpha\beta} \]

\[ M_{\omega,k}^{\alpha\beta} = i \int \frac{d\omega'}{(2\pi)^{2}} g_{k,q}^{2} g_{k,q}^{2} \chi_{\omega',\omega}^{'*} \chi_{\omega',\omega}^{*} \]

and integration of the magnon loop, see Fig. 1, is our primary task.

The frequency integration is simple and keeping real part in the answer we have

\[ \int \frac{d\omega'}{(2\pi)^{2}} \chi_{\omega',\omega}^{'*} \chi_{\omega',\omega}^{*} = \frac{1}{\omega - 2J\tilde{\kappa}^{2}q_{k}^{2}/k_{s}} \] (13)

The \( \tilde{q} \) integral in turn is complicated. At low frequencies important for phonon dispersion

\[ M_{\omega,k}^{\alpha\beta} = \omega I_{k}^{\alpha\beta} f_{k} \quad I_{k}^{\alpha\beta} = g_{k}^{2} g_{k}^{2} \delta_{\alpha\beta} + \cos k_{x}^{\alpha} \cos k_{y}^{\alpha} \frac{2}{2\pi J^{2}a^{2}} \] (14)

and it has the pole

\[ f_{k} = \frac{\sin^{2} k_{x}^{\alpha}/k_{s}^{2} - \sin^{2} k_{y}^{\alpha}/k_{s}^{2}}{\sin^{2} k_{x}^{\alpha} + \sin^{2} k_{y}^{\alpha}} + \text{non-singular term} \] (15)

where \( \sin^{2} k_{x}^{\alpha}/k_{s}^{2} > \sin^{2} k_{y}^{\alpha}/k_{s}^{2} \) and one should interchange \( k^{x} \) with \( k^{y} \) when \( \sin^{2} k_{x}^{\alpha}/k_{s}^{2} < \sin^{2} k_{y}^{\alpha}/k_{s}^{2} \).

There are two branches of the phonon dispersion, as obtained from Eqs. (12), (14), and \( \det D_{\omega,k}^{-1} = 0 \). Near the pole of \( f_{k} \) one branch is the original phonon dispersion \( \omega = \omega_{0}(k) \) and another branch is

\[ \frac{\omega^{2} - \omega_{0}^{2}(k)}{(\kappa_{k}^{2})^{2}} - \omega[I_{k}^{\alpha\beta} + I_{k}^{\beta\alpha}]f_{k} + \text{n.s.t.} = 0 \] (16)

where n.s.t. stands for non-singular terms. Our result Eq. (1) with all prefactors reads

\[ \omega = (\kappa_{k}^{2})^{2}[I_{k}^{\alpha\beta} + I_{k}^{\beta\alpha}]f_{k} \] (17)

valid for \( \omega \ll J(\kappa_{k}^{2})^{2} \) - condition for \( \omega \)-expansion of \( M_{\omega,k}^{\alpha\beta} \).

In conclusions the phonon dispersion is modified by interaction with spin waves; the effect is strong for large phonon wave numbers (new branch goes \( \propto k^{3} \)) and should be observed experimentally. The phonon dispersion becomes singular along \( k_{x} = \pm k_{y} \) lines opening a lot of room for electron pairing, that could be key solution for high-temperature superconductivity. This work has been inspired by discussion at Physics department of Stanford University. The experiment showed that low \( k \) part of the phonon spectrum depends strongly on electron density where as high \( k \) part is completely insensitive. This is in agreement with our results, because the renormalization of \( D_{\omega,k}^{(0)} \) by electron-phonon interaction does not change \( \omega(k) \) given by Eq. (17).