# MOTTNESS
# AND STRONG COUPLING

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**based on various papers**
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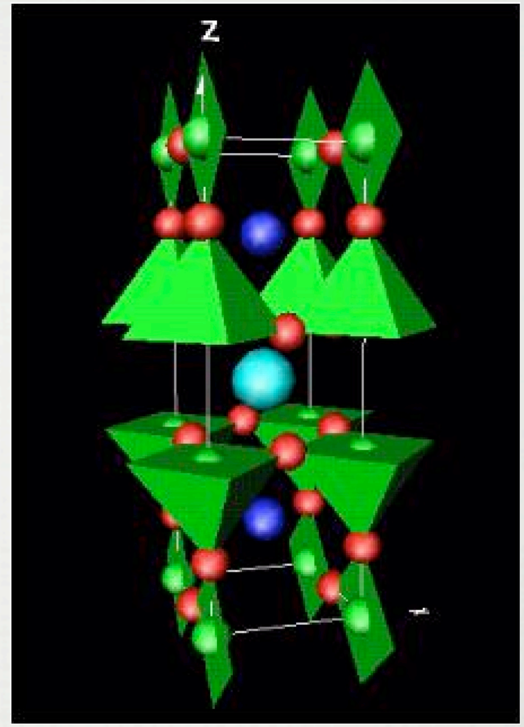
**PRL 99 (2007) 046404**
**PRB 77 (2008) 014512**
**PRB 77 (2008) 104524**
**0802.3405**

Rutgers University
April 2008

# High $T_c$ Materials

- superconductivity was discovered about 20 years ago in copper oxide materials, with rather high critical temperatures
- electronic properties can be changed by 'doping' with rogue atoms -- these are thought of as supplying or removing extra electrons from the system
- because of the electronic orbital structure, it is a good approximation to take the electrons to move in a 2d plane
  - *idealize as electrons hopping between sites of a square lattice*
  - *a useful model Hamiltonian is the Hubbard model, for reasons that we will explore shortly*

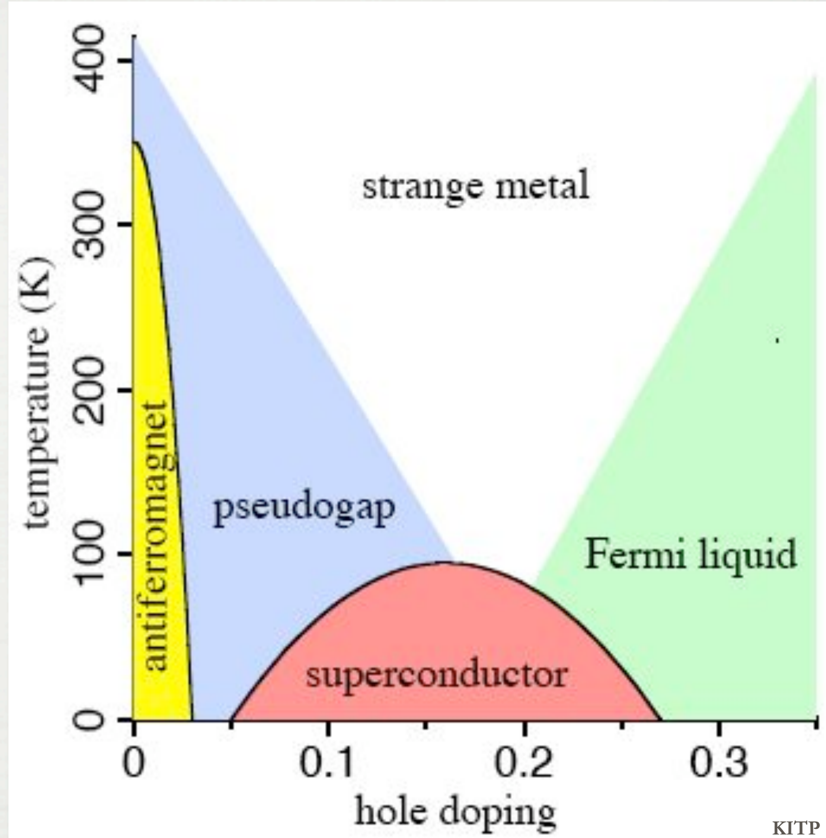


# High $T_c$ Materials: Phases

- different phases are encountered depending on temperature, magnetic field and ***filling***
  - *filling refers to number of electrons on lattice*
  - *half-filling = zero doping = one electron per site*

- half of the phase diagram (at zero magnetic field) is shown
  - *anti-ferromagnetic near half-filling*
  - *superconducting dome*
  - *'pseudogap' in between (density of states exhibits a dip, but no clear gap)*

$x$ = number of holes per site (compared to half filling) = $1-n$




KITP

# BCS Theory

**FERMI LIQUID:**
interacting theory consists essentially of 'renormalized' electrons

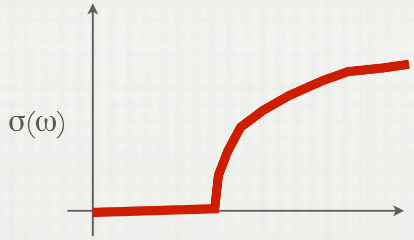
- the low temperature superconductors are well described by the BCS theory
  - *normal state is a Fermi liquid, and there is a phonon-induced pairing mechanism which leads to U(1)-violating condensation*
  - *the robustness of the pairing can be traced to the existence of a (non-trivial) relevant perturbation as one renormalizes to the Fermi surface*

- the phase diagram of the cuprates cannot be explained by BCS, for a variety of reasons
  - *critical temperature of the superconducting transition is too high*
  - *the 'normal state' has exotic features, and is in fact an insulator, rather than a conductor*
    - will argue that this should not be thought of as a Fermi liquid

- the first step, as in the case of BCS, is to understand the normal state
  - *with luck, this will lead to new possibilities for a description of the superconducting state as well*

# Mott Insulators

- normal metals are conducting because there are gapless excitations above the ground state (Fermi surface)
  - *i.e., an unfilled band (and weak interactions)*
- normal insulators don't conduct because they are gapped
  - *i.e, a filled band*




- such materials are well described by Fermi liquid theory
  - *i.e., more or less free quasiparticles (~dressed electrons) carry charge (or not)*
  - *i.e., RG towards Fermi surface is not exotic, interactions are irrelevant*
- Mott insulators insulate only through strong coupling effects
  - *electronic picture has only partially filled bands, with no apparent gap*
  - *the prototype model is the Hubbard model, with less than two electrons per site*

# Hubbard model

- square lattice, up to two electrons per site (spin 1/2)

$$H_{\mathrm{Hubb}} = -t\sum_{i,j,\sigma} g_{ij}c^\dagger_{i,\sigma}c_{j,\sigma} + U\sum_{i,\sigma} c^\dagger_{i,\uparrow}c^\dagger_{i,\downarrow}c_{i,\downarrow}c_{i,\uparrow}$$

(multi-band models also exist)

- $t, U$ are energy scales that should be determined experimentally
- if $U \ll t$, this would be a simple model with a weak 4-fermi interaction
- in the cuprates, typical values are $U \sim 4-5eV,\ t \sim 0.5eV$
- thus the system is inherently ***strongly coupled***
- we would then expect that this is an insulator at half-filling, because there is such a large energy cost to doubly occupy sites (and that is the only way to move electrons around at half filling)
- *away from half-filling, the insulating property would go away*
- *in fact, a gap persists away from half-filling, and many interesting properties*

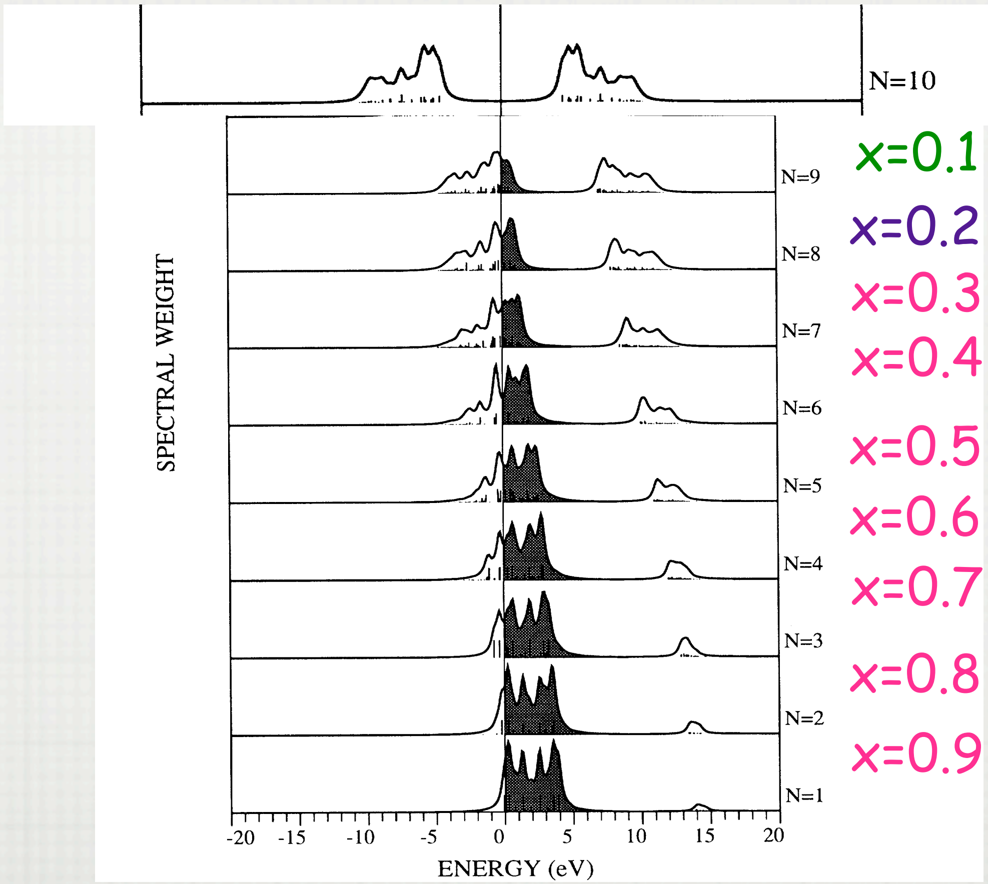
# ‘UV-IR Mixing’

- one of the interesting features of this system is the behaviour of the density of states as we change the filling/ doping
  - *the density of states changes shape (‘spectral weight transfer’)*
  - *states that were at high energy come down to low energy*
- in a sense, the electron splits into two pieces, one moving in the LHB, one moving in the UHB

$$c_{i,\sigma} = c_{i,\sigma}(1 - n_{i,-\sigma}) + c_{i,\sigma} n_{i,-\sigma}$$

- these ‘pieces’ are non-canonical
- in fact, I want to argue that this can be taken to imply that new degrees of freedom emerge at low energies, that cannot be thought of as electrons
  - *that is, this is not a Fermi liquid*
- to do so, we consider the single particle density of states carefully

# Spectral weight transfer



# Fermi Liquid

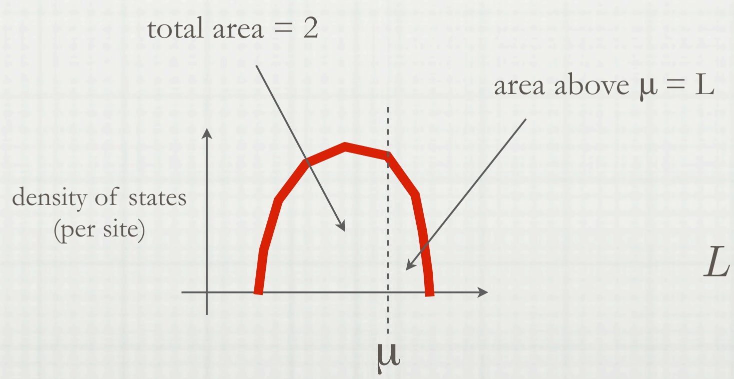
- let's begin with free spin ½ fermions on N sites
  - *if we have* $n = 1$, *we could add N particles to the system (to get to* $n = 2$, *fully filled)*
  - *if we have* $n = 1 - x$, *we could add* $N(1 + x)$ *particles to the system*
  - *thus the number of particles that we can add to the system (at low energies) is* $n_h = 1 + x$
- as we change the filling, the Fermi surface contracts
  - *L states remain above the Fermi surface (chemical potential)*
  - *this is just* $L = 2 - n = 1 + x$
- thus $L/n_h = 1$

$n$ = number of electrons per site

$x$ = number of holes per site

$n_h$ = number of electrons that can be added (at low energy)

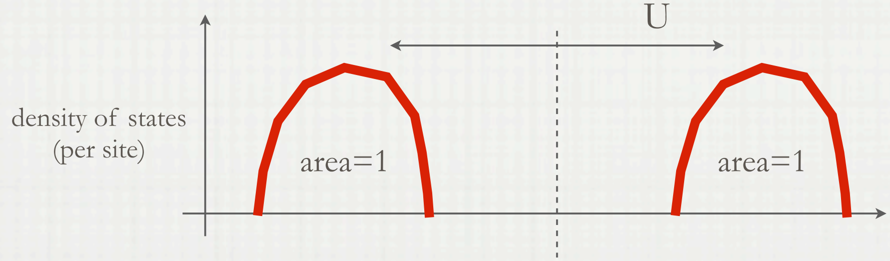
$L$ = density of states above chemical potential




$$L = \int_{\mu}^{\Lambda} d\omega N(\omega)$$

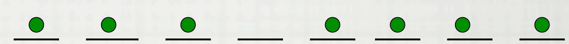
# Hubbard Model - Infinite U

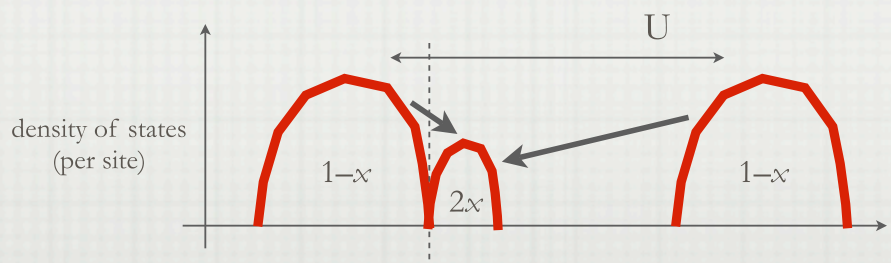
- it is also simple to analyze the strong coupling limit, where $U = \infty$
  - *in this limit, there is no hopping*
  - *at* half filling, *there is one particle on each site*
  - *if we add particles to the system, they are all at high energy, thus* $L = n_h = 0$




half filling

- if we dope the system with holes, when we add particles, there are two (spin) states at low energy per hole
  - *states come down from high energy*





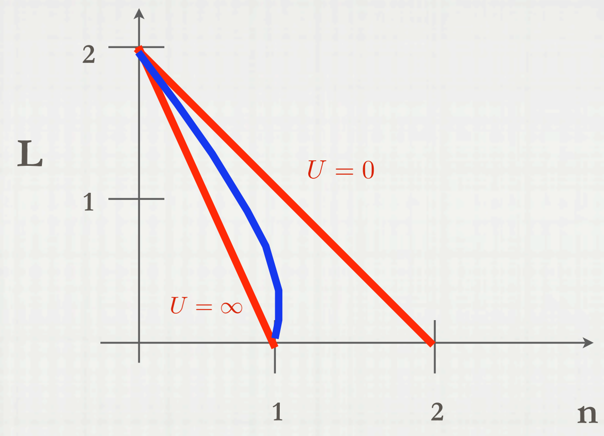

hole doped

$$L = n_h = 2(1 - n)$$

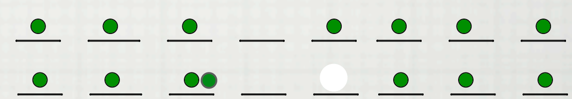
$$\boxed{L/n_h = 1}$$

# Finite Hopping

- one way to understand these results is via the following plot




- at finite U, the ground state will contain admixtures (suppressed by t/U) of configurations with doubly occupied sites
- thus, when we dope the system, not only do we get low energy states because there are empty sites, but there are configurations in the ground state in which even more empty sites are available
- $n_h$ remains $2x$, but $L$ increases, which implies $\boxed{L/n_h > 1}$



- we conclude that if we dope the system at finite t/U, there is more spectral weight at low energy than is accounted for by counting particles
  - **— new degrees of freedom must emerge**

# A Low Energy Description

- we wish to develop a low energy description of the Hubbard model
    - *"integrate out the upper Hubbard band"*
- because of our discussion, this is not a straightforward matter
- a traditional approach to this problem is by **projection**
- by a similarity transformation on the electron operators, one can block diagonalize the Hamiltonian
- *the energy eigenvalues of states in different blocks are separated at order U (for large U/t)*
- *one obtains a simple spin model, the* tJ*–model as a first approximation*

$$\mathcal{H}_{\text{Hubbard}} \to \mathcal{H}_{tJ} + \text{ stuff}$$

- the tJ–model is often taken as the starting point for the cuprates
- *however, this is dangerous for a variety of reasons*
    - the fermionic operators of the tJ model are not electrons, they are complicated admixtures of multi-particle operators
    - the extra 'stuff' is important for a description of many important experimental phenomena
- note also that limits $U \to \infty, \quad N \to \infty$ do not commute
- is there a better way? can we construct an **effective** theory?

# Integrating out UHB

- in the course of developing a low energy description of the Hubbard model, we will find new degrees of freedom emerging at low energy which cannot be thought of in terms of electrons
  - strong analogue to non-linear sigma model
    - *Lagrange multiplier field grows dynamics in IR, determines vacuum structure*

- **the problem**: the UHB is associated with multi-particle states (doubly-occupied sites)
  - *it's not clear how to do the 'integration' over the UHB*
  - *the theory is strongly coupled*

- **proposed solution**:
  - *extend Hilbert space -- introduce new degree of freedom representing the doubly occupied states*
  - *i.e., isolate these states in 'elementary massive field' (which may be integrated out)*
  - *include constraint such that the extended model is* **equivalent** *to the Hubbard model*

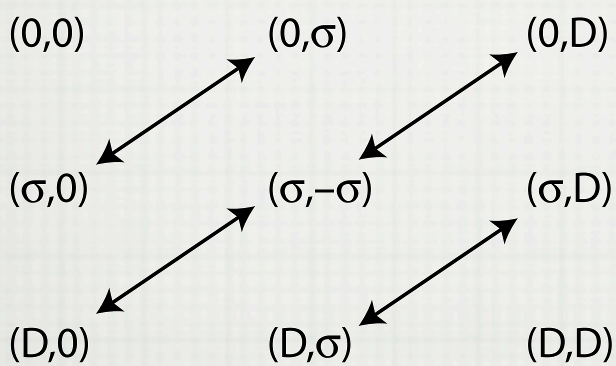
analogue approach electron gas collective behaviour
D. Bohm and D. Pines, Phys. Rev. 92 (1953) 609.

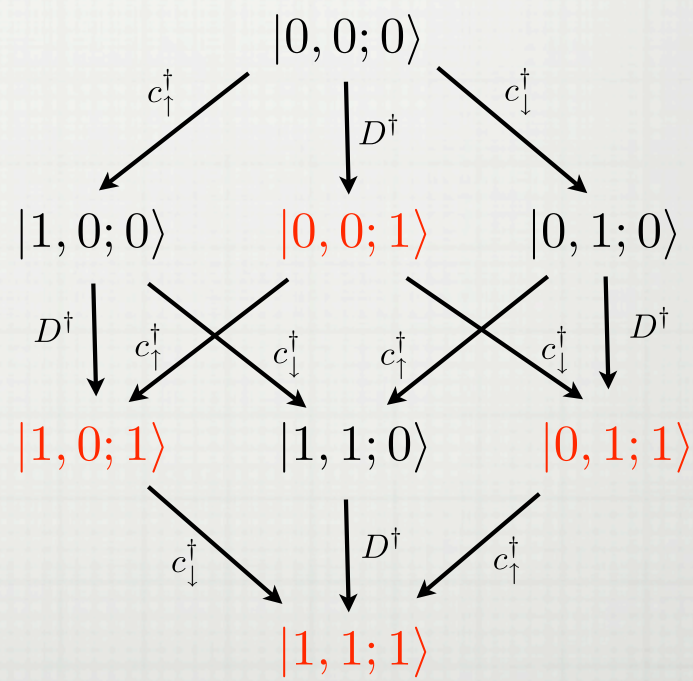
# Extended Hilbert Space

- introduce fermionic oscillator $D$

$$\otimes_i \left(\mathcal{F}_\uparrow \otimes \mathcal{F}_\downarrow\right) \longrightarrow \otimes_i \left(\mathcal{F}_\uparrow \otimes \mathcal{F}_\downarrow \otimes \mathcal{F}_D\right)$$

- introduce Hamiltonian which contains terms corresponding to hops in and out of doubly occupied states (which are replaced by D-oscillators)



# Extended Hamiltonian (hole-doped)

- we'll think in terms of a path integral
- because $D$ is fermionic, introduce Grassmann parameter to keep track of statistics

$$L = \int d^2\theta \left[ \bar{\theta}\theta \sum_{i\sigma} (1 - n_{i-\sigma}) c^\dagger_{i\sigma} \dot{c}_{i\sigma} + \sum_i D^\dagger_i \dot{D}_i \right.$$

$$+U \sum_j D^\dagger_j D_j + H_{\text{con}}$$

U dependence

$$\left. -t \sum_{i,j,\sigma} g_{ij} \left[ C_{ij\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + D^\dagger_i c^\dagger_{j,\sigma} c_{i,\sigma} D_j + (D^\dagger_j \theta c_{i,\sigma} V_\sigma c_{j,-\sigma} + h.c.) \right] \right],$$

- appropriate constraint $H_{\text{con}} = s\bar{\theta} \sum_j \varphi^\dagger_j (D_j - \theta c_{j,\uparrow} c_{j,\downarrow}) + h.c.$

bosonic Lagrange multiplier

- after manipulations, the Grassmann parameters will disappear
- can show that this is *equivalent* to the Hubbard model

# Extended Hamiltonian

- integrate over $\varphi \longrightarrow$ solve constraint (linear in $D$) $\longrightarrow$ Hubbard model

$$\delta[D - \theta c_\uparrow c_\downarrow]$$

- Hamiltonian is quadratic in $D$ — ($D$ has 'mass' $U$)
  - *integrating over $D$ gives low energy theory* $H_{eff}[c, c^\dagger, \varphi]$
  - *this can be done exactly, because theory is Gaussian in $D$*

$$\tilde{H}_{\text{int}} = -\frac{t^2}{U}\sum_{j,k} b_j^\dagger (\mathcal{M}^{-1})_{jk} b_k - \frac{s^2}{U}\sum_{i,j}\varphi_i^\dagger (\mathcal{M}^{-1})_{ij}\varphi_j - s\sum_j \varphi_j^\dagger c_{j,\uparrow} c_{j,\downarrow} + \frac{st}{U}\sum_{i,j}\varphi_i^\dagger (\mathcal{M}^{-1})_{ij} b_j + h.c.,$$
$$+ tr\ \log \mathcal{M}$$

**ω dependence hidden**

- we identify $s \sim t$
- $\varphi$ is a charge $2e$ classical scalar field
- we expect it to contribute to dynamics in the IR (for large lattice), **in some sense**

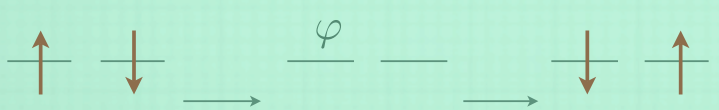
$$b_i = \sum_j b_{ij} = \sum_{j\sigma} g_{ij} c_{j,\sigma} V_\sigma c_{i,-\sigma}$$

$$\mathcal{M}_{ij} = \delta_{ij} - \frac{t}{U} g_{ij} \sum_\sigma c_{j,\sigma}^\dagger c_{i,\sigma}$$

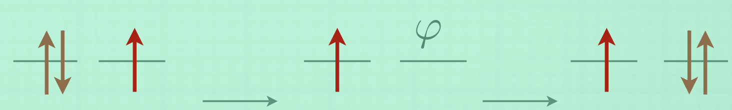
# Comments

- $\varphi$ is a charge $2e$ scalar, without dynamical term at tree-level
- the theory is still interacting, so the physics is not immediately apparent
- if $s$ were large, would make sense to integrate out $\varphi$
  - *this leads directly back to the UV theory (Hubbard model)*
  - *not a surprise, because integrations can be done* **exactly**
- dynamics of electrons is amongst non-doubly occupied sites only
  - *but doubly occupied sites can be 'unblocked' by conversion to boson occupation*
  - *important mechanism for conduction*

$$\mathcal{L}_{kin} = \sum_{\sigma} (1 - n_{i,-\sigma}) c^{\dagger}_{i,\sigma} \dot{c}_{i,\sigma}$$




SPIN FLIP




'DOUBLON' MOTION

# Comments

- as $U \to \infty$ , projected model is recovered
  - $\varphi$ *integration reduces to* $\delta(c_{i,\uparrow} c_{i,\downarrow})$
  - *i.e., no double occupancy*
  - *or, if we simply set* $\varphi \longrightarrow 0$, *the tJ model is recovered --* $\varphi$ *represents non-projective physics*

- this can be made more precise by comparing our theory to projection + perturbation theory
- such a procedure generates complicated multi-particle effects
  - *these are subsumed into simpler interactions involving the scalar field*

- **what is the physics at low energies?**
- one might suppose the simplest thing -- that the scalar field grows dynamics radiatively and becomes a propagating degree of freedom
- early on, we made this supposition and analyzed mean field theory
  - *e.g., might have expected a condensate of the scalar field to drive superconductivity*
  - *however, it seems difficult to generate the proper (d-wave) spatial symmetry with this condensate, among other problems*
- there is another possibility...

# Bound States

- consider again the derivation of the theory
- one can ask: what object would give the electron upon return to the Hubbard model?
- in fact, it is non-trivial

$$c^\dagger_{i,\sigma} \rightarrow (1-n_{i,-\sigma})c^\dagger_{i,\sigma} + V_\sigma \frac{t}{U} b^\dagger_i \mathcal{M}^{-1}_{ij} c_{j,-\sigma} - V_\sigma \frac{s}{U} \boxed{\varphi^\dagger_i \mathcal{M}^{-1}_{ij} c_{j,-\sigma}}$$

new charge *e* operator

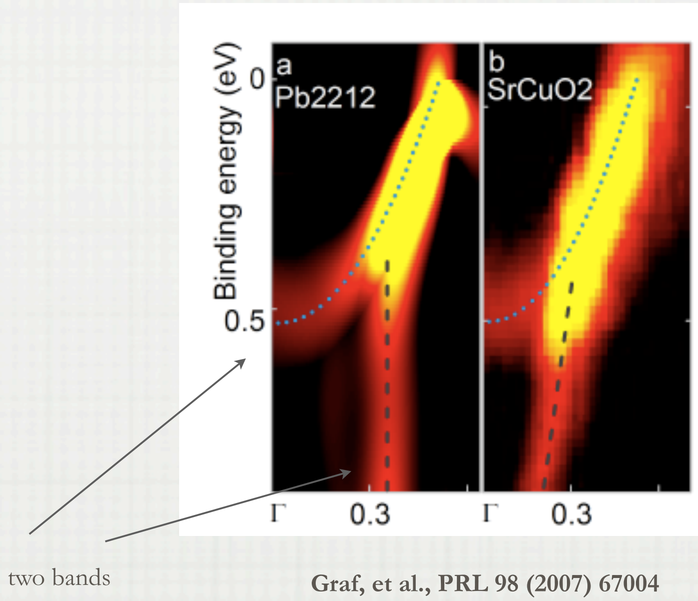
- correspondingly, the EM current takes the form

$$J_{i,j} = ie\left[\sum_\sigma g_{ij}\alpha_{ij\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + \frac{s}{U}\varphi^\dagger_i b_{ij} + \frac{t}{U} b^\dagger_i b_{ij} - h.c. + \ldots\right]$$

- we take this as some indication that $\varphi^\dagger c$ may act as a separate degree of freedom in the low energy theory
  - *this has the same quantum numbers as* $c^\dagger$

# Spectral Function

- in fact there is some evidence for this
  - *experimental data probing the single-particle density of states sees a bifurcation below the chemical potential*



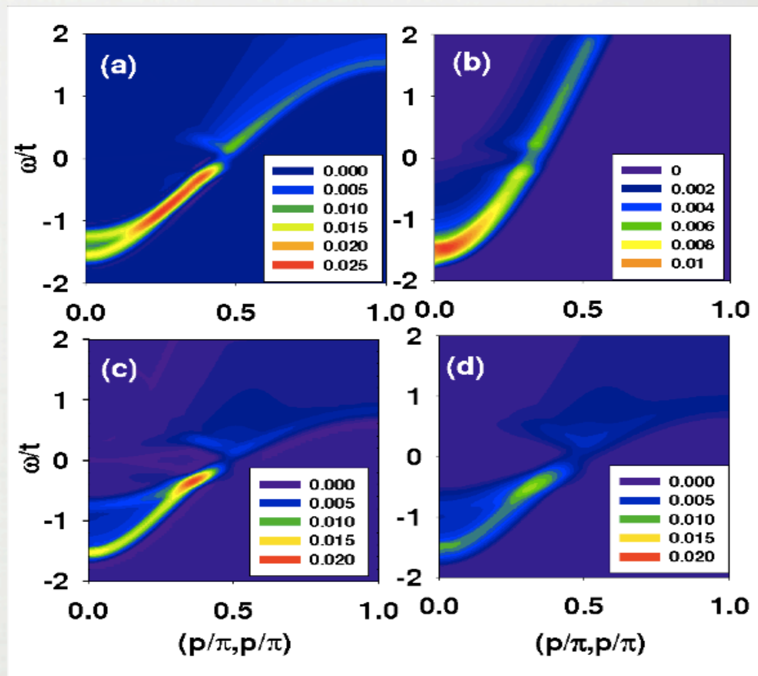

**Graf, et al., PRL 98 (2007) 67004**

# Spectral Function

- in fact, a simple simulation in the low energy theory reveals kinks and a bifurcation in the single particle density of states
- the bifurcation goes away for large doping
- determined by *t*-scale physics
- the two branches come from the ordinary electron, and a 'bound state' $\sim \varphi^\dagger c$
  - *$\varphi$ itself is non-dynamical*
- the ordinary branch gives the *2x* part of the spectral weight transfer, while new branch gives dynamical part
- (a full understanding of the binding mechanism has not been established) — Bethe-Salpeter?

SINGLE PARTICLE DISPERSION

$n = 0.8$ $n = 0.4$




$U = 10t$ $U = 20t$



saddle point (couldn't be consistent with 2 modes)
mean field (would not allow for bound states)
est thing to do is consider electron 2pt function in

# Pseudogap

- recall the pseudogap -- a dip in the density of states
- the formation of the composite excitation appears to be consistent with a pseudogap
    - *in fact, can see this in the plots*
- because of the pseudogap, would also expect divergence in DC resistivity as T goes to zero.
    - *indeed, simulations show this (and it goes away if we remove the boson by hand)*
- note that, because $\varphi$ is associated in some sense with double-occupancy, we might associate this with a 'binding' of doublons to holes

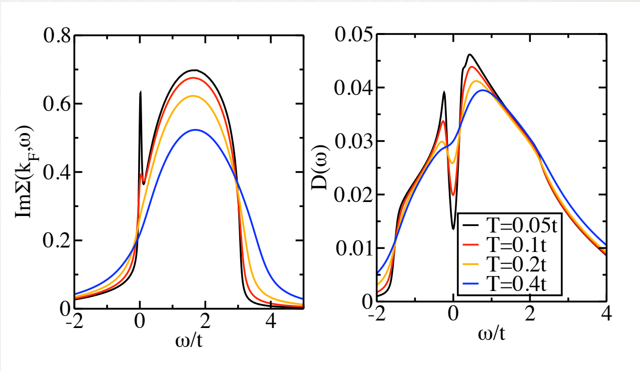
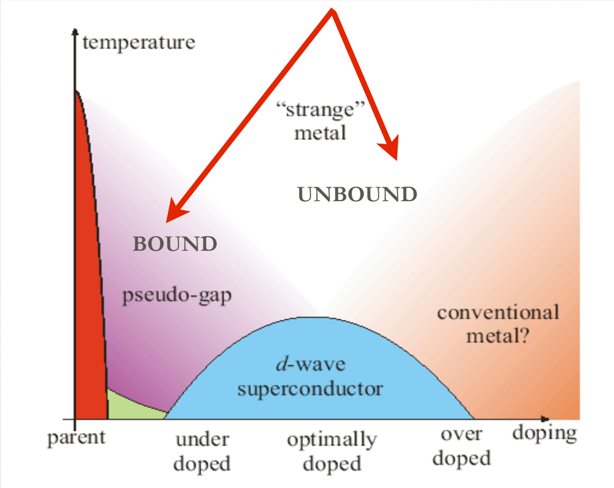



FIG. 5: The imaginary part of the self energy as the function of temperature for $n = 0.7$. A peak is developed at $\omega = 0$ at low temperature which is the signature of the opening of the pseudogap. The density of states explicitly showing the pseudogap is shown in adjacent figure.

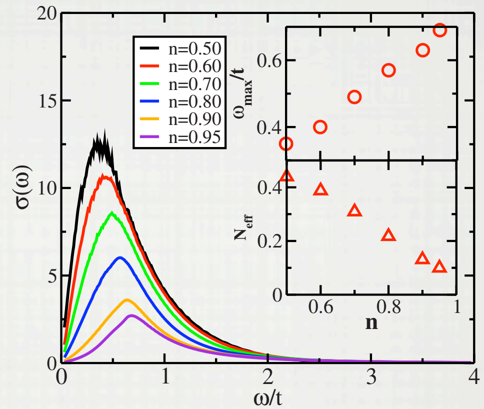
# Linear T Resistivity

- in the strange metal regime, it is found that resistivity scales linearly with temperature
    - *in fact, in normal metals, electron-phonon scattering gives linear in T behaviour above the Debye temperature*
    - *the scales involved in that physics are all wrong for this system though*
- in fact, it has been argued that Fermi liquid theory could not possibly give rise to this effect (Polchinski; Shankar)
- in our low energy theory, as we increase the doping, we expect that the binding mechanism disappears above some critical doping
    - *if above this critical value, charge 2e bosons can be produced, boson-electron scattering could give rise to linear T resistivity, much as for phonon scattering*

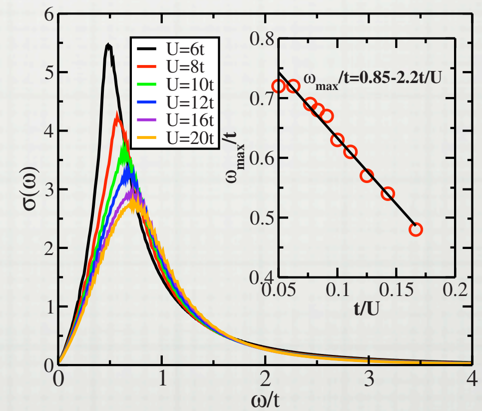


# Optical Conductivity

- another test of the theory is in the two particle channel
  - *e.g., optical conductivity governed by current-current correlators via Kubo*
- an important feature is a 'mid-infrared band' in the conductivity
  - *this is an unexpected feature, because the natural energy scales are in the UV (U) and far IR (J)*
- simulations based on our low energy theory give such a feature, and its presence is due to mobile double occupancy (accounted for by charge 2e bosons) in the lower Hubbard band
  - *fairly insensitive to U — determined by t-scale physics*
- consequences of the low energy theory would also be expected to show up in related quantities
  - *e.g. dielectric function*




vs. filling




vs. U

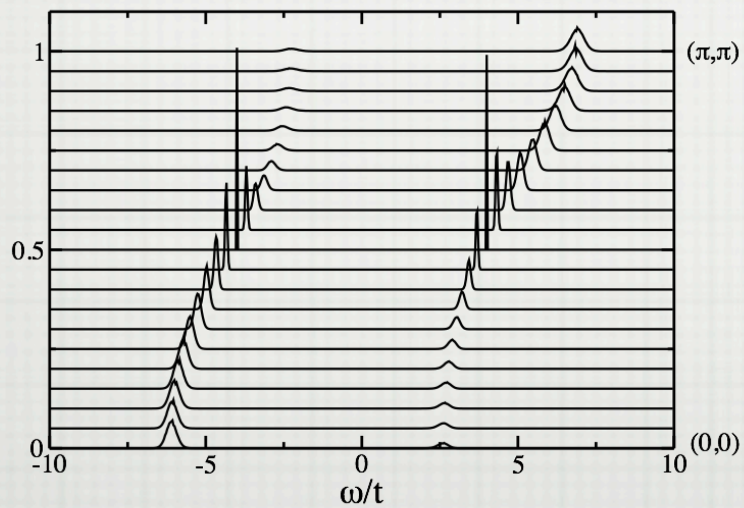
# Comments

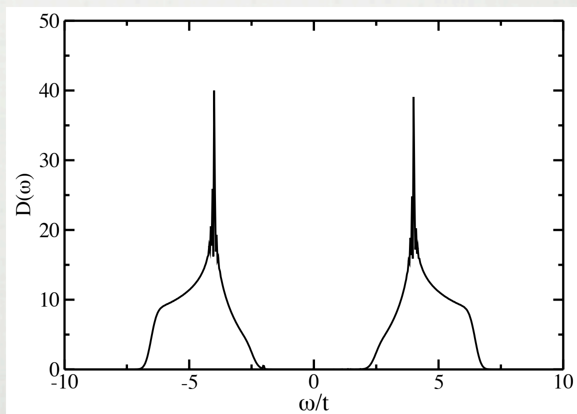
- the version of the theory that I've shown here is appropriate to hole doping. There is a similar version for electron doping, and a version applicable to the half-filled state.
- Anti-ferromagnetic order
  - *near zero-doping, antiferromagnetic order is seen experimentally*
  - *in the low energy theory, this might be associated with condensation of* $\langle \varphi_i^\dagger c_{i,\sigma} V_\sigma c_{j,-\sigma} \rangle$ *, which has zero charge, and staggered spins*
  - *the Mott gap itself might be explained by the binding up of charge in this way*

- Superconductivity
  - *the low energy theory provides possible new channels for pairing and charged condensates* $\langle c \cdot c \rangle$ $\langle c \cdot \varphi c^\dagger \rangle$
  - *(under investigation)*

# The Mott Gap

- at half filling, the low energy theory is very simple (no $\mathcal{M}_{ij}$ factors)
- using the low energy theory, we can derive the spectral function (Im G(k,ω)) at half-filling
  - *extremely simple calculation if we just drop spin-spin interactions*
- the result has the expected form (!)
  - *Mott gap*
  - *k-dependent spectral function*
  - *Re G(k, ω) changes sign at would-be Fermi surface*
- gives confidence that the low energy theory is capturing the correct physics



# Conclusions

- we have constructed systematically a low energy theory of the Hubbard model in the strongly coupled regime
- this low energy theory contains an emergent degree of freedom which carries electric charge and makes important contributions to a variety of phenomena
- the precise nature of the normal state is under investigation
  - *good results with some simple assumptions (that we hope to firm up a posteriori)*
- promising possibilities for a description of the superconducting phase