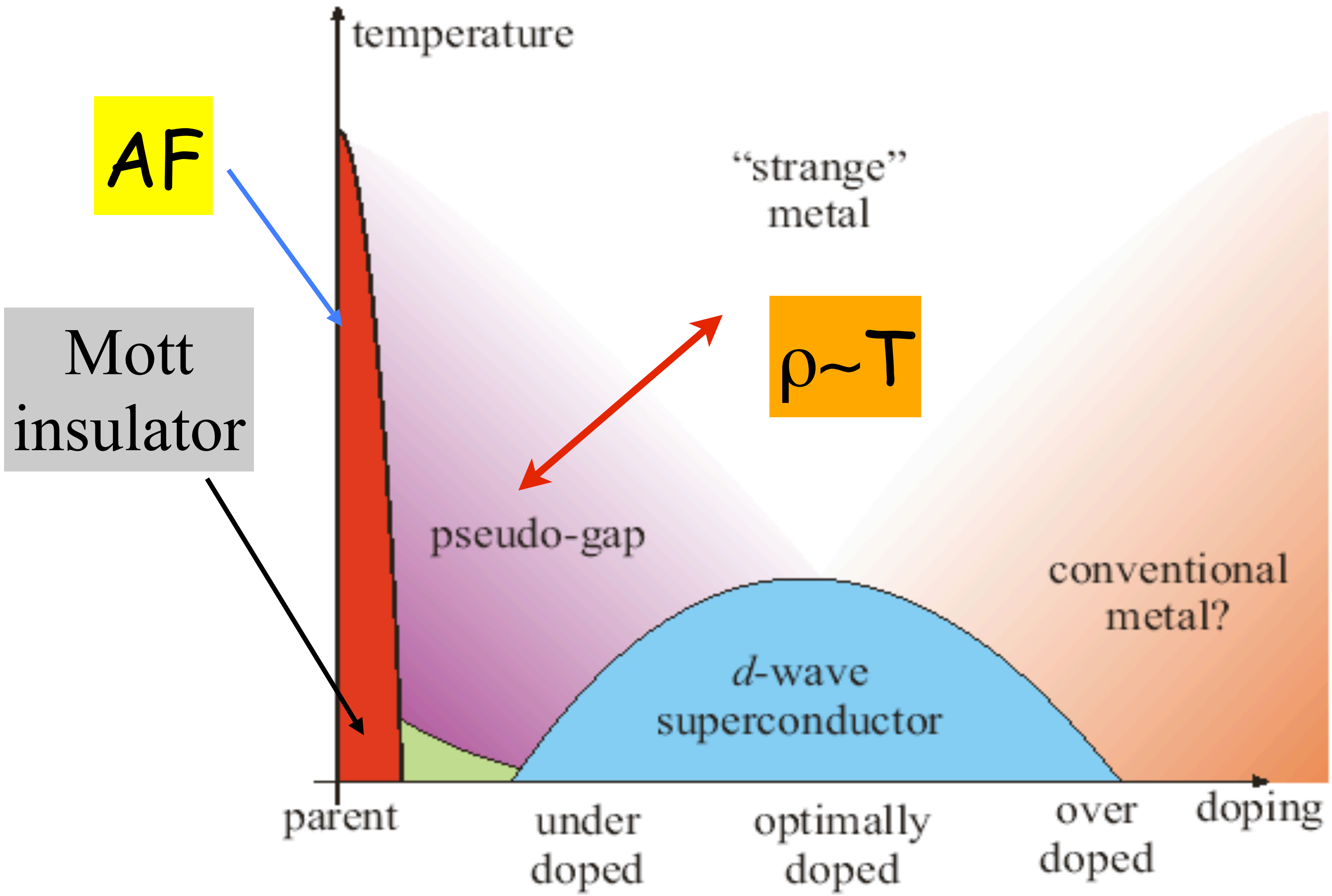
Hidden Charge 2e Boson in Doped Mott insulators:

Field theory of Mottness

Thanks to: T.-P. Choy, R. Leigh
(PRL, 99, 46404 (2007) and
arxiv:0707.1554, PRB in press)

Key Message: 2 distinct
charge e excitations
at low energy in a DMI

0.) Normal State: Charge Degrees of Freedom?



approach

Isolate the relevant degrees of freedom

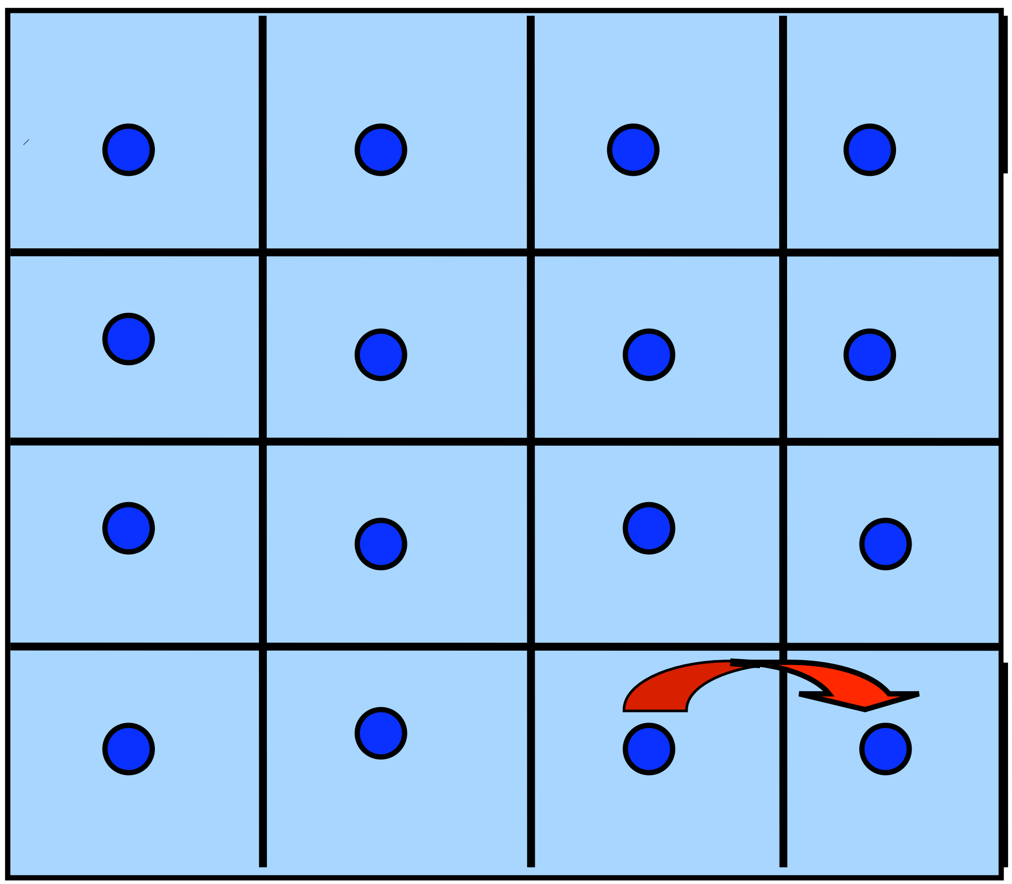
↓

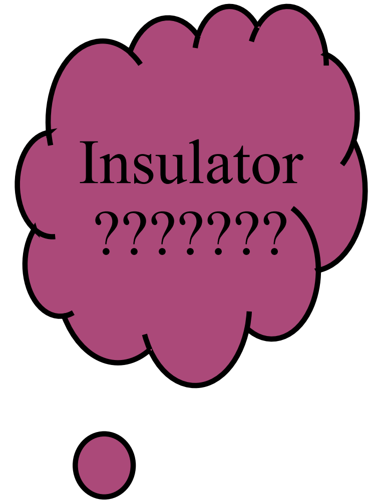
Construct low-energy theory

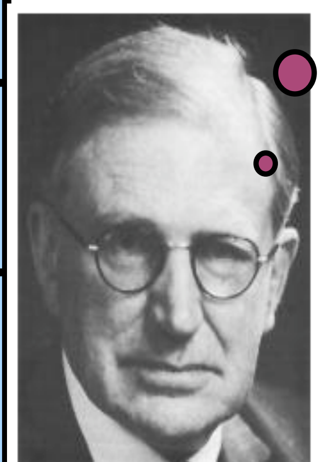
(Spectral Weight Transfer)

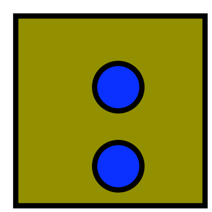
Mott Problem: NiO

Station Q floor plan (N rooms N theorists)



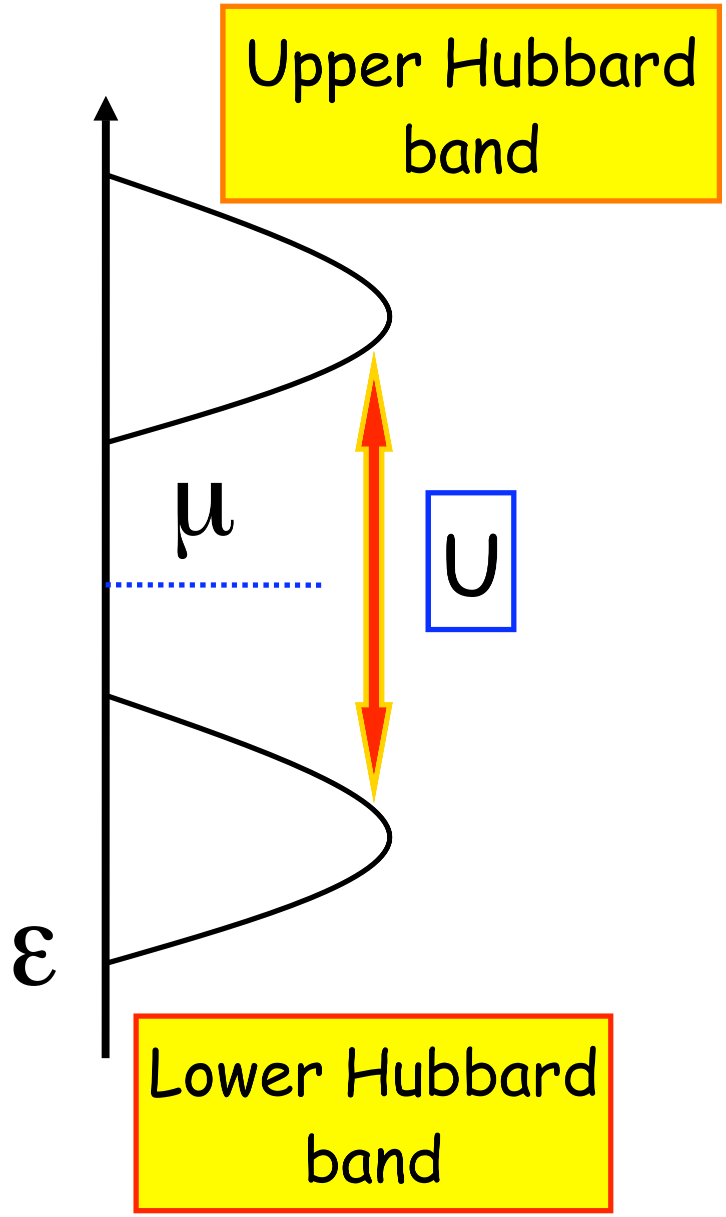




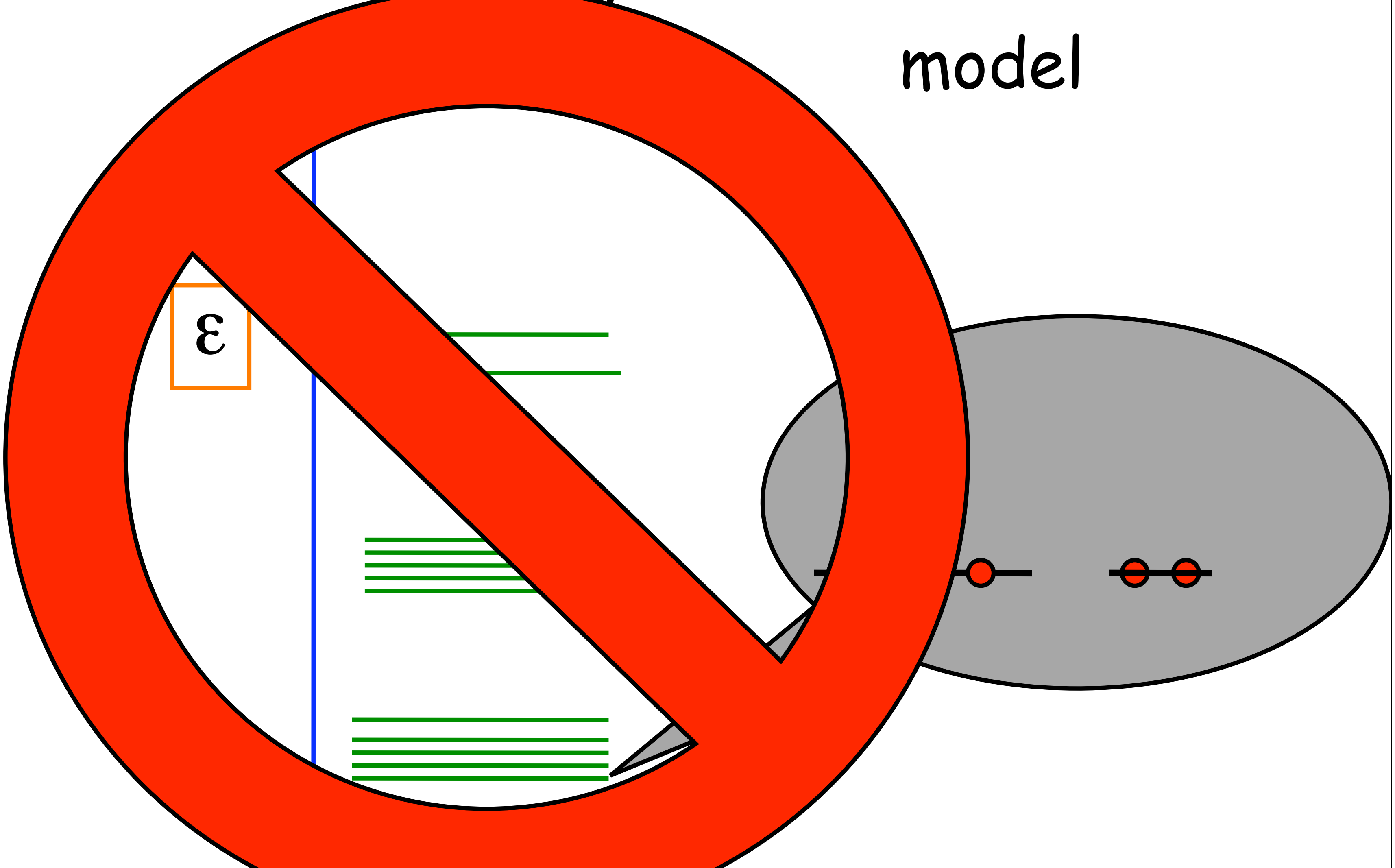


$\Delta E = U \gg K.E.$

Low-energy Theory?



Order eigenstates of Hubbard model



Only possible for small systems

Low-energy Theories:

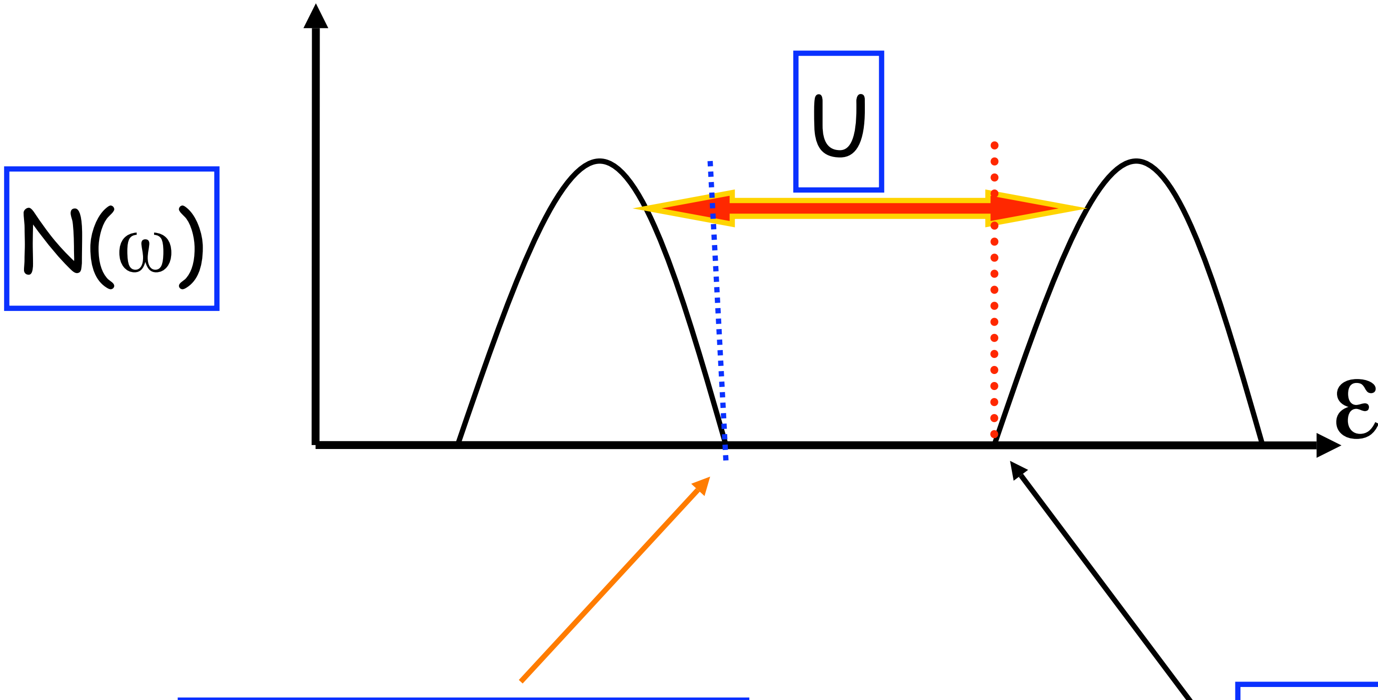
$S(\phi)$

Integrate Out high Energy fields

$\phi = \phi_L + \phi_H$

$$e^{-S_{\rm eff}[\phi_L]} = \int d\phi_H \exp - S(\phi_L, \phi_H)$$

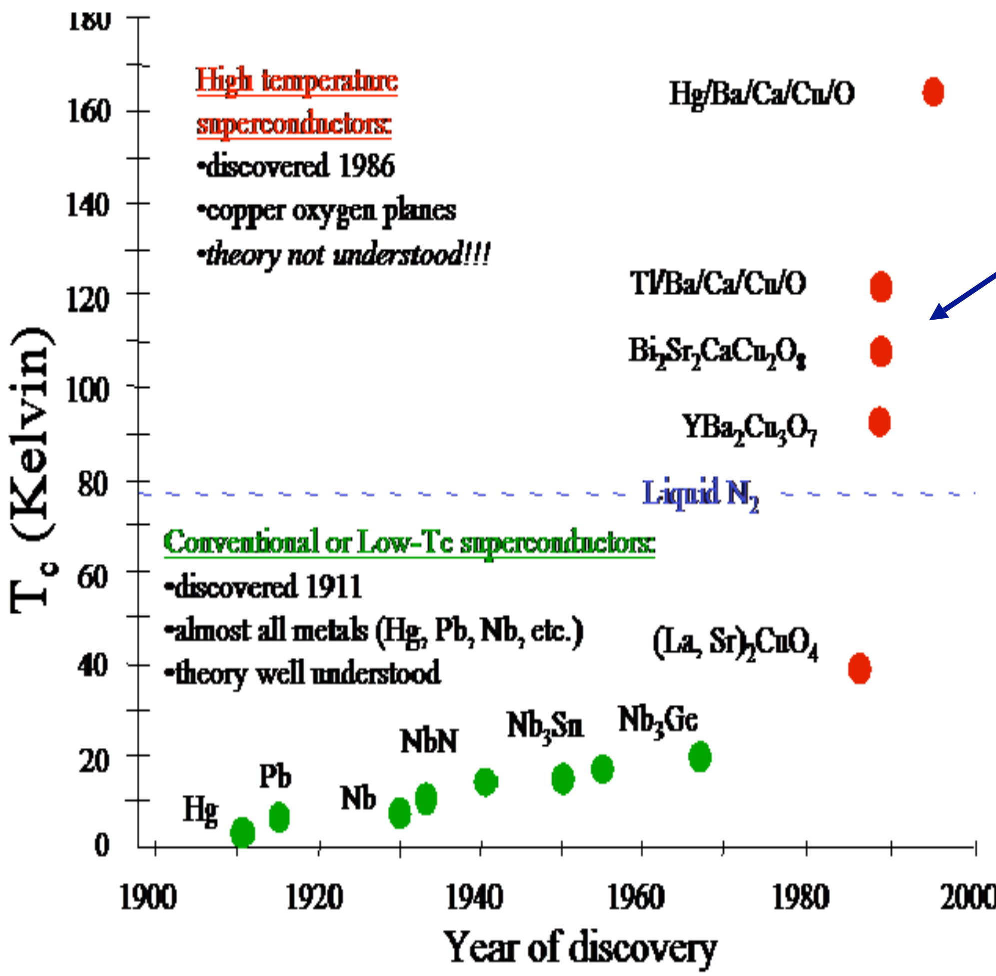
Low-energy theory



Hole doping: Integrate out UHB

e-doping: Integrate out LH B

Goal: Identify high-energy field



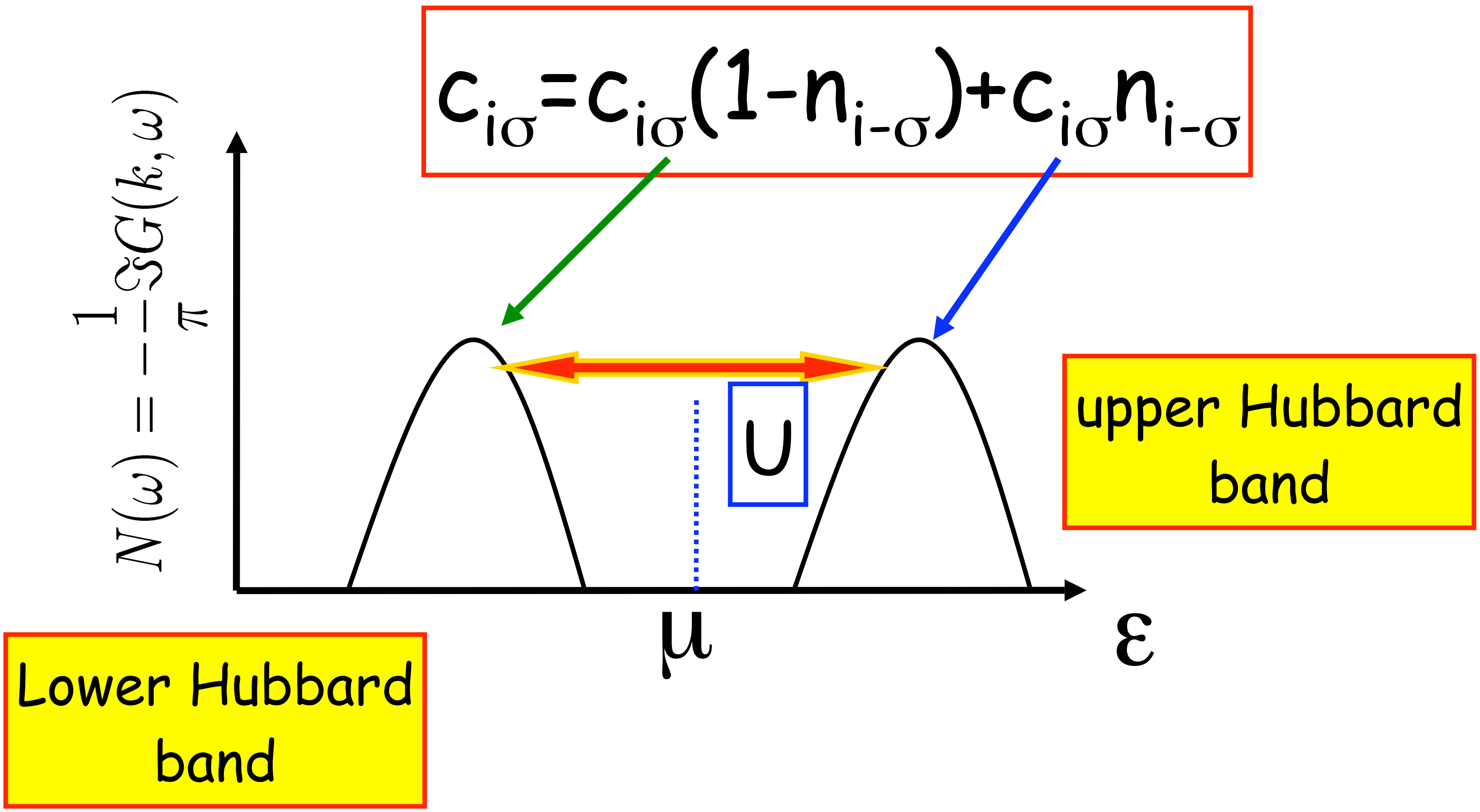
20 years after: Has the U-scale been Integrated out?

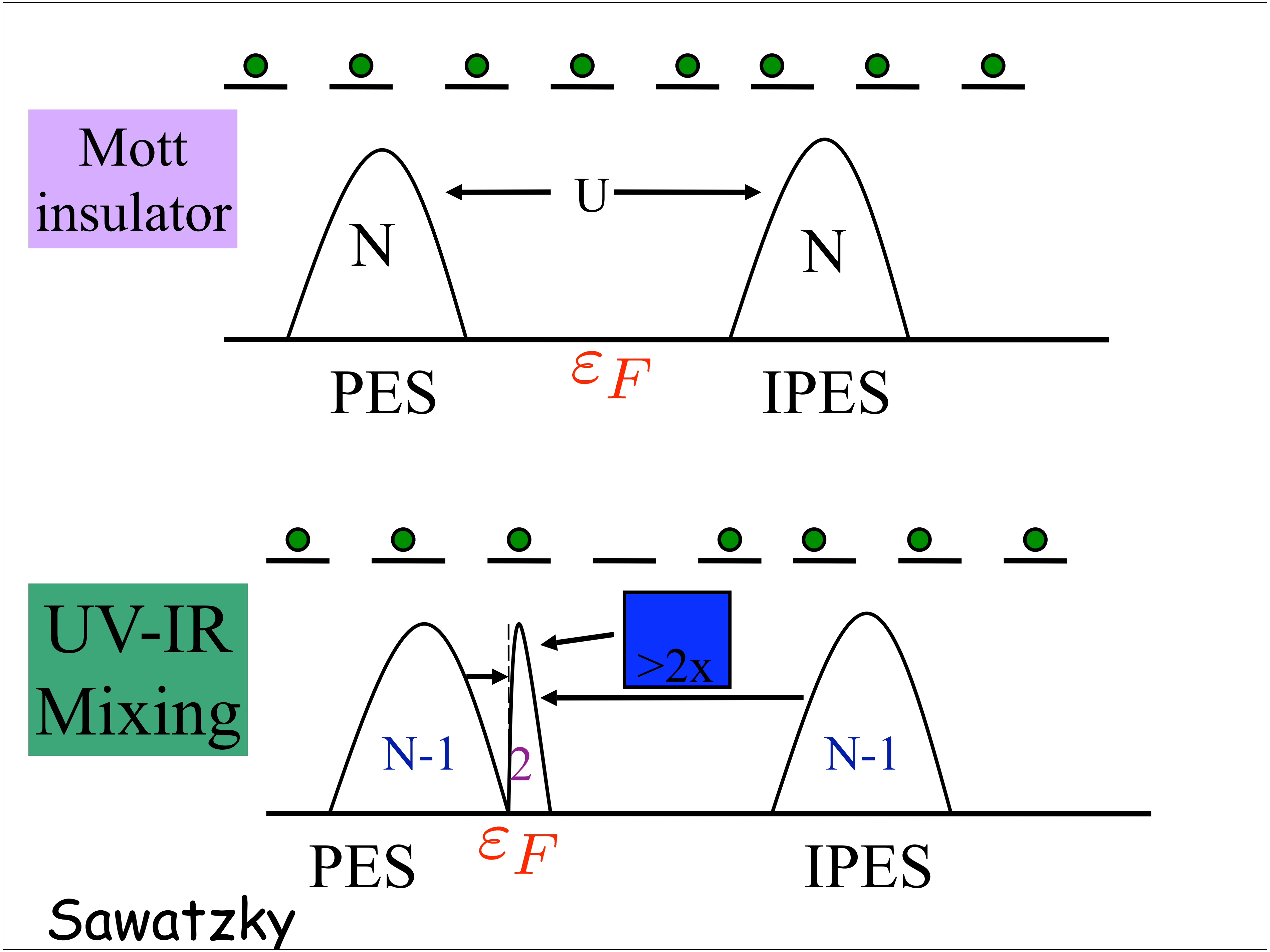
No!

Two problems

- U-scale physics is neither fermionic nor bosonic: $U n_{i\uparrow} n_{i\downarrow}$
- Spectral weight transfer: UHB and LHB are not orthogonal

Spectral weight transfer

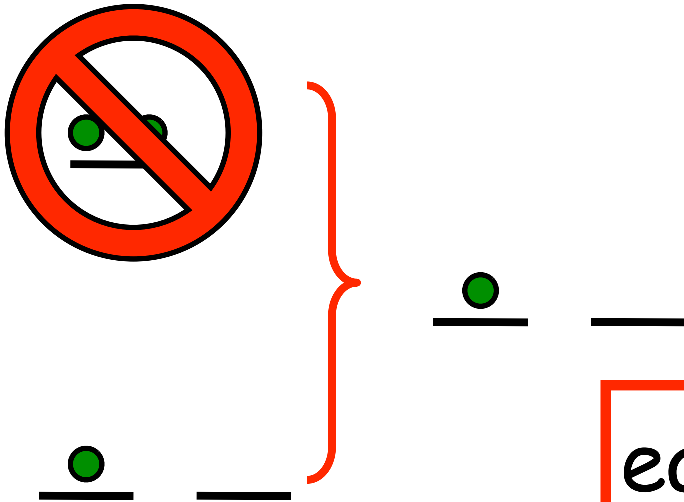



Mott
insulator
U
N
N
PES
εF
IPES
UV-IR
Mixing
>2x
N-1
2
N-1
PES
εF
IPES
Sawatzky

How can we preserve the 2x sum rule without the high-energy scale ?

new particle statistics

?



$$a^\dagger_{i\uparrow} a^\dagger_{i\downarrow} |0\rangle = 0$$

each $a_{i\sigma}$ excitation blocks two states

$$P_0 e^{iS} H e^{-iS} P_0$$

$$H_{tJ} = -t \sum_{ij\sigma} g_{ij} a^\dagger_{i\sigma} a_{j\sigma} + J S_i \cdot S_j$$

$$H_{tJ} = -t \sum_{ij\sigma} g_{ij} a^{\dagger}_{i\sigma} a_{j\sigma} + J S_i \cdot S_j$$

Half-filling

$$J \sum_{ij} S_i \cdot S_j$$

Local SU(2) symmetry

Not in original model

applicability

Incoherent broadening of LHB does not fill in the charge gap

$$tN_{\text{sites}} < U$$

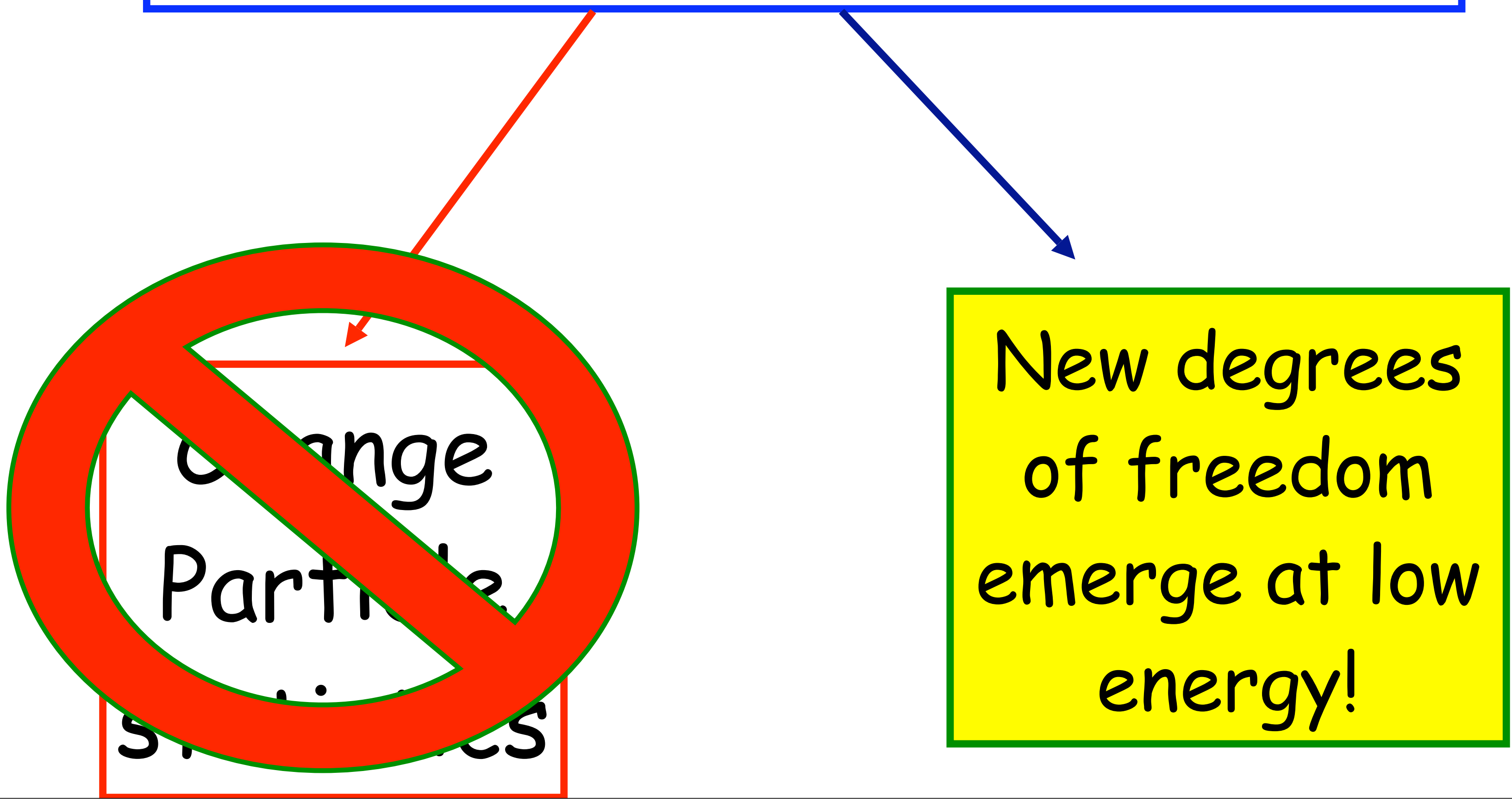
$U \to \infty$ $L \to \infty$ do not commute

Projection is not integration:

Integration does not change the number of states per site

Local SU(2) symmetry is An artifact of projection

How can we preserve the 2x sum rule without the high-energy scale (UHB)



e

φ (charge 2e boson)

$$(c_{i\sigma}^{\dagger}, c_{i\bar{\sigma}}\varphi_i^{\dagger})$$

remnant of high energy

new bound state
(charge e)

2 states are annihilated

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Spectral-weight transfer: Breakdown of low-energy-scale sum rules in correlated systems

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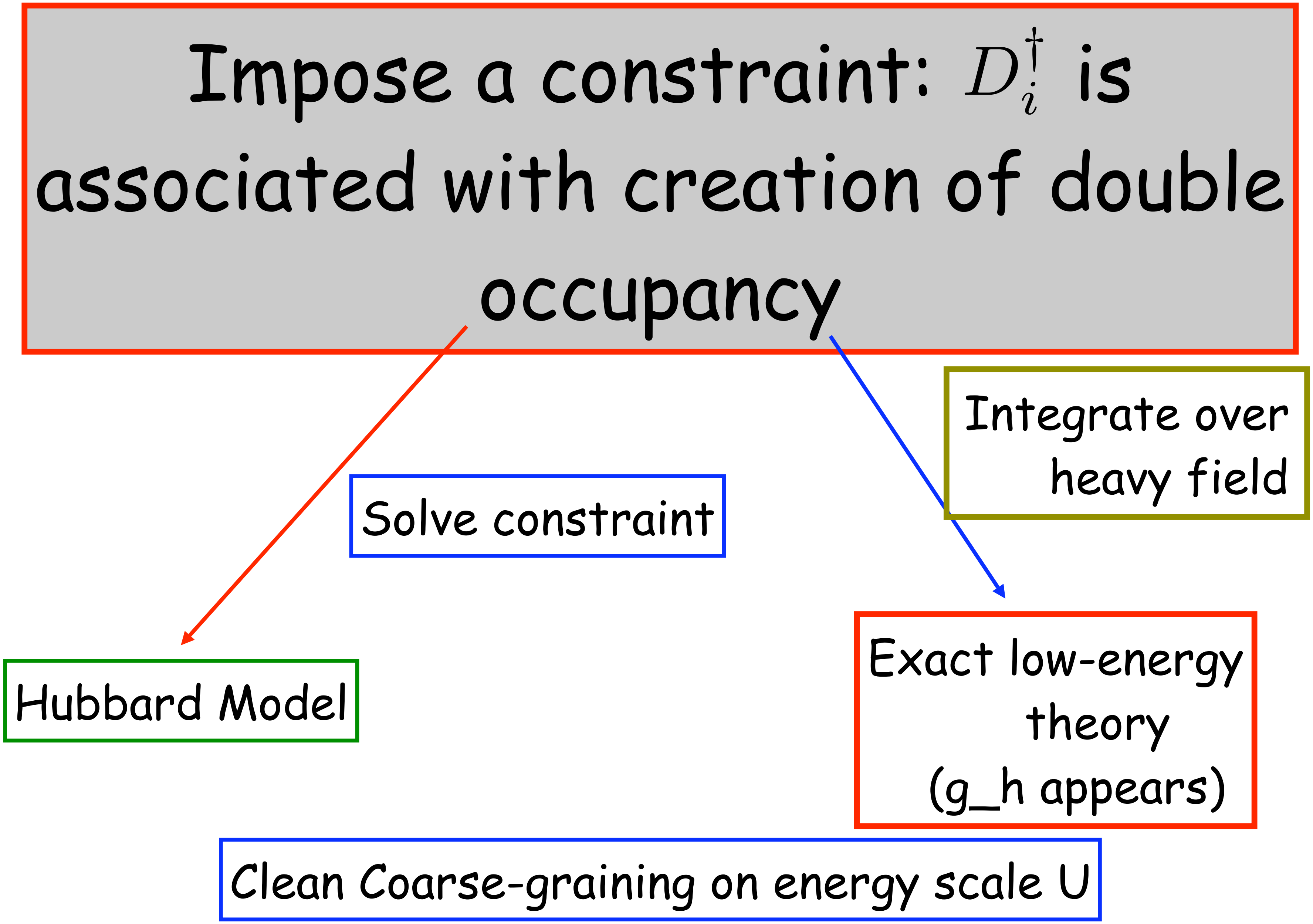
(Received 4 March 1993)

In this paper we study the spectral-weight transfer from the high- to the low-energy scale by means of exact diagonalization of finite clusters for the Mott-Hubbard and charge-transfer model. We find that the spectral-weight transfer is very sensitive to the hybridization strength as well as to the amount of doping. This implies that the effective number of low-energy degrees of freedom is a function of the hybridization and therefore of the volume and temperature. In this sense it is not possible to define a Hamiltonian which describes the low-energy-scale physics unless one accepts an effective nonparticle conservation.

Key idea:

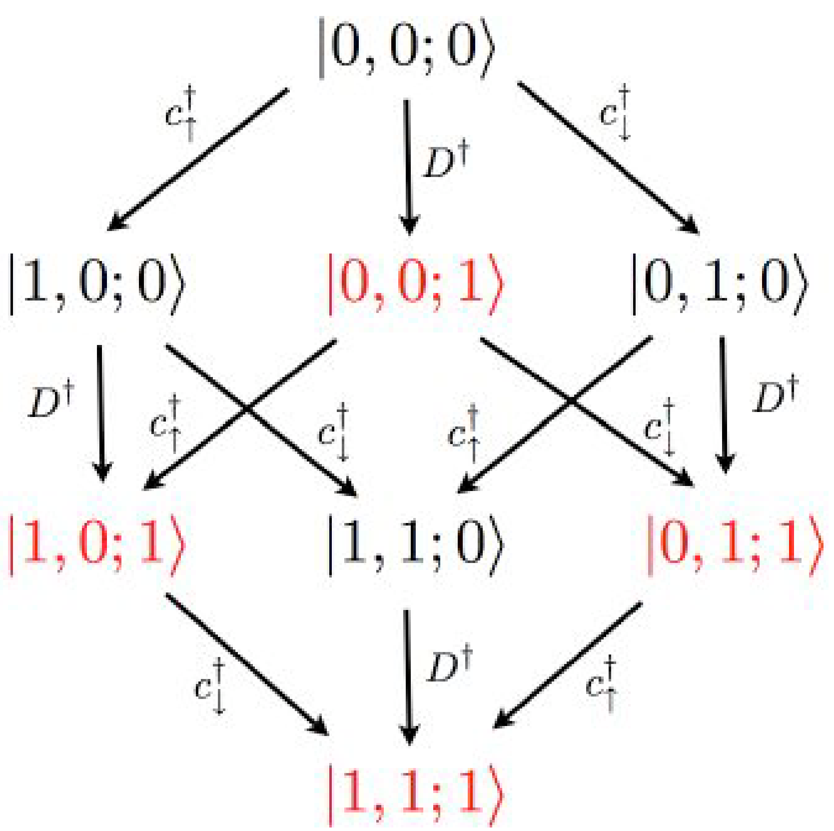
Extend the Hilbert space:
Associate with U-scale a new
Fermionic oscillator

Impose a constraint in such
A way that all unphysical states
Are removed


Impose a constraint: $D_i^\dagger$ is associated with creation of double occupancy
Integrate over heavy field
Solve constraint
Hubbard Model
Exact low-energy theory (g_h appears)
Clean Coarse-graining on energy scale U

Extend Hilbert Space

$$\bigotimes_i \left(\mathcal{F}_\uparrow \otimes \mathcal{F}_\downarrow\right) \rightarrow \bigotimes_i \left(\mathcal{F}_\uparrow \otimes \mathcal{F}_\downarrow \otimes \mathcal{F}_D\right)$$



$$\Psi = \begin{pmatrix} c_\uparrow & c_\downarrow \\ c_\downarrow^\dagger & -c_\uparrow^\dagger \end{pmatrix}$$

$$S = \Psi^\dagger \Psi$$

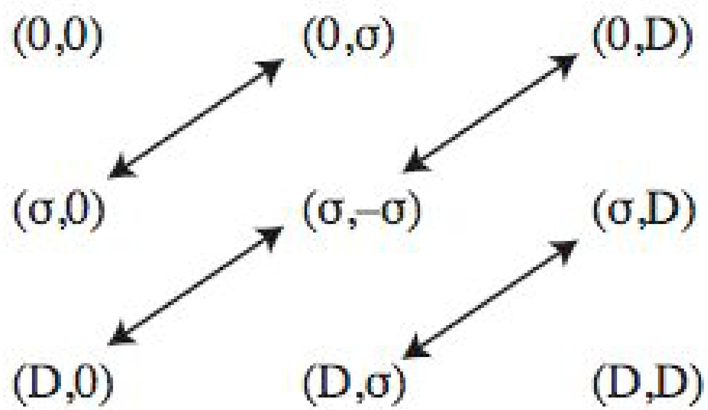
local SU(2)

$$\Psi = h\Psi \qquad h = \begin{pmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{pmatrix}$$

$$|\alpha|^2 + |\beta|^2 = 1$$

$$S- > \Psi^\dagger h^\dagger h \Psi = S$$

Allowed Hops: Hole Doping



Construct Lagrangian

Lagrangian

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

$$+U \sum_j D^\dagger_j D_j$$

$$-t \sum_{i,j,\sigma} g_{ij} \left[C_{ij\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} \; + D^\dagger_i c^\dagger_{j,\sigma} c_{i,\sigma} D_j \right.$$

$$\left. \left. + \left(D^\dagger_j \eta c_{i,\sigma} V_\sigma c_{j,-\sigma} + h.c. \right) \right] + H_{\text{con}} \right]$$

Grass-mann Integra-tion

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

$$V_\uparrow = 1 \quad , V_\downarrow = -1,$$

Couples to singlet

$$C_{ij\sigma} \equiv \bar{\eta}\eta \alpha_{ij\sigma} \equiv \bar{\eta}\eta (1 - n_{i,-\sigma})(1 - n_{j,-\sigma})$$

Solve Constraint:

$$Z = \int [\mathcal{D}c\, \mathcal{D}c^\dagger\ \mathcal{D}D\ \mathcal{D}D^\dagger\ \mathcal{D}\varphi\ \mathcal{D}\varphi^\dagger]\, \exp^{-\int_0^\tau L dt}$$

a.) Integrate over φ_i

$$\int d\eta \delta(D_i - \eta c_{i\uparrow} c_{i\downarrow})$$

b.) integrate over D_i

$$\int d^2\eta\ \bar{\eta}\eta L_{\text{Hubb}} = \sum_{i\sigma} c_{i\sigma}^\dagger \dot{c}_{i\sigma} + H_{\text{Hubb}} = L_{\text{Hubb}}$$

UV theory = Hubbard model

$$
\begin{aligned}
L \quad &= \int d^2\eta \Bigg[\bar{\eta}\eta \sum_{i\sigma} (1 - n_{i\bar{\sigma}}) c^\dagger_{i\sigma} \dot{c}_{i\sigma} + \sum_i D^\dagger_i \dot{D}_i \\
&+ U \sum_j D^\dagger_j D_j - t \sum_{i,j,\sigma} g_{ij} \Big[C_{ij\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + D^\dagger_i c^\dagger_{j,\sigma} c_{i,\sigma} D_j \\
&+ \; (D^\dagger_j \eta c_{i,\sigma} V_\sigma c_{j,\bar{\sigma}} + h.c.) \Big] + H_{\rm con} \Bigg] ,
\end{aligned}
$$

Integrate over D_j: heavy field

Fermionic Guassian integral: Do exactly!!

Exact Low-energy theory

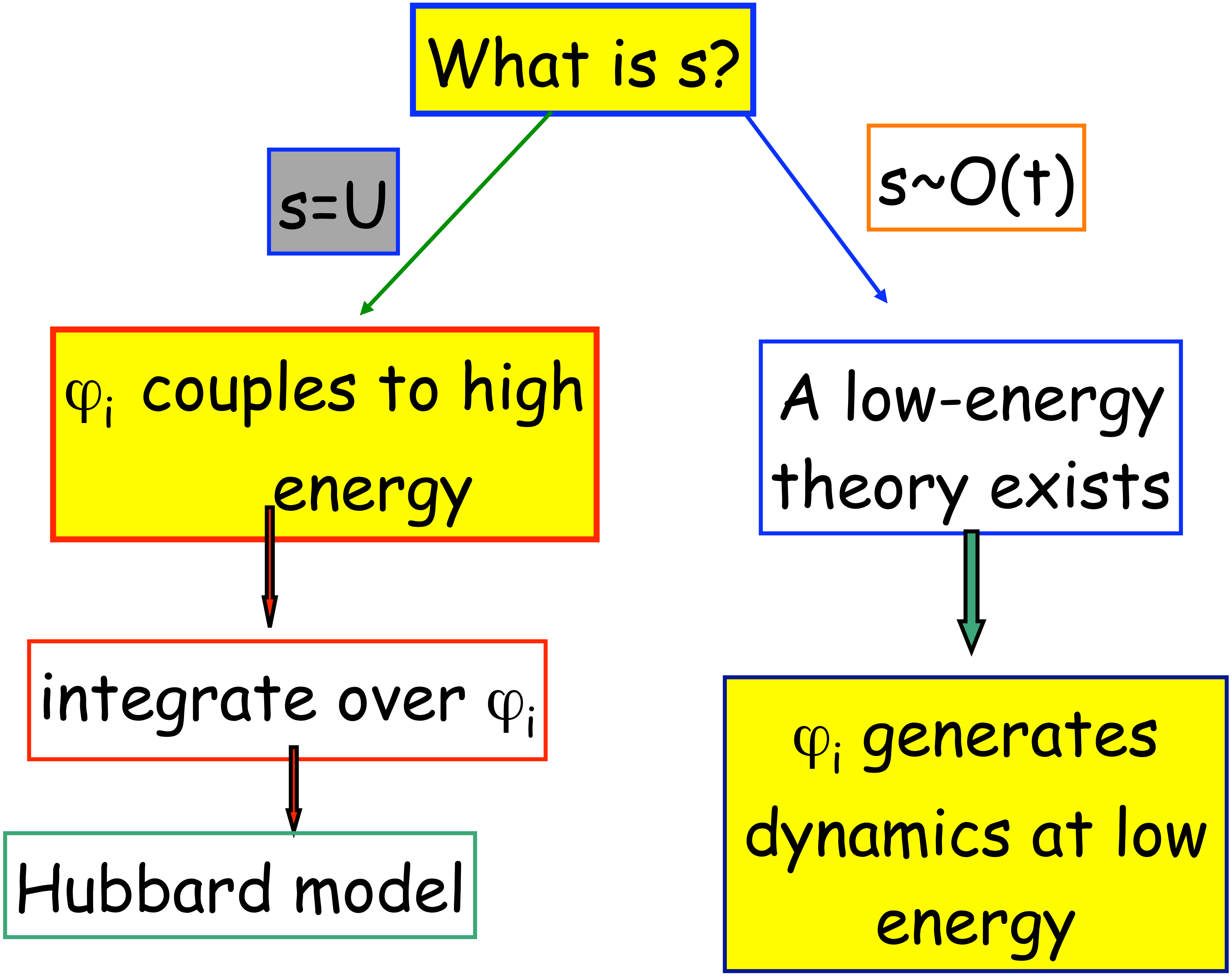
$$H_h^{IR} = -t\sum_{i,j,\sigma} g_{ij}\alpha_{ij\sigma}c^\dagger_{i,\sigma}c_{j,\sigma} + H_{\rm int} - \frac{Tr\ln\mathcal{M}}{\beta}$$

$$H_{\rm int} = -\frac{t^2}{U}\sum_{j,k} b_j^\dagger(\mathcal{M}^{-1})_{jk}b_k - \frac{s^2}{U}\sum_{i,j}\varphi_i^\dagger(\mathcal{M}^{-1})_{ij}\varphi_j$$

$$-s\sum_i \varphi_j^\dagger c_{j,\uparrow}c_{j,\downarrow} + \frac{st}{U}\sum_{i,j}\varphi_i^\dagger(\mathcal{M}^{-1})_{ij}b_j + h.c. \quad ,$$

$$\mathcal{M}_{ij} = \left(\delta_{ij} - \frac{t}{U}g_{ij}\sum_\sigma c^\dagger_{j,\sigma}c_{i,\sigma}\right)$$

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



What is s?
s=U
s~O(t)
φ_i couples to high energy
A low-energy theory exists
integrate over φ_i
φ_i generates dynamics at low energy
Hubbard model

a.) $U \to \infty$?

$$H_{\text{int}} \to t \sum_j \varphi_j^\dagger c_{j,\uparrow} c_{j,\downarrow} \qquad \int d\varphi_i d\varphi_i^\dagger \longrightarrow \delta(c_{j,\uparrow} c_{j,\downarrow})$$

No double occupancy

b.) Conserved Charge: bosons+fermions

$$Q = \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} + 2 \sum_i \varphi_i^\dagger \varphi_i$$

$$\left.\begin{aligned} c_{i\sigma} &\longrightarrow e^{i\alpha_i} c_{i\sigma} \\ \varphi_i &\longrightarrow e^{i\theta_i} \varphi_i \end{aligned}\right\} \theta_i = 2\alpha_i \to U(1) \times U(1) \to U(1)_{\text{EM}}$$

$$\sum_i b_i^\dagger b_i = \sum_{ij\ell\sigma\sigma'} g_{ij} g_{j\ell} c_{i,\sigma}^\dagger V_\sigma c_{j,-\sigma}^\dagger c_{\ell,\sigma'} V_{\sigma'} c_{j,-\sigma'} \propto -(S_i \cdot S_j - n_i n_j / 4)$$

two-site terms

Spin exchange

$$H_h^{IR} = -t \sum_{i,j,\sigma} g_{ij} \alpha_{ij\sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + H_{\rm int}$$

$$H_{\rm int} = -\frac{t^2}{U} \sum_{j,k} b_j^\dagger (\mathcal{M}^{-1})_{jk} b_k - \frac{t^2}{U} \sum_{i,j} \varphi_i^\dagger (\mathcal{M}^{-1})_{ij} \varphi_j$$

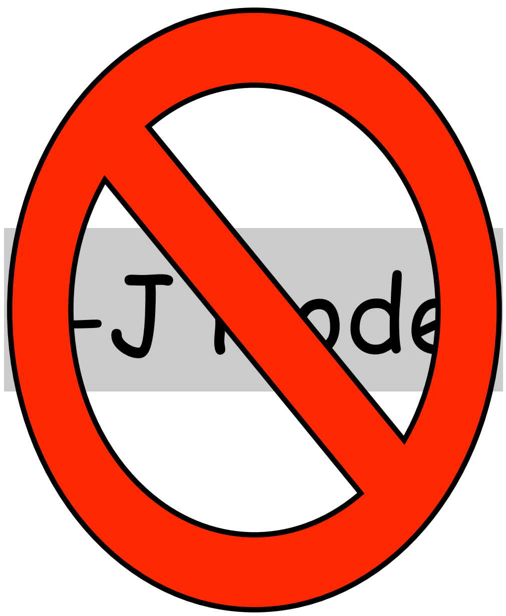
$$-t \sum_j \varphi_j^\dagger c_{j,\uparrow} c_{j,\downarrow} + \frac{t^2}{U} \sum_{i,j} \varphi_i^\dagger (\mathcal{M}^{-1})_{ij} b_j + h.c. \quad ,$$

let $M^{-1}{}_{ij} = \delta_{ij}$

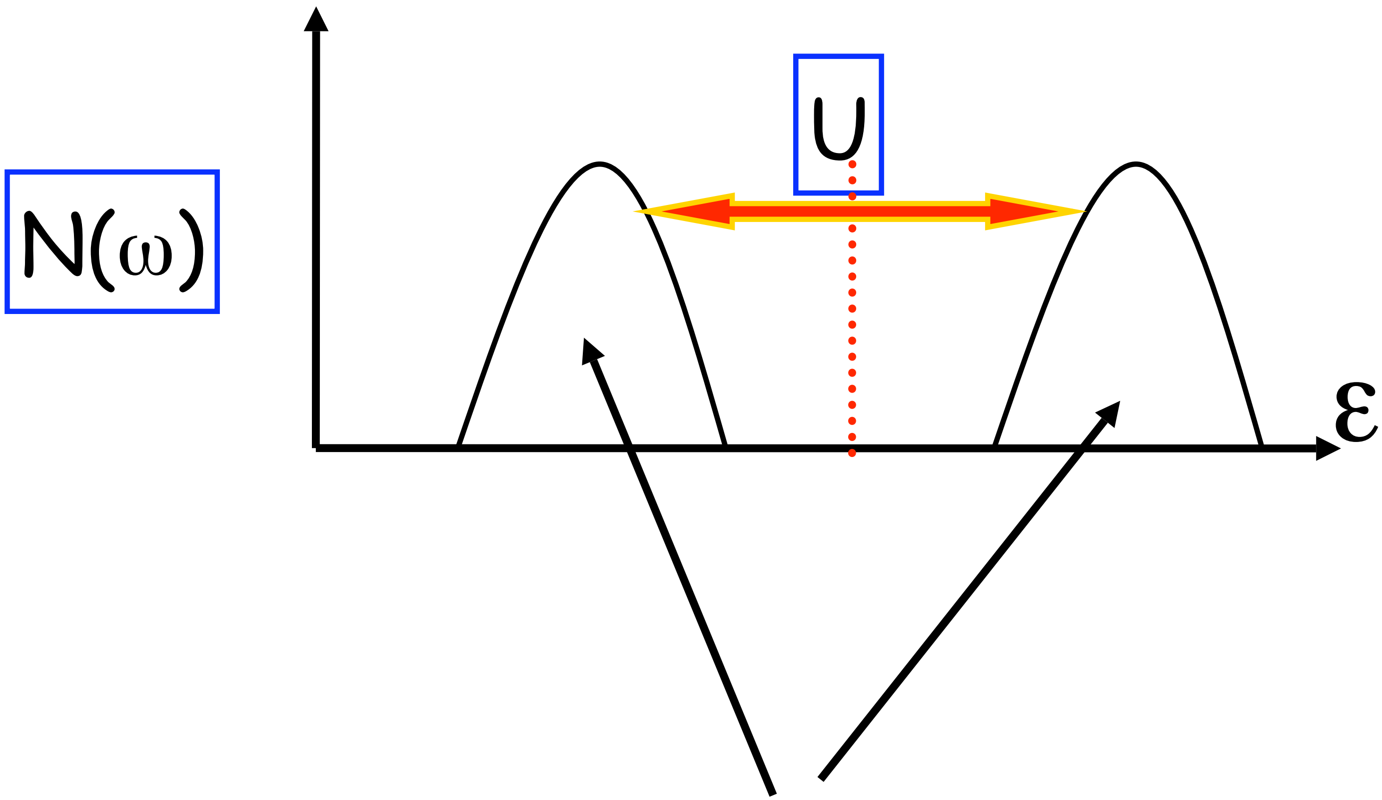
$$H_h^{IR} = H_{t-J} - \frac{t^2}{U} \sum_i \varphi_i^\dagger \varphi_i - t \sum_j \varphi_j^\dagger c_{j,\uparrow} c_{j,\downarrow} + \frac{t^2}{U} \sum_{i,j} \varphi_i^\dagger b_i + h.c. \quad ,$$

Non-projective

Low energy
Limit of Hubbard model



Half-filling



Integrate out both

$$
\begin{aligned}
H &= \int d^2\theta \left[\frac{1}{2} U \sum_j (D_j^\dagger D_j - \tilde{D}_j \tilde{D}_j^\dagger) \right. \\
&\left. - t \sum_{i,j,\sigma} g_{ij} \left(+(D_j^\dagger \theta c_{i,\sigma} V_\sigma c_{j,-\sigma} + h.c. + \bar{\theta} c_{i,\sigma} V_\sigma c_{j,-\sigma} \tilde{D}_i + h.c. \right) + H_{\mathrm{con}} \right]
\end{aligned}
$$

Note no $D^\dagger$...D terms

$$
H_{con} = s\bar{\theta} \sum_i \varphi_i^\dagger (D_i - \theta c_{i,\uparrow} c_{i,\downarrow}) + h.c. + \tilde{s} \sum_i \bar{\theta} \tilde{\varphi}_i (\tilde{D}_i - \theta c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger) + h.c.
$$

No M Matrix: Closed Form

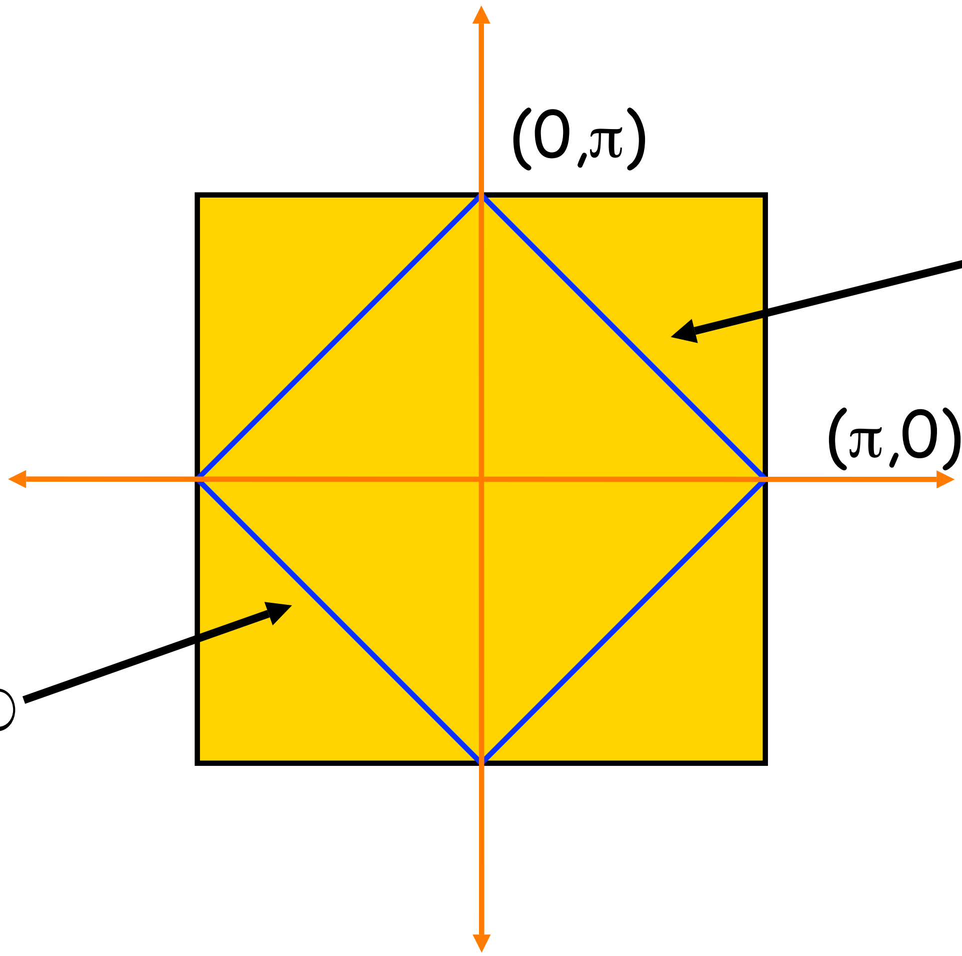
$$
\begin{aligned}
H_{\text{int}} \quad = \quad & -\frac{t^2}{2U}\sum_j b_j^\dagger b_j - \frac{t^2}{U}\sum_i \varphi_i^\dagger \varphi_i \\
& -t\sum_j \varphi_j^\dagger c_{j,\uparrow} c_{j,\downarrow} - \frac{t^2}{U}\sum_{i,j} \varphi_i^\dagger b_i + h.c. \quad , \\
& -\frac{t^2}{2U}\sum_j b_j^\dagger b_j - \frac{t^2}{U}\sum_i \tilde{\varphi}_i^\dagger \tilde{\varphi}_i \\
& -t\sum_j \tilde{\varphi}_j^\dagger c_{j,\uparrow} c_{j,\downarrow} + \frac{t^2}{U}\sum_{i,j} \tilde{\varphi}_i^\dagger b_i + h.c.
\end{aligned}
$$

$$H_{IR}(n=1) \neq H_{\mathrm{spinmodel}}$$

Why?

Boson breaks local SU(2) symmetry Of Heisenberg model!!

Much ado about zeros



$G(0,p=p_F)=0$

Mott insulator

$\Sigma = \infty$

$$ReG(0,p) = \int_{-\infty}^{-\Delta_-} \frac{A(\omega',p)d\omega'}{-\omega'} + \int_{\Delta_+}^{\infty} \frac{A(\omega',p)d\omega'}{-\omega'}$$

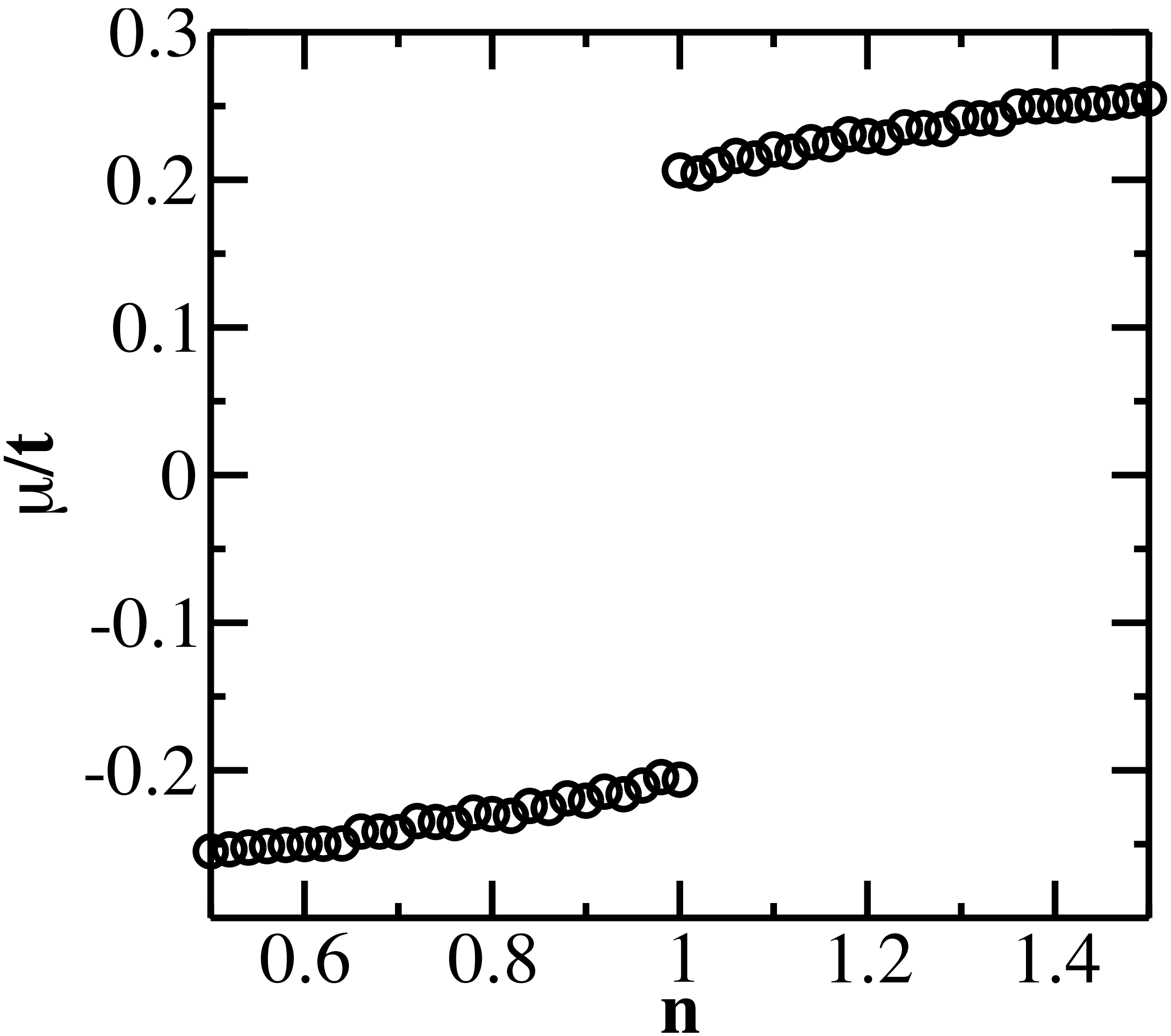
Ze

No $ReG(0,p) \neq 0$

p)=0

Non-projective terms
Preserve the zeros

Low-energy theory preserves 'Mott gap'



Wavefunction

$$\psi = \Pi_{i<j} f(z_i - z_j) e^{-\frac{U}{t}\int d^2\theta \sum_i |D_i|^2}$$

UV

IR

$$\psi = \Pi_{i<j} f(z_i - z_j)\left(1 - (1 - e^{-\frac{U}{t}}) n_{i\uparrow} n_{\downarrow}\right)$$

Gutzwiller at $U = \infty$

$$|\psi\rangle^{IR} \quad = \quad e^{-\frac{t}{U}\sum_i |\varphi_i + b_i|^2} \Pi_{i<j} f(r_i - r_j) b^\dagger_{ij} |0\rangle$$

What is the electron operator?

$$H \longrightarrow H + \sum_{i\sigma} J_i((1-n_{i\bar{\sigma}})c^\dagger_{i\sigma} + \bar{\sigma} D^\dagger_i c_{i\bar{\sigma}}\eta) + h.c.$$

UV

$$H_{hubb} + Jc^\dagger_{i\sigma} + h.c.$$

IR

$$c^\dagger_{i\sigma} \rightarrow (1-n_{i\bar{\sigma}})c^\dagger_{i\sigma} + \bar{\sigma}\frac{t}{U} b^\dagger_i c_{i\bar{\sigma}} + \bar{\sigma}\frac{t}{U}\phi^\dagger_i c_{i\bar{\sigma}}$$

new charge e bound state?

Spectral function

$$G(k,\omega) = FT \int D[\phi_i^*]D[\phi_i] \int D[c_i^*]D[c_i]Tc_i(t)c_j(0)^* \exp^{-\int L[c,\phi]dt}$$

↓

Bosonic field ~ independent of space

$$G(k,\omega) = \int D[\phi^*]D[\phi]FT\left(\int D[c_i^*]D[c_i]Tc_i(t)c_j(0)^* \exp^{-\int L[c,\phi]dt}\right)$$

$$G(k,\omega) = \int D[\phi^*]D[\phi]G(k,\omega,\phi) \exp^{-L_{eff}}$$

$$G(k,\omega,\phi) = \frac{\sin^2\theta_k}{\omega + E(k,\phi)} + \frac{\cos^2\theta_k}{\omega - E(k,\phi)}$$

$$E(k,\phi) = \sqrt{\varepsilon(k)^2 + t^2\phi^2(1 - \frac{2t}{U}(\cos(k_x) + \cos(k_y))^2}$$

$$L_{\text{eff}} = \sum_k (E_0 + E_k - \lambda_k - \frac{2}{\beta}\ln(1 + \exp^{-\beta\lambda_k})$$

$$\alpha_k = 2(\cos k_x + \cos k_y) \quad (1)$$

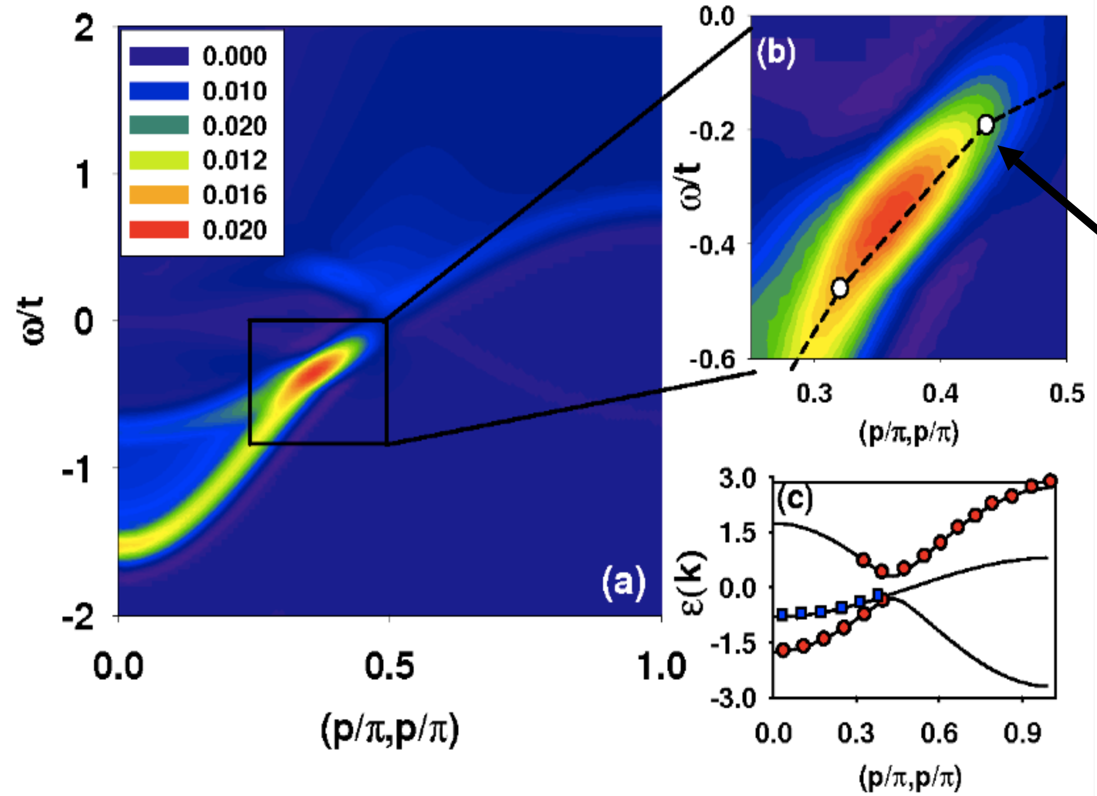
$$E_0 = -(2\mu + \frac{t^2}{U}) \quad (2)$$

$$E_k = -g_t t\alpha_k - \mu \quad (3)$$

$$\lambda_k = \sqrt{E_k^2 + \Delta_k^2} \quad (4)$$

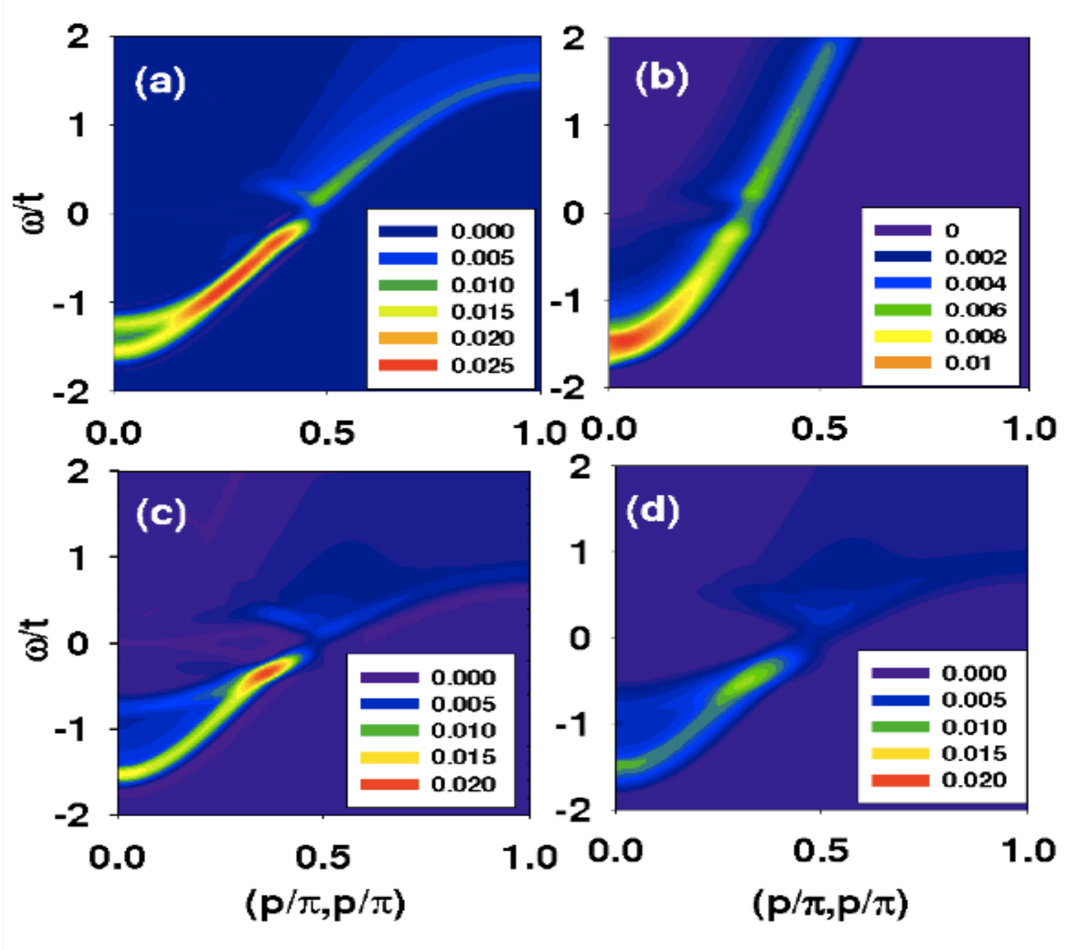
$$\Delta_k = t\phi^*(1 - \frac{2t}{U}\alpha_k) \quad (5)$$

$$(6)$$



0.000
0.010
0.020
0.012
0.016
0.020
2
1
0
-1
-2
ω/t
0.0
0.5
1.0
(p/π,p/π)
(a)
(b)
0.0
-0.2
-0.4
-0.6
0.3
0.4
0.5
(c)
3.0
1.5
0.0
-1.5
-3.0
ε(k)
0.0
0.3
0.6
0.9

t^2/U~60meV


(a)
(b)
(c)
(d)
ω/t
ω/t
(p/π,p/π)
(p/π,p/π)
0.000
0.005
0.010
0.015
0.020
0.025
0
0.002
0.004
0.006
0.008
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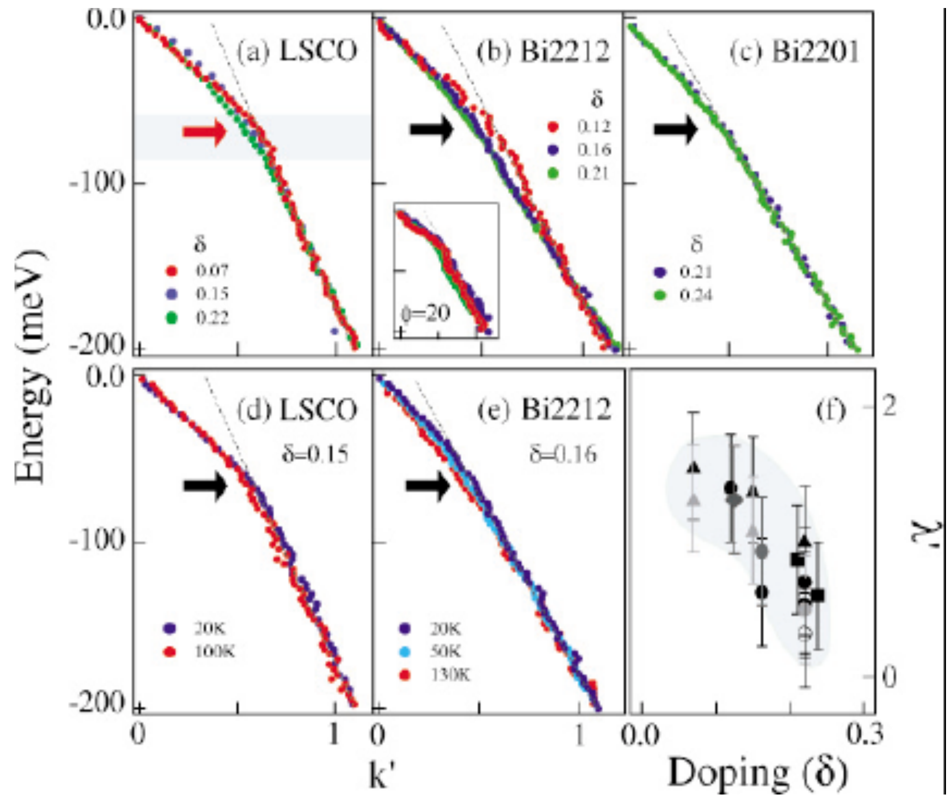
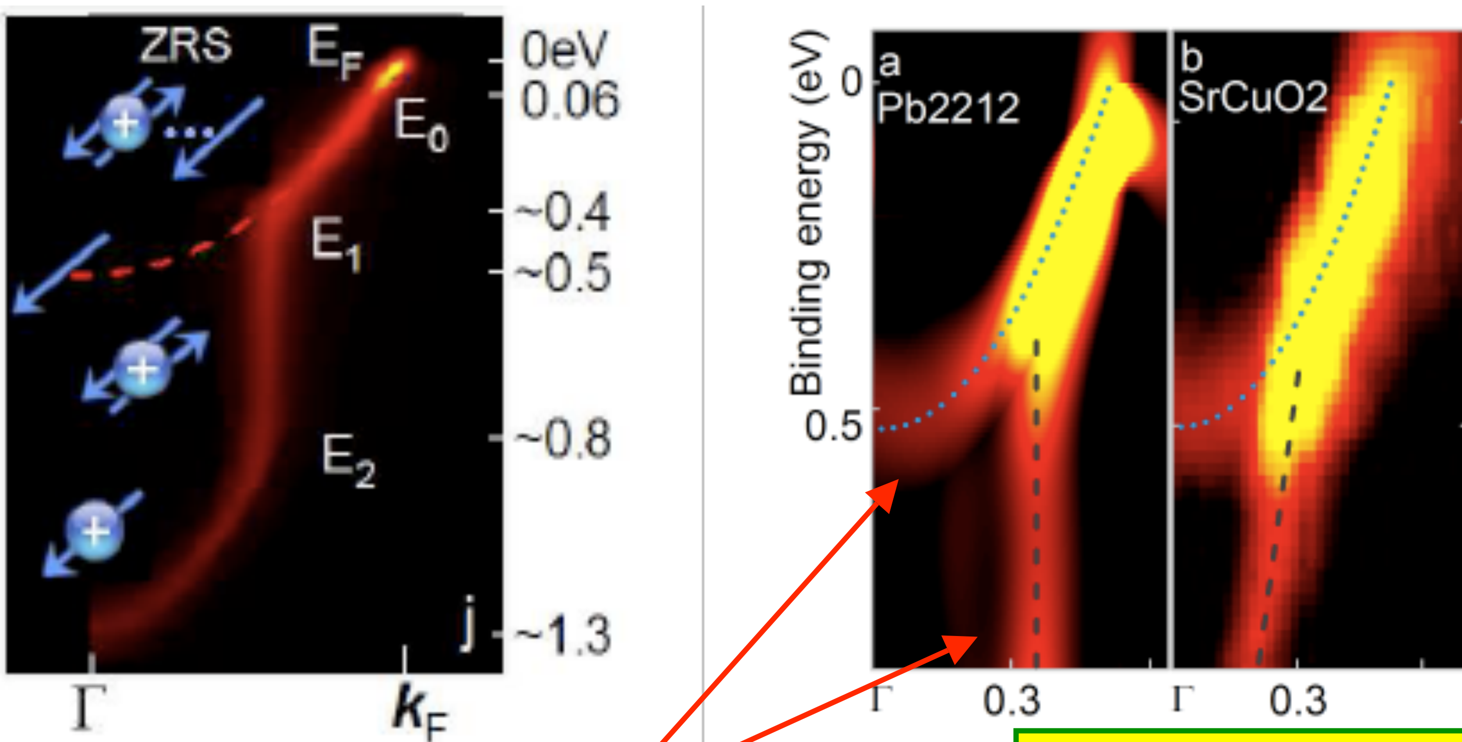


Lanzara et. al.

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



Two bands!!

Spin-charge separation?

Origin of two bands

Two charge e excitations

$c_{i\sigma}$

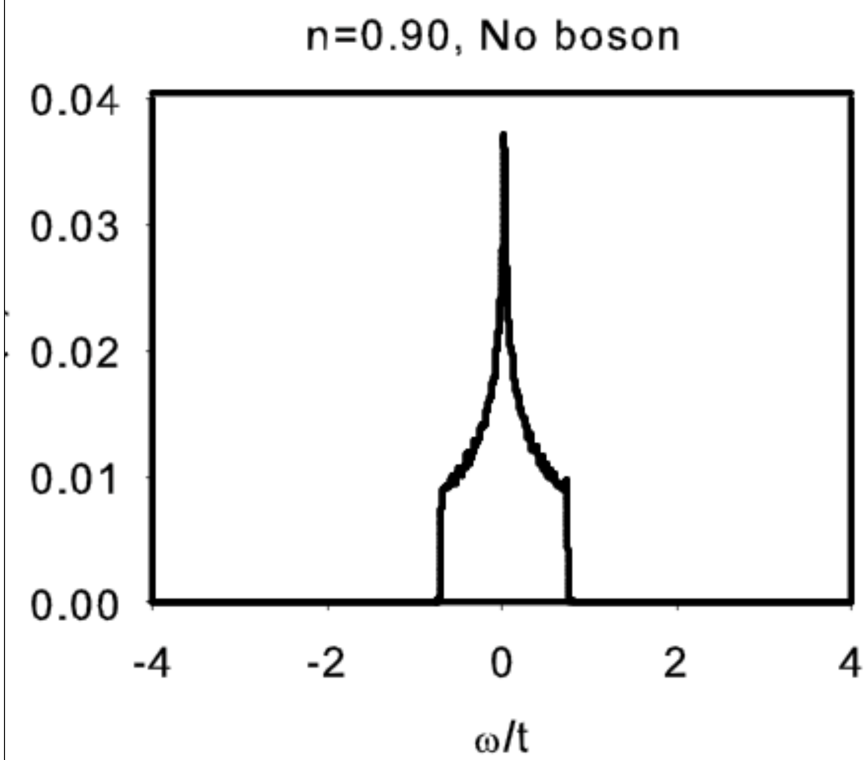
$\varphi_i^\dagger c_{i\bar{\sigma}}$

φ_i is confined

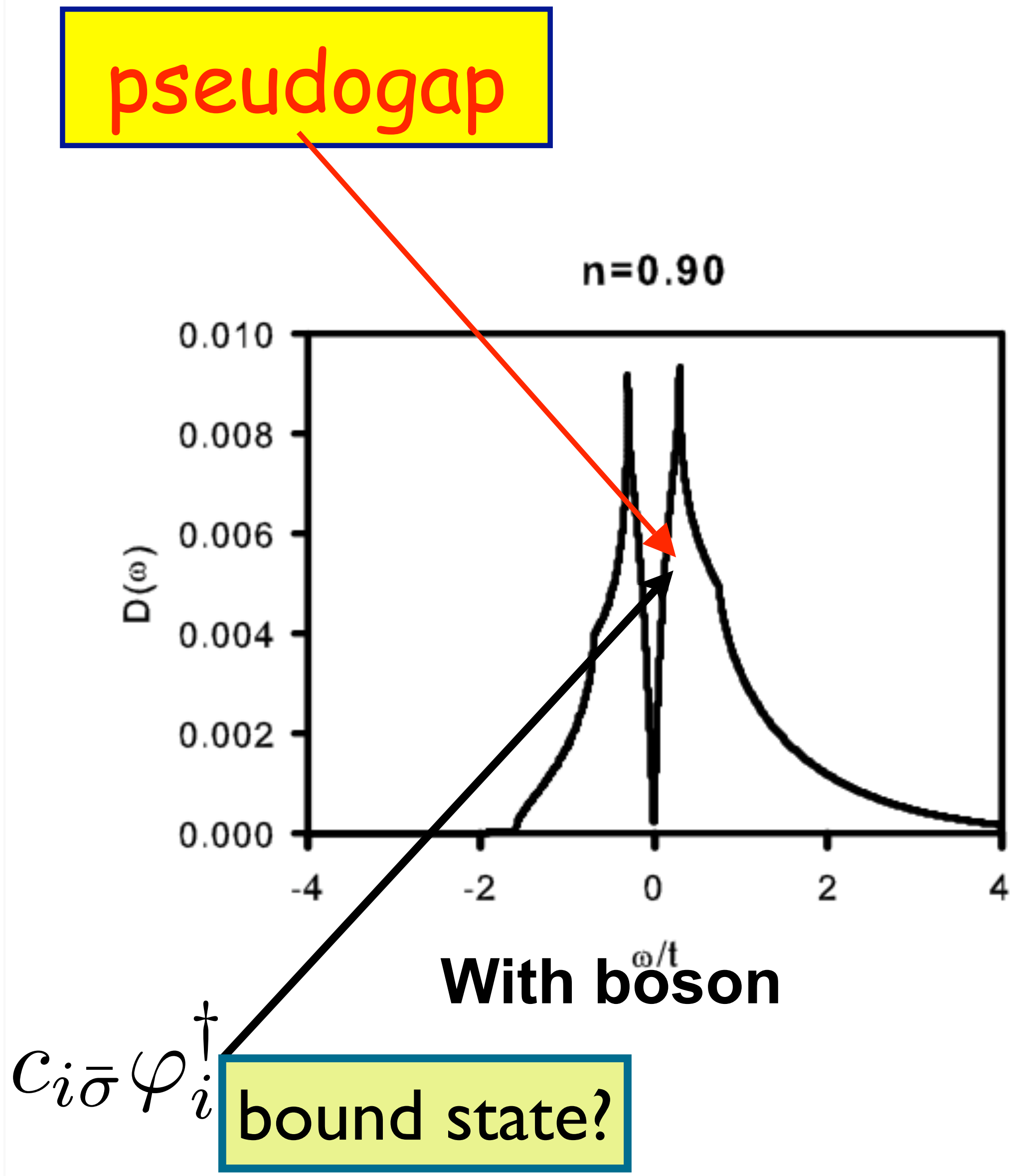
?

New bound state

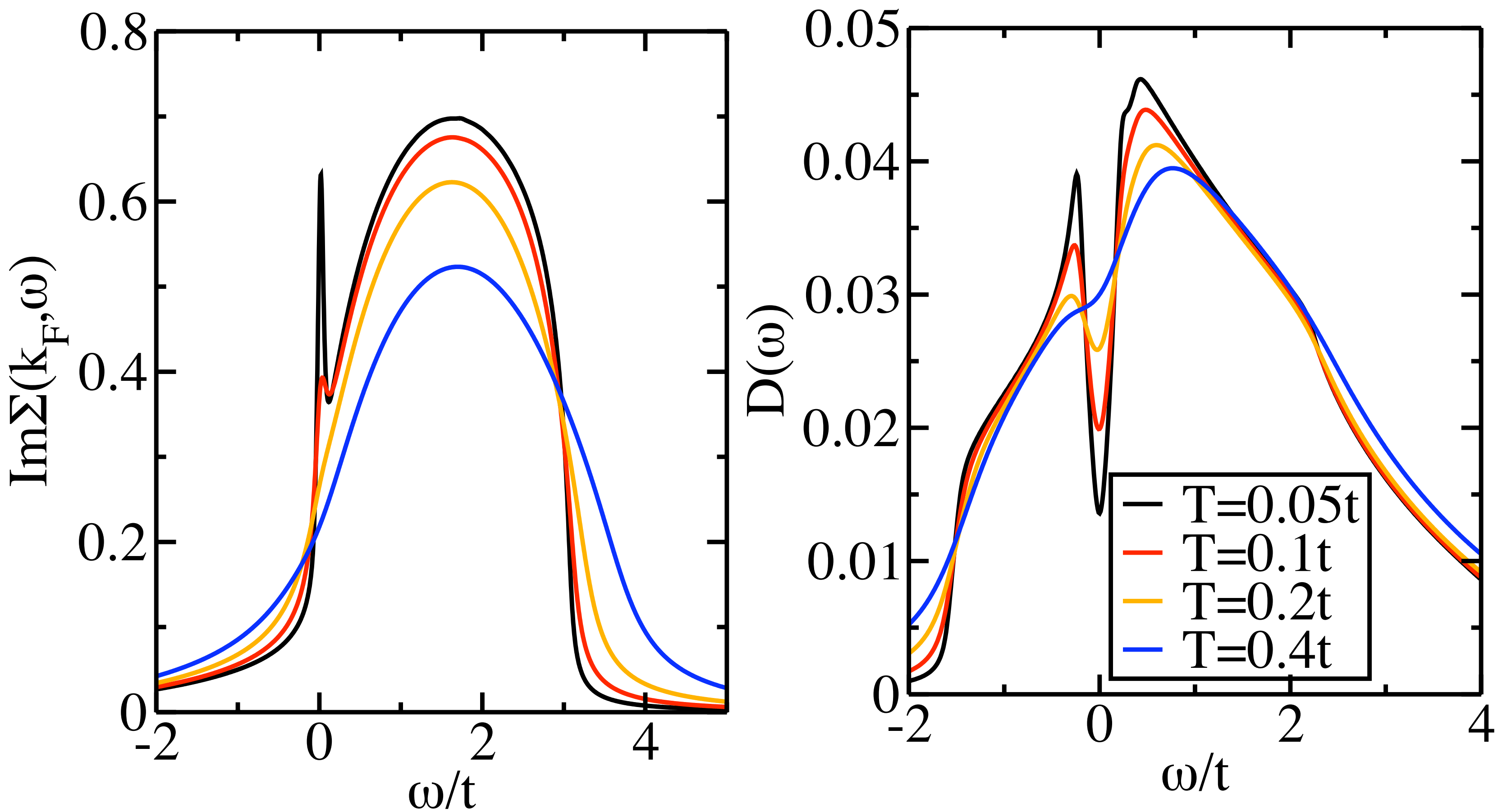
Density of States



Without boson

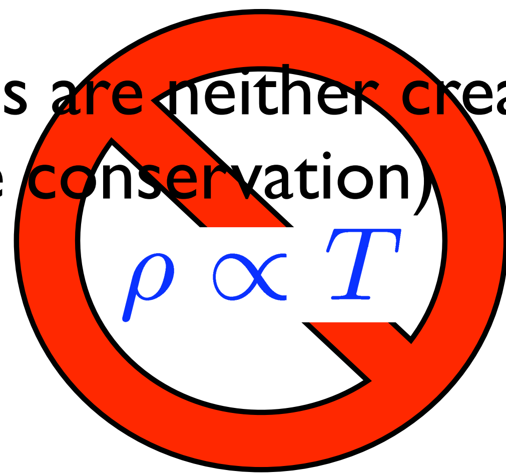


With boson


0.8
0.6
0.4
0.2
0
-2
0
2
4
ImΣ(k_F,ω)
ω/t
0.05
0.04
0.03
0.02
0.01
0
-2
0
2
4
D(ω)
ω/t
T=0.05t
T=0.1t
T=0.2t
T=0.4t

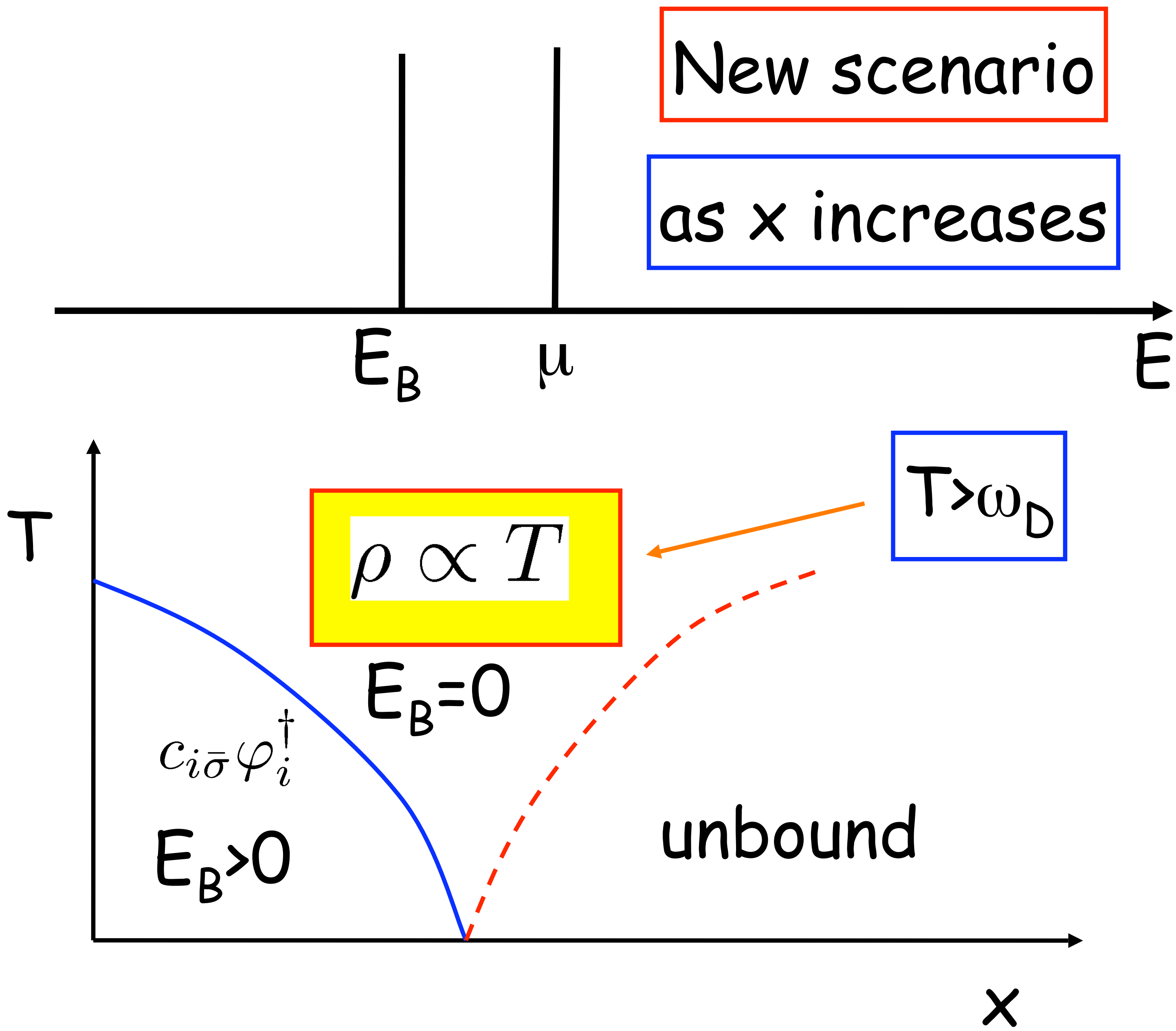
T-linear resistivity

- One critical length scale
- Charges are critical
- Charges are neither created nor annihilated (charge conservation)

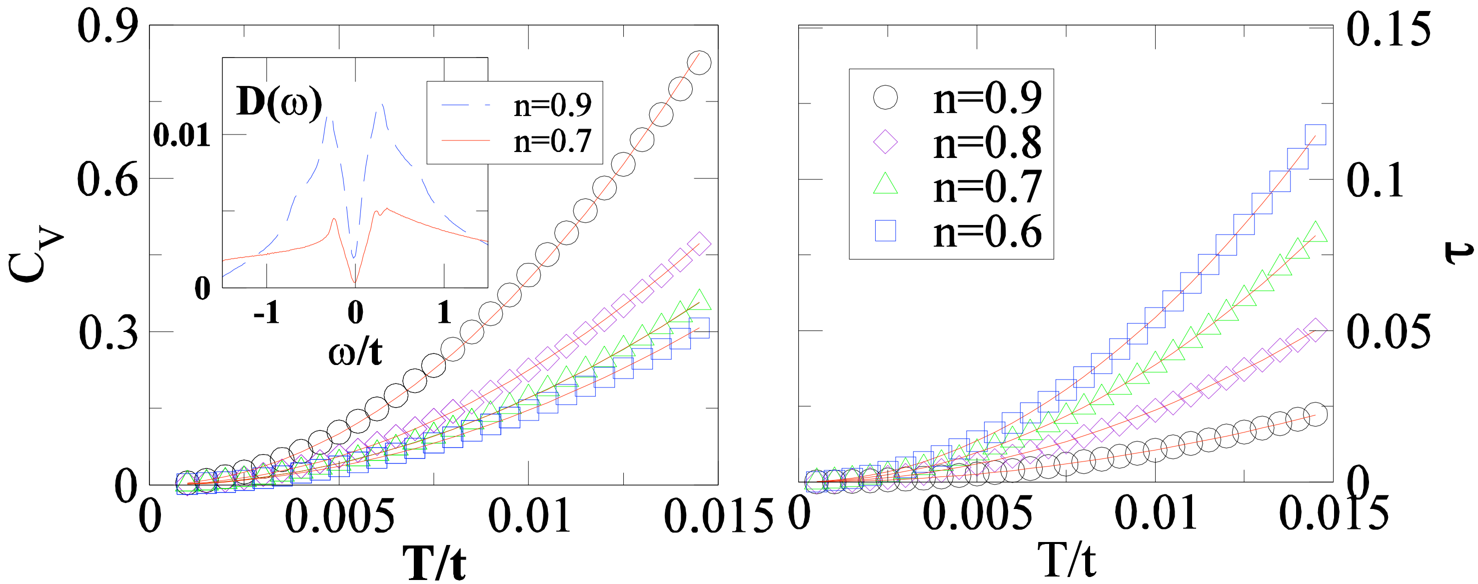


$$\sigma(\omega, T) = \frac{Q^2}{\hbar} T^{(d-2)/z} f\left(\frac{\hbar\omega}{k_B T}\right)$$

PP, CC, PRL, vol. 95, 107002 (2005)

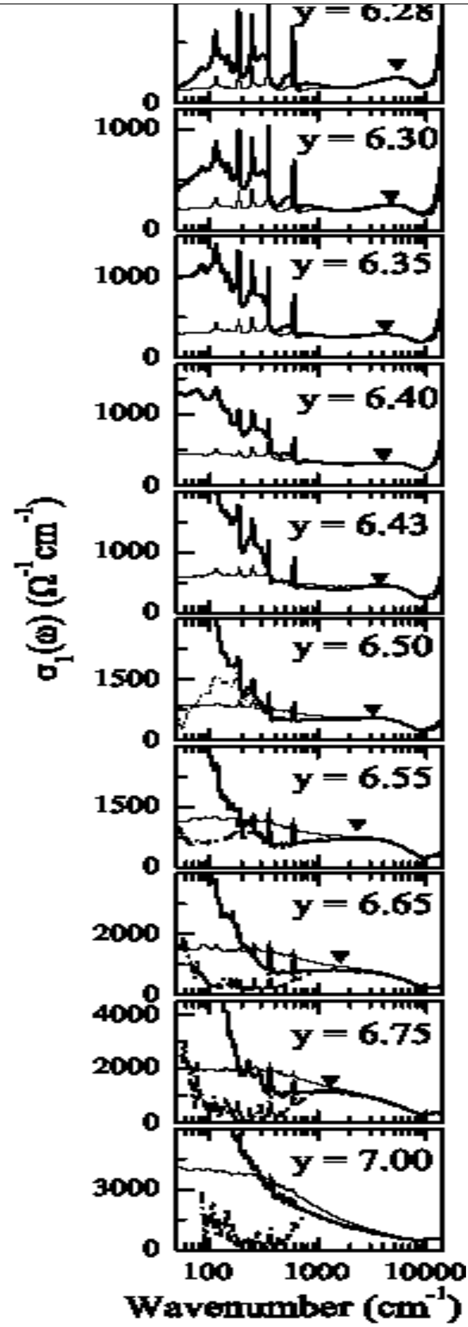

New scenario
as x increases
E_B
μ
E
T
$\rho \propto T$
$T > \omega_D$
$E_B=0$
$c_{i\bar{\sigma}}\varphi_i^\dagger$
$E_B>0$
unbound
x

Thermal effects



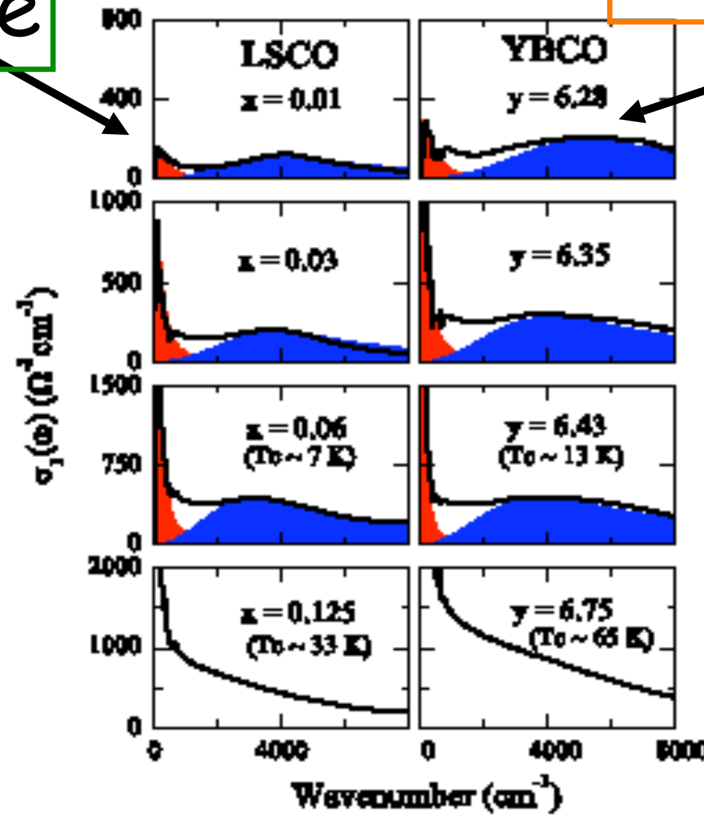
C_v~T ^{2}

Optical conductivity



Drude

Mid-IR

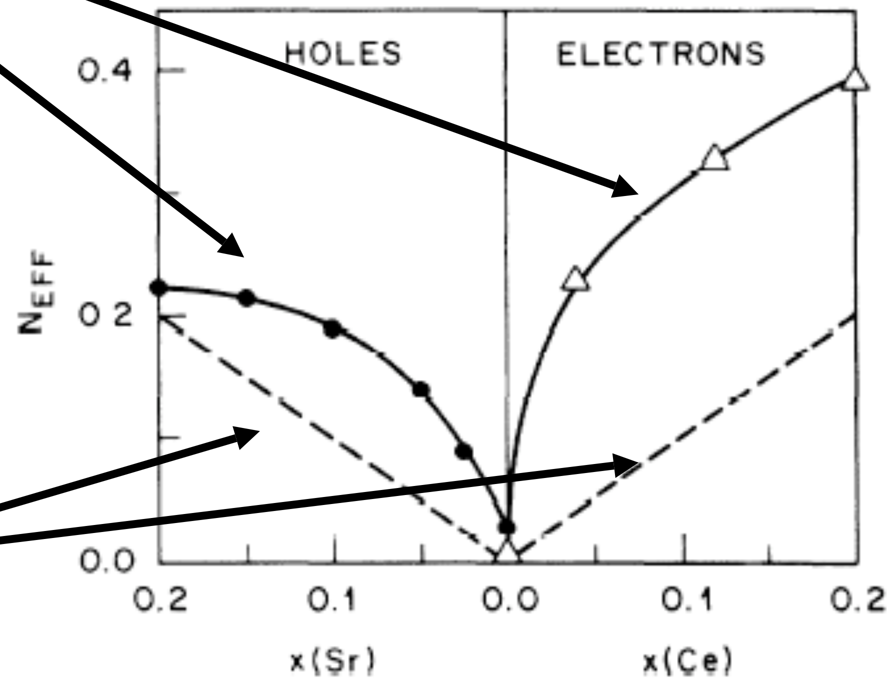


Basov, et. al. 2005

Two-components

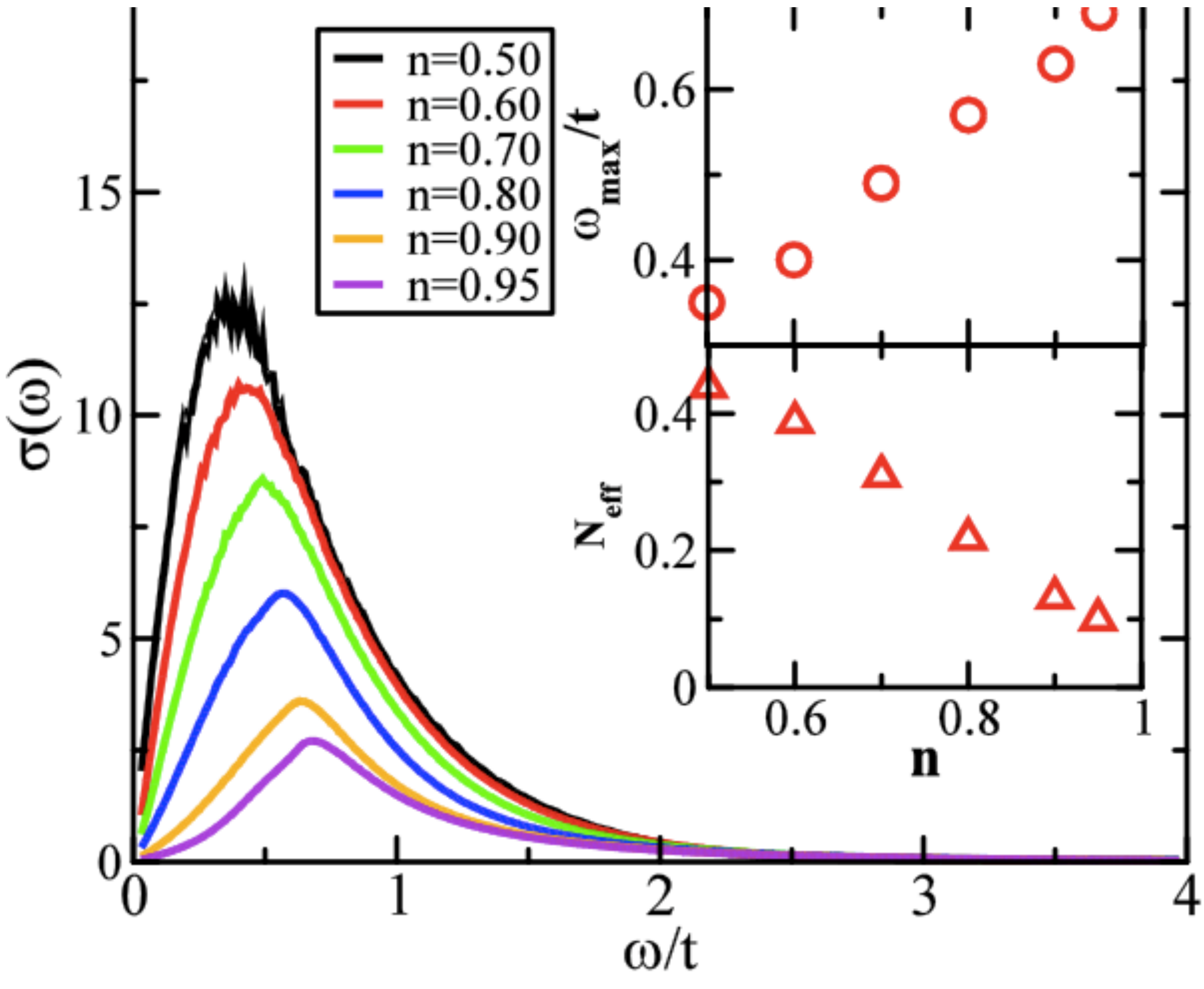
cuprates

Cooper, et al. PRB 41, 11605 (1990)



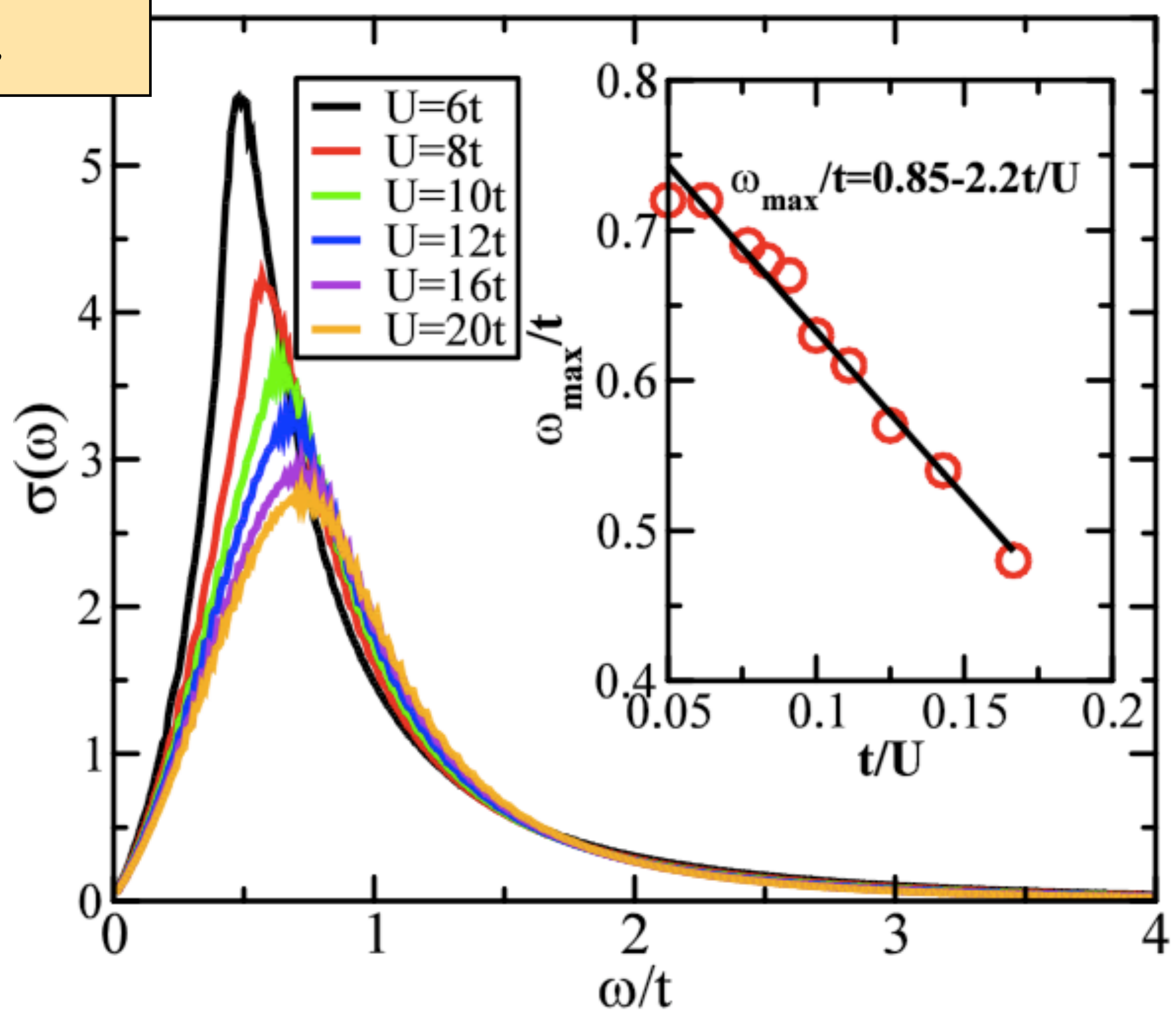
Semiconductors:
Si:P: N~x

From where do the extra Degrees of freedom originate?

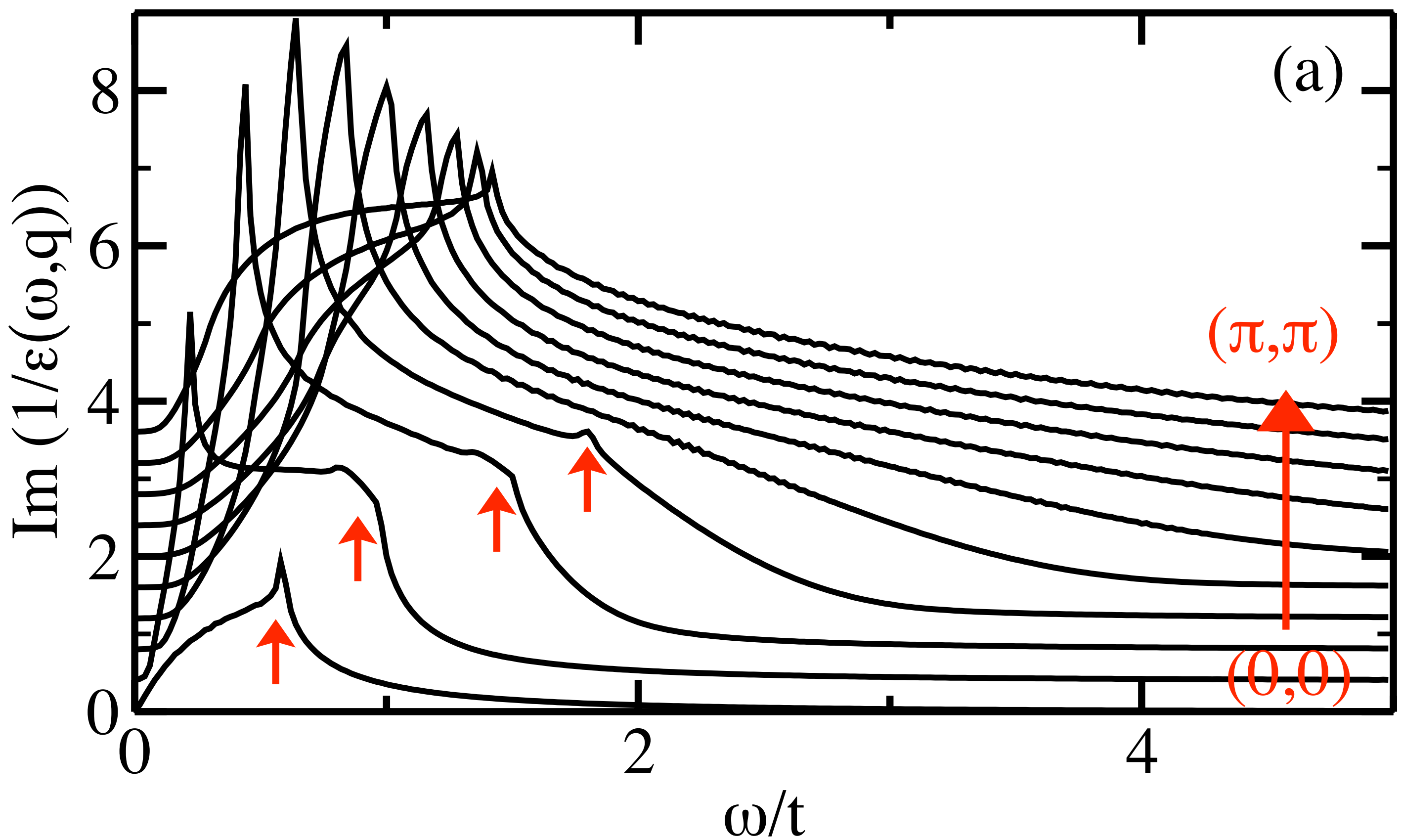


n=0.50
n=0.60
n=0.70
n=0.80
n=0.90
n=0.95
σ(ω)
ω/t
0
5
10
15
0
1
2
3
4
ω_max/t
0.4
0.6
N_eff
0
0.2
0.4
0.6
0.8
1
n

MID-IR=
New bound
state



Prediction: dielectric function

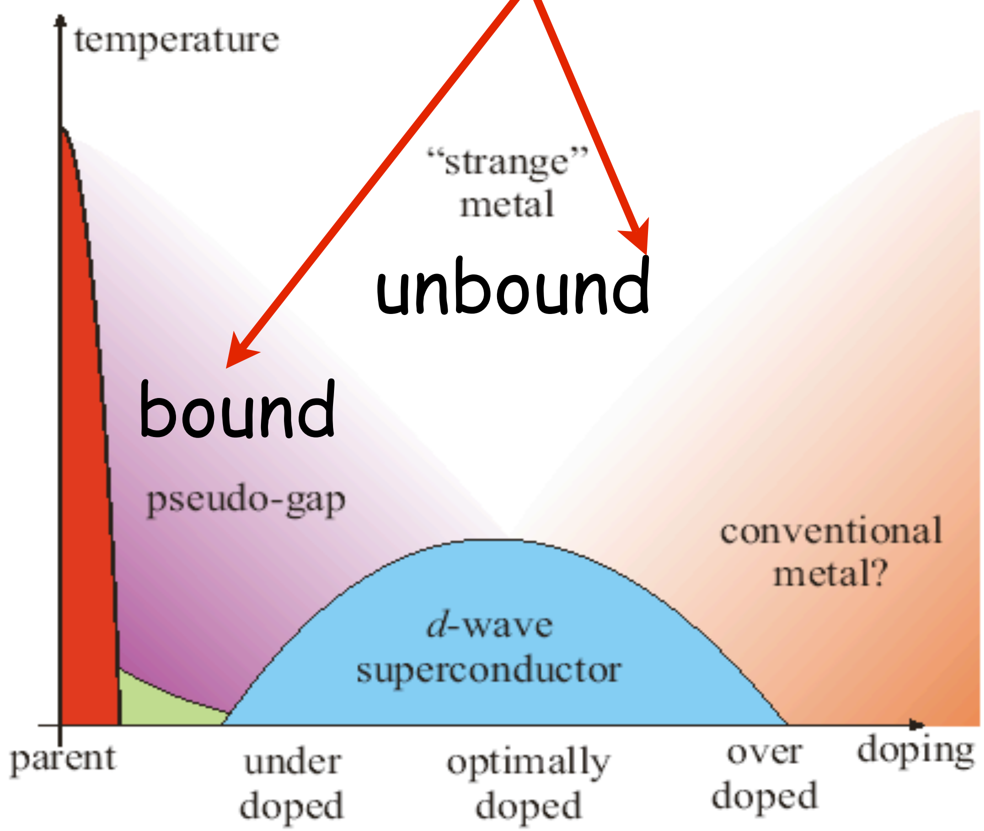


2 particle-hole branches

Hubbard model

integrate high energy

$$e \approx e_L + e_H(c_{i\bar{\sigma}}\varphi_i^\dagger)$$



summary

low-energy theory: non-electron

Quantum numbers emerge---

SC boson-fermion model

Boson=normal state properties of cuprates

Thanks to R. G. Leigh and
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and DMR-NSF