Philip Phillips (University of Illinois)

Beyond $U = \infty$: Hidden Charge 2e boson

Thanks to: T.-P. Choy, R. G. Leigh, S. Chakraborty
PRL, 99, 46404 (2007);
PRB, 77, 14512 (2008); ibid, 77, 104524 (2008));
ibid, 79,245120 (2009);...., DMR/NSF-ACIF

KITP Higher Tc Conference, June 25, 2009

Mott gap

dynamical spectral weight transfer

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mediated by

composite or bound states not in UV theory

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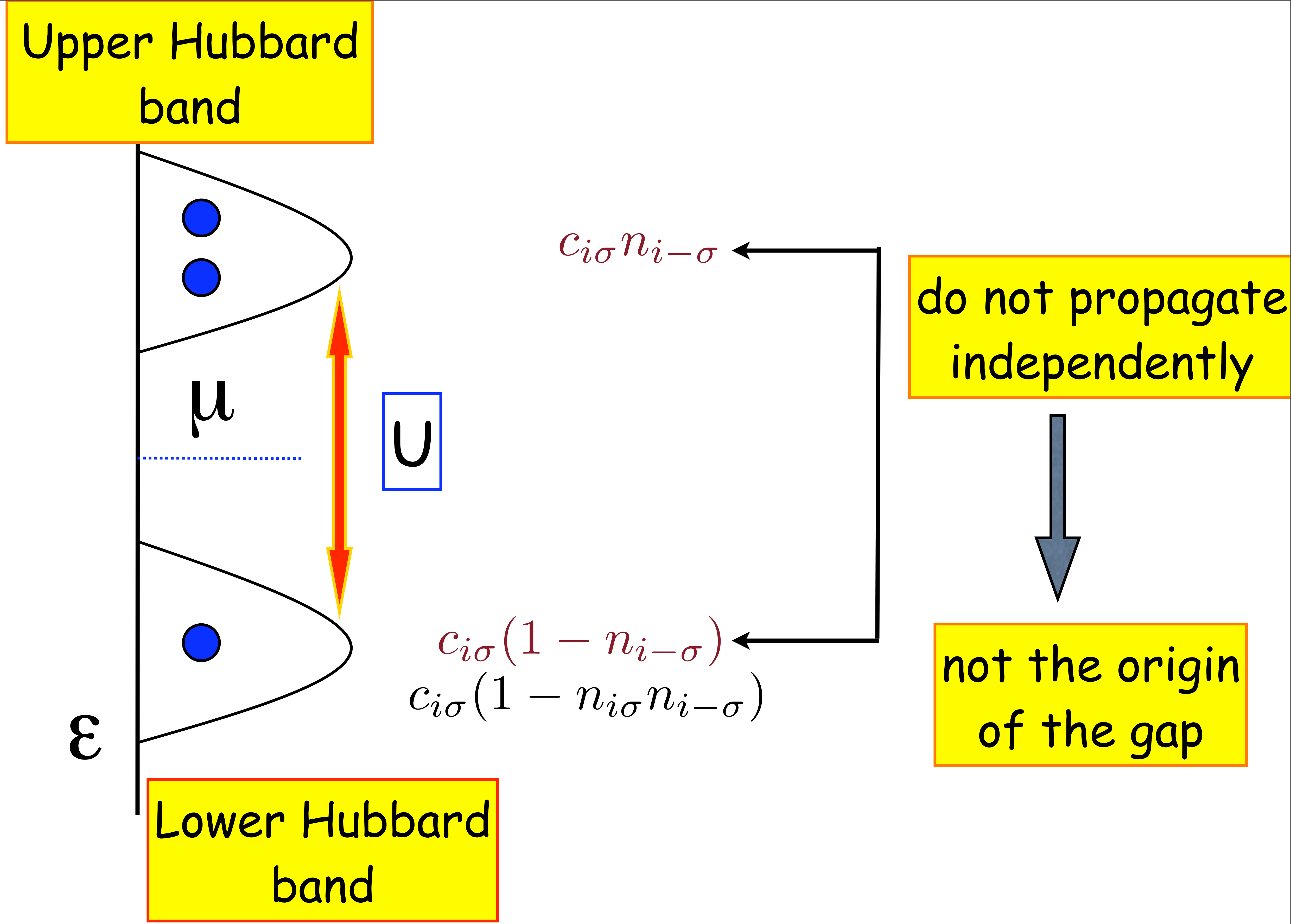
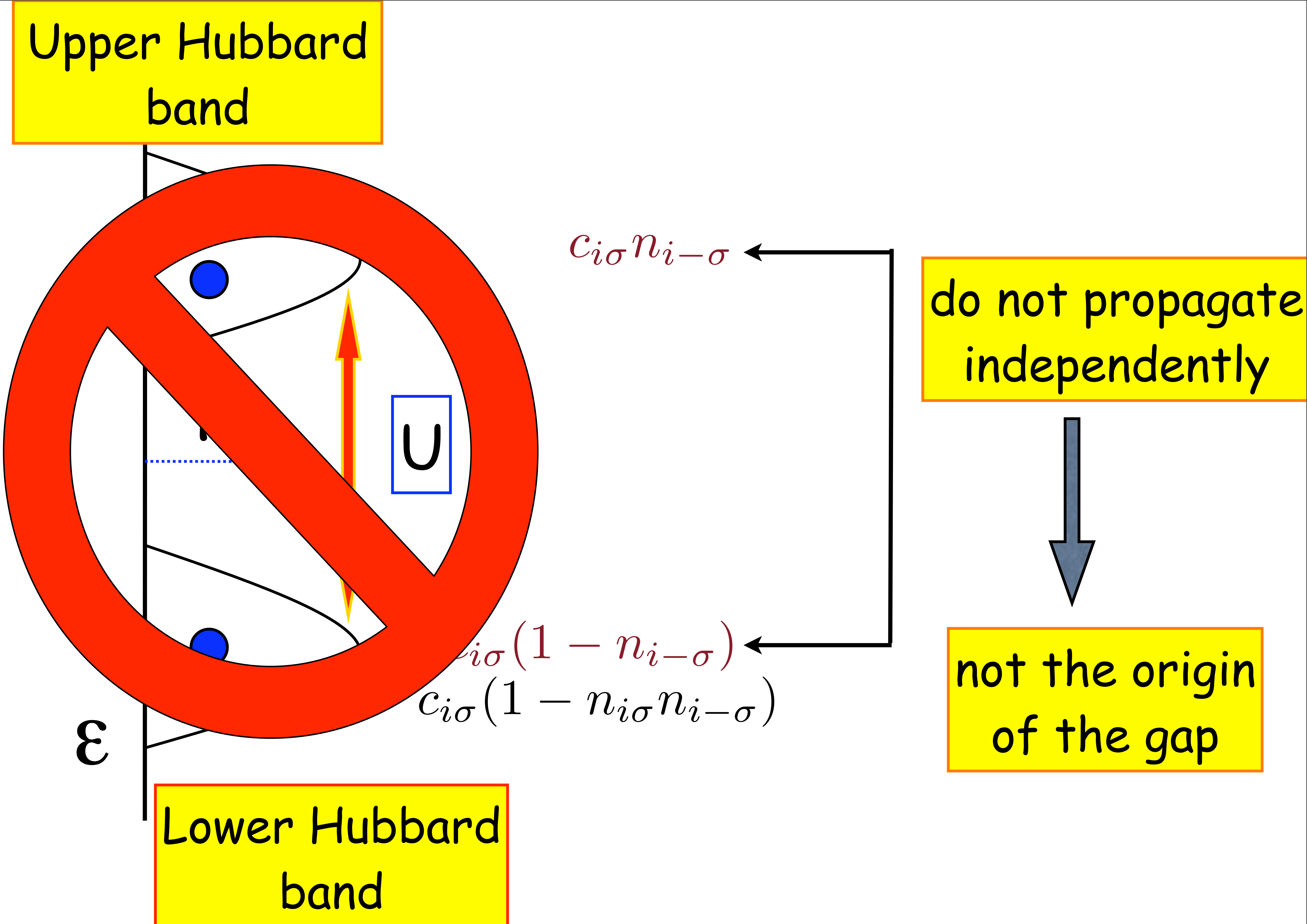
Strong Coupling

First Problem: Mott gap


Upper Hubbard band
μ
U
ε
Lower Hubbard band
$c_{i\sigma} n_{i-\sigma}$
$c_{i\sigma}(1-n_{i-\sigma})$
$c_{i\sigma}(1-n_{i\sigma} n_{i-\sigma})$
do not propagate independently
not the origin of the gap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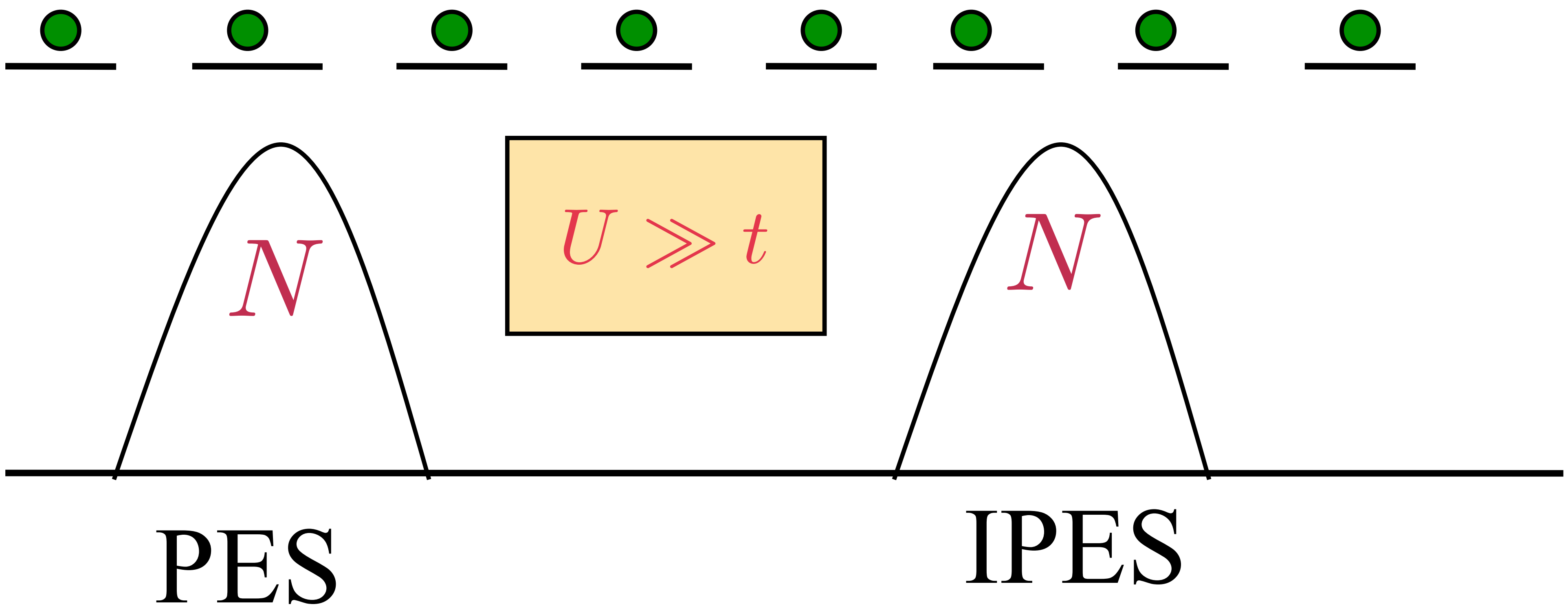
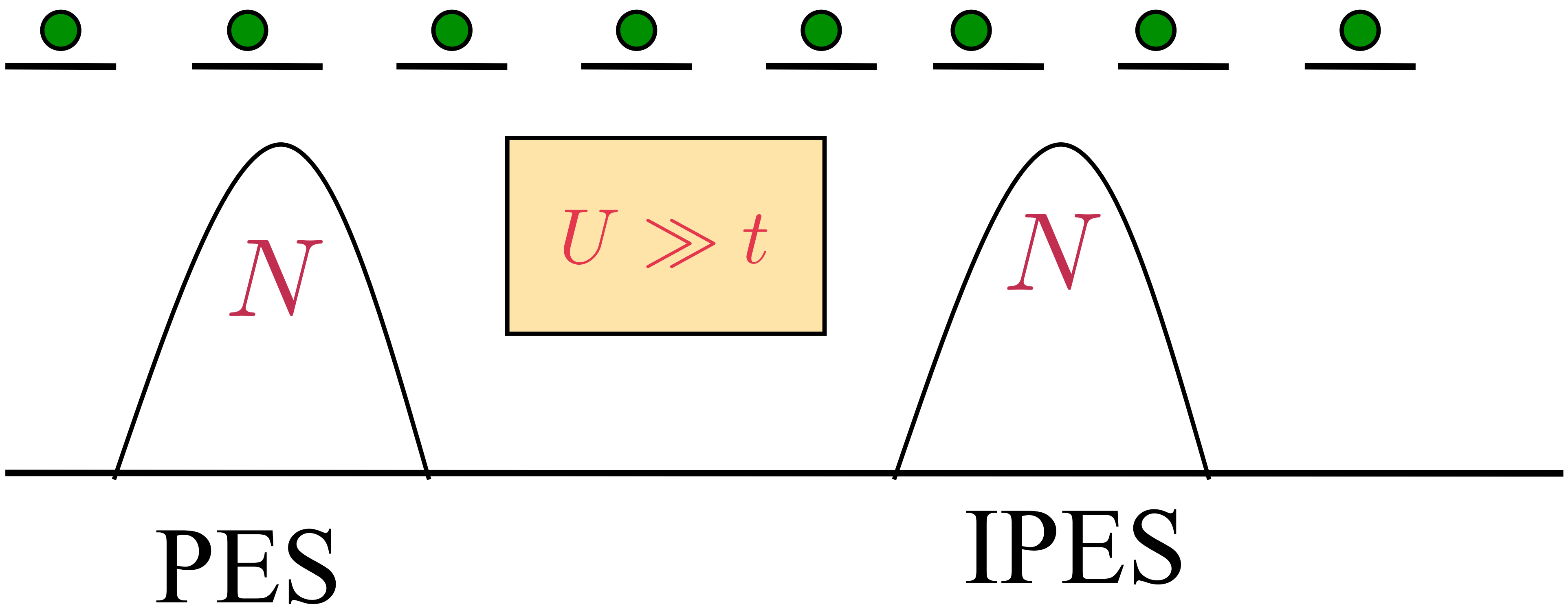
Mott Problem

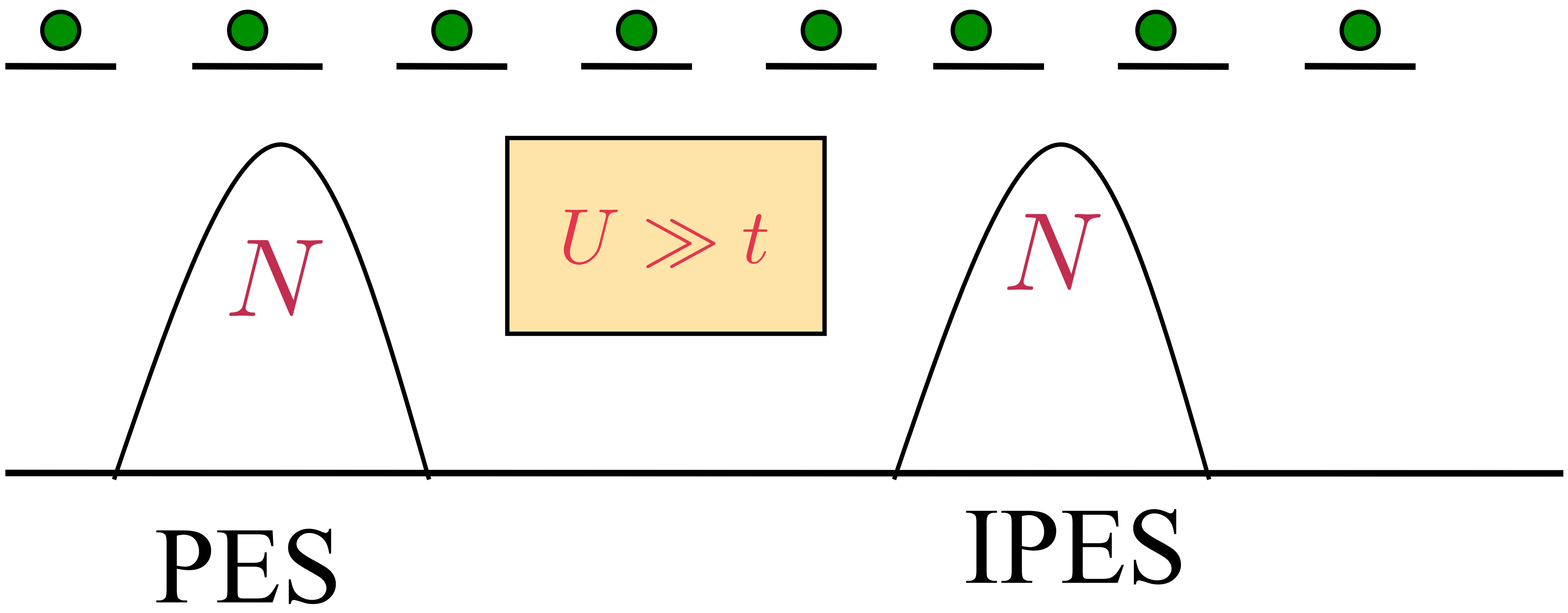


Mott Problem



What are the propagating degrees of freedom that produce the gapped spectrum?

Mott Problem



What are the propagating degrees of freedom that produce the gapped spectrum?

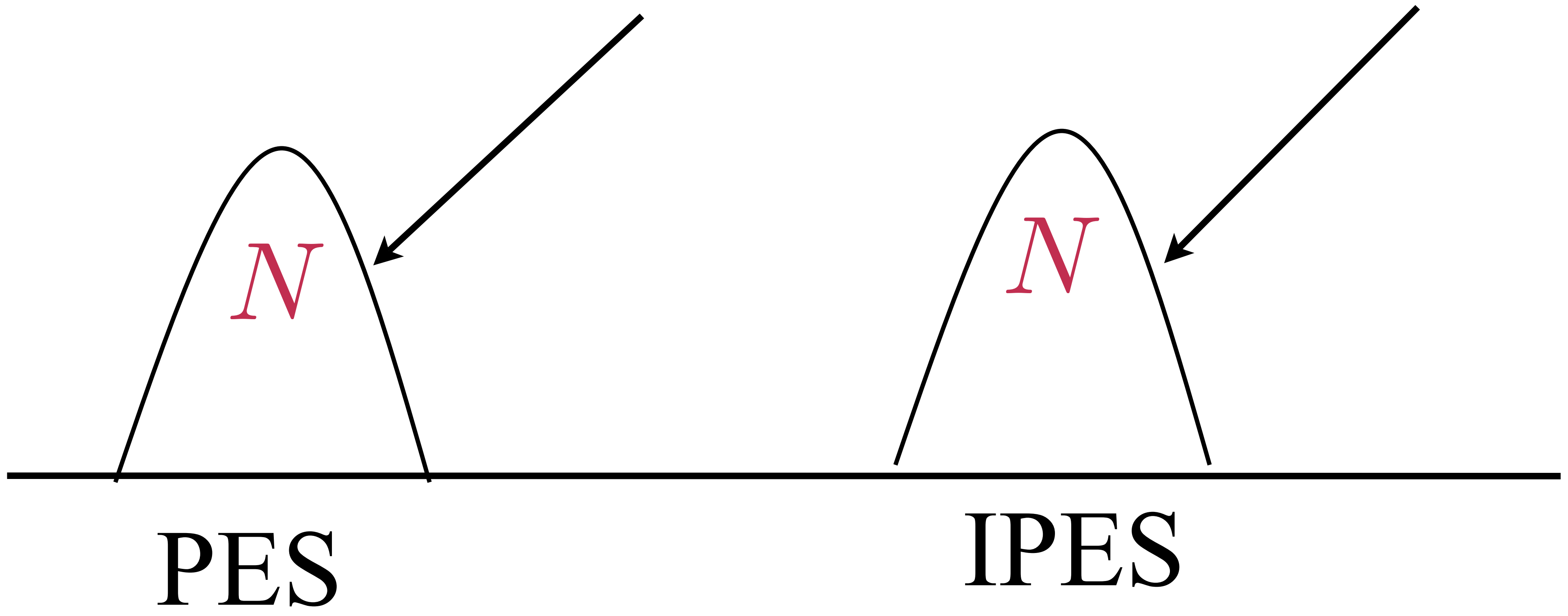
not electrons: $G(\omega = 0, p = p_L) = 0$

Fermi-liquid analogy

$$L_{\mathrm{FL}} \propto (\omega - \epsilon_k)|\psi_k|^2$$

Mott Problem?

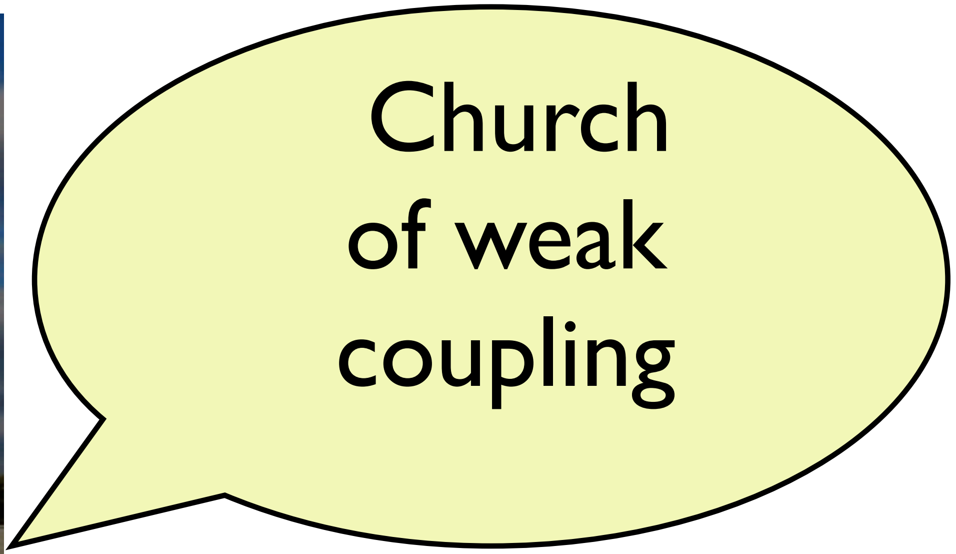
$$L_{\mathrm{MI}} = (\omega - E_{\mathrm{LHB}}(k))|\overset{?}{\eta_k}|^2 + (\omega - E_{\mathrm{UHB}}(k))|\overset{?}{\tilde{\eta}_k}|^2$$



A Critique of Two Metals

R. B. Laughlin

idea is either missing or improperly understood. Another indicator that something is deeply wrong is the inability of anyone to describe the elementary excitation spectrum of the Mott insulator precisely even as pure phenomenology. Nowhere can one find a quantitative band structure of the elementary particle whose spectrum becomes gapped. Nowhere can one find precise information about the particle whose gapless spectrum causes the paramagnetism. Nowhere can one find information about the interactions among these particles or of their potential bound state spectroscopies. Nowhere can one find precise definitions of Mott insulator terminology. The upper and lower Hubbard bands, for example, are vague analogues of the valence and conduction bands of a semiconductor, except that they coexist and mix with soft magnetic excitations no one knows how to describe very well.



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Church of weak coupling

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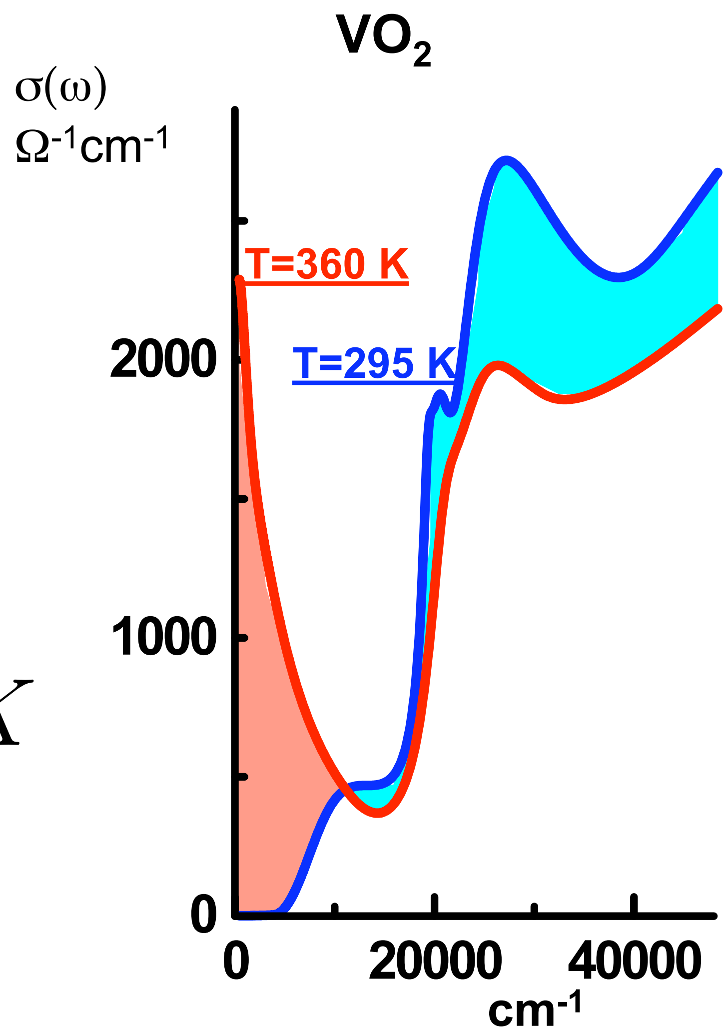
Beliefs:
Mott gap is heresy?
HF is the way!
No UHB and LHB!

$$\Delta = 0.6eV > \Delta_{\text{dimerization}}$$ (Mott, 1976)

Recall,
$eV = 10^4 K$



transfer
of spectral
weight to
high energies
beyond any ordering
scale

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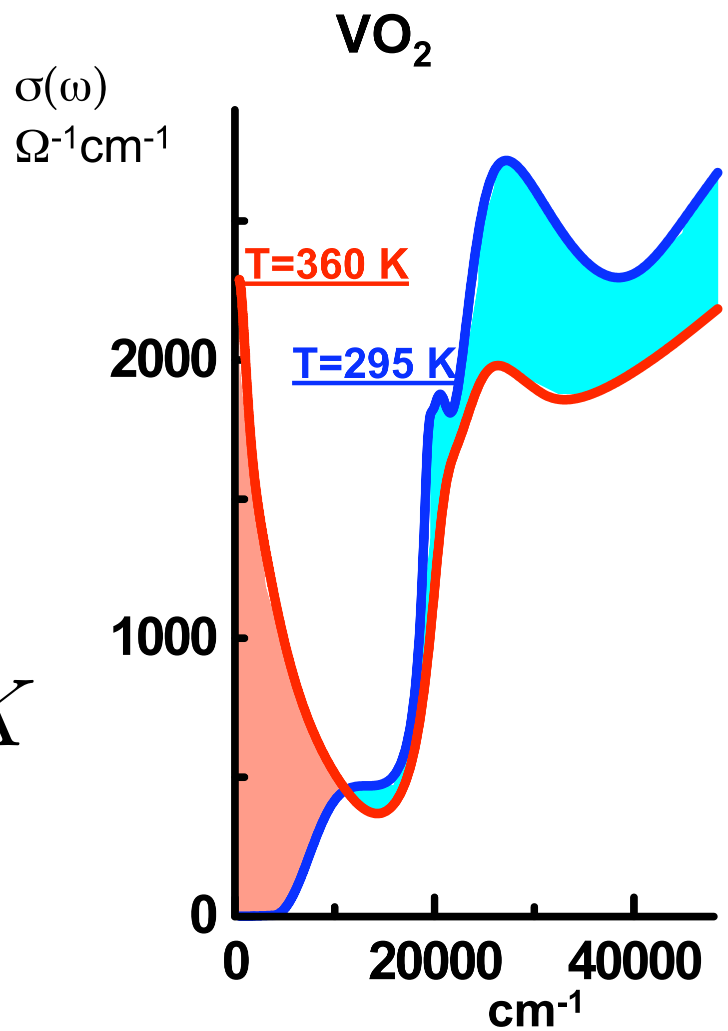

M. M. Qazilbash, K. S. Burch, D. Whisler, D. Shrekenhamer, B. G. Chae, H. T. Kim, and D. N. Basov PRB 74, 205118 (2006)

transfer
of spectral
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high energies
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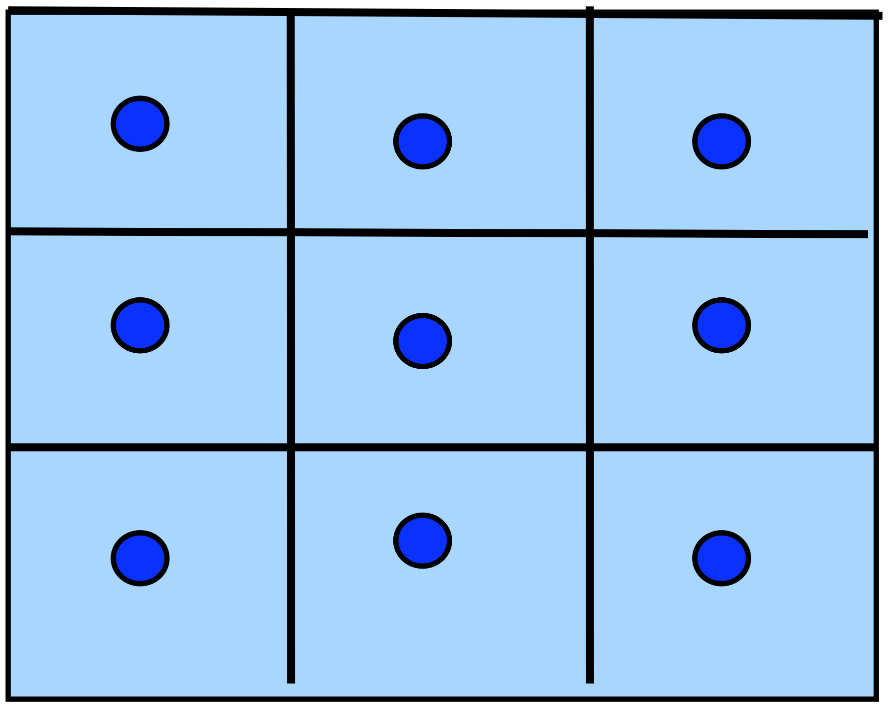
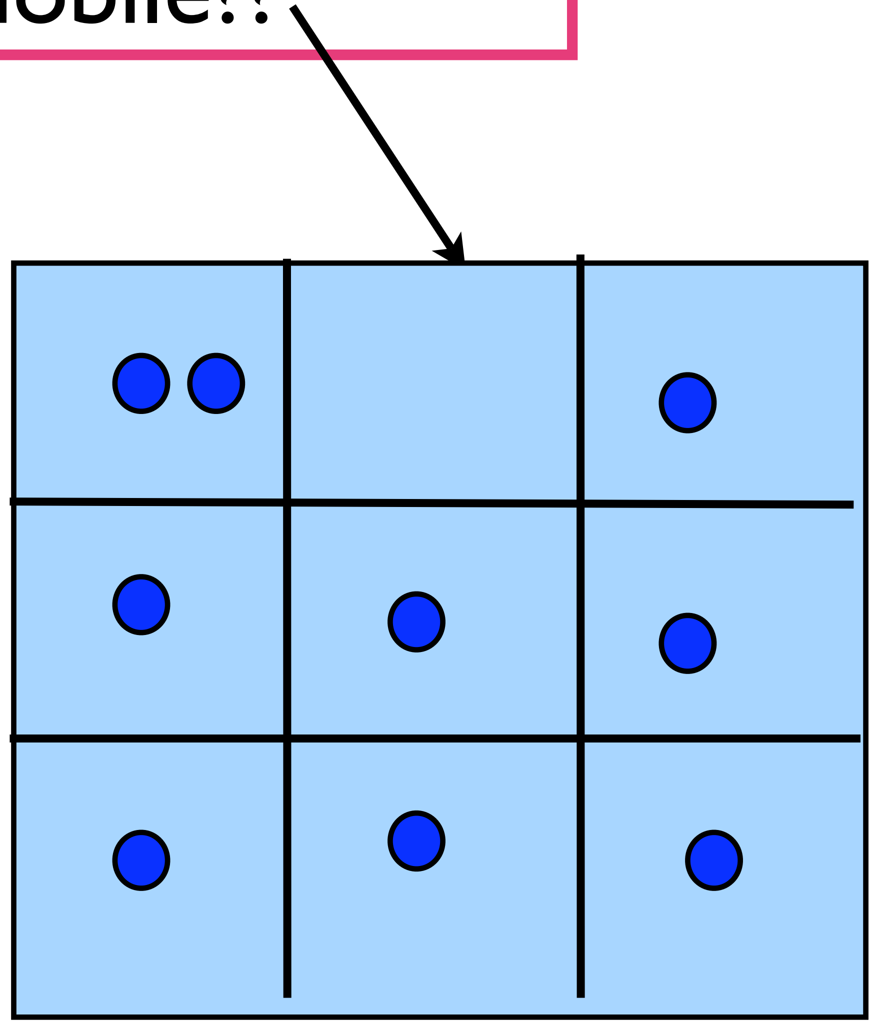
Collective Phenomena

is the empty site mobile??



+ t/U



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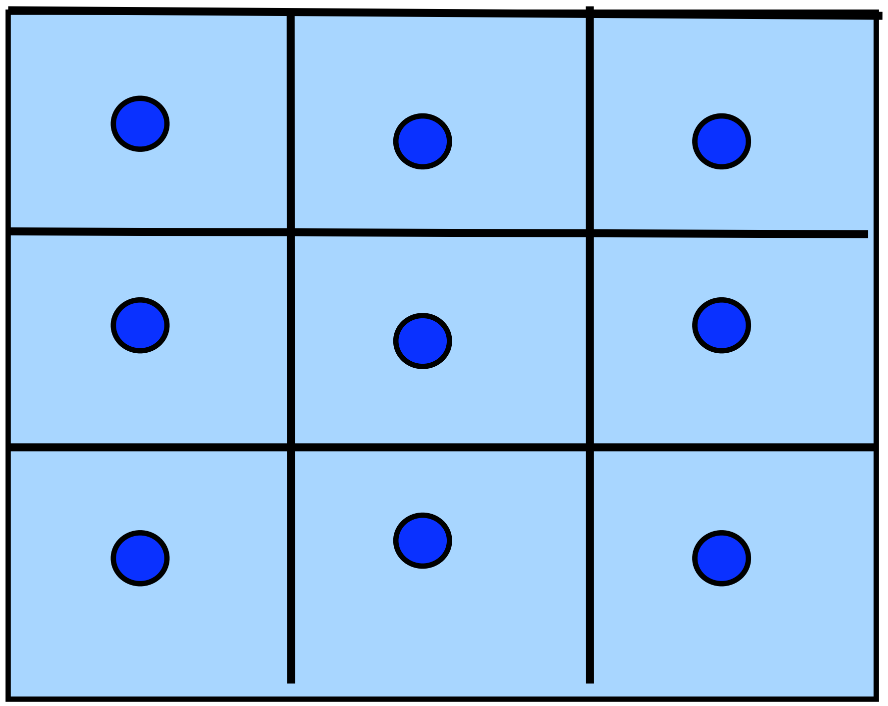

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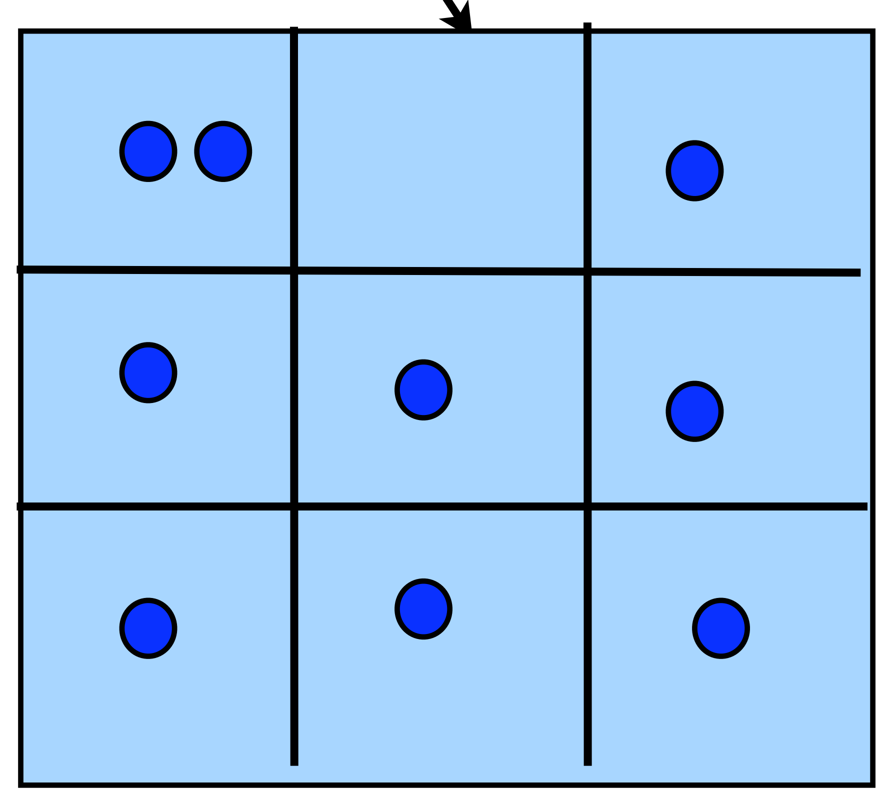

if yes, then 1.)
Mott insulator is a metal,
2.) no magnetic order

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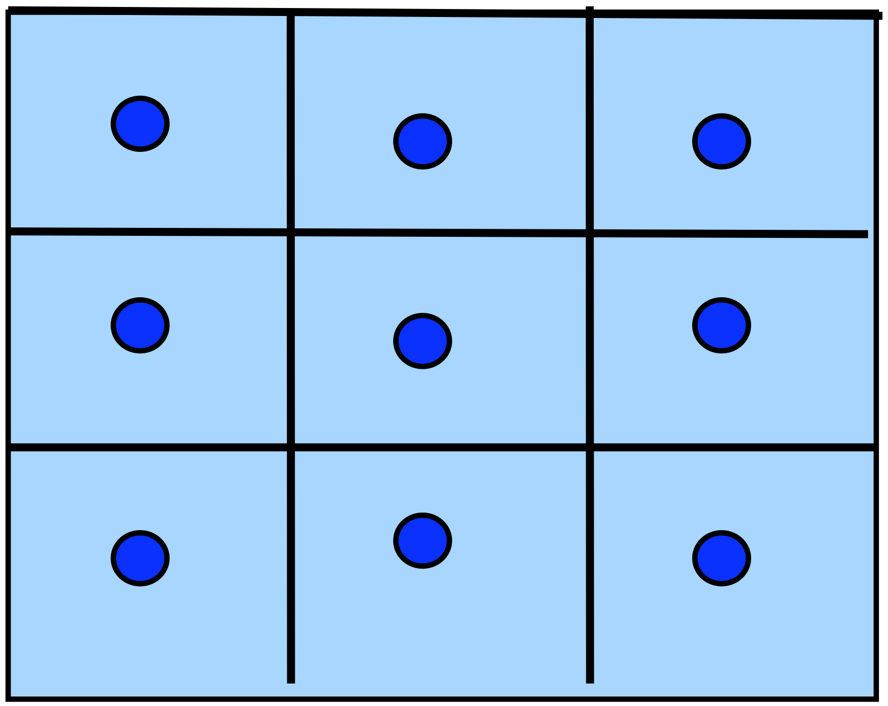

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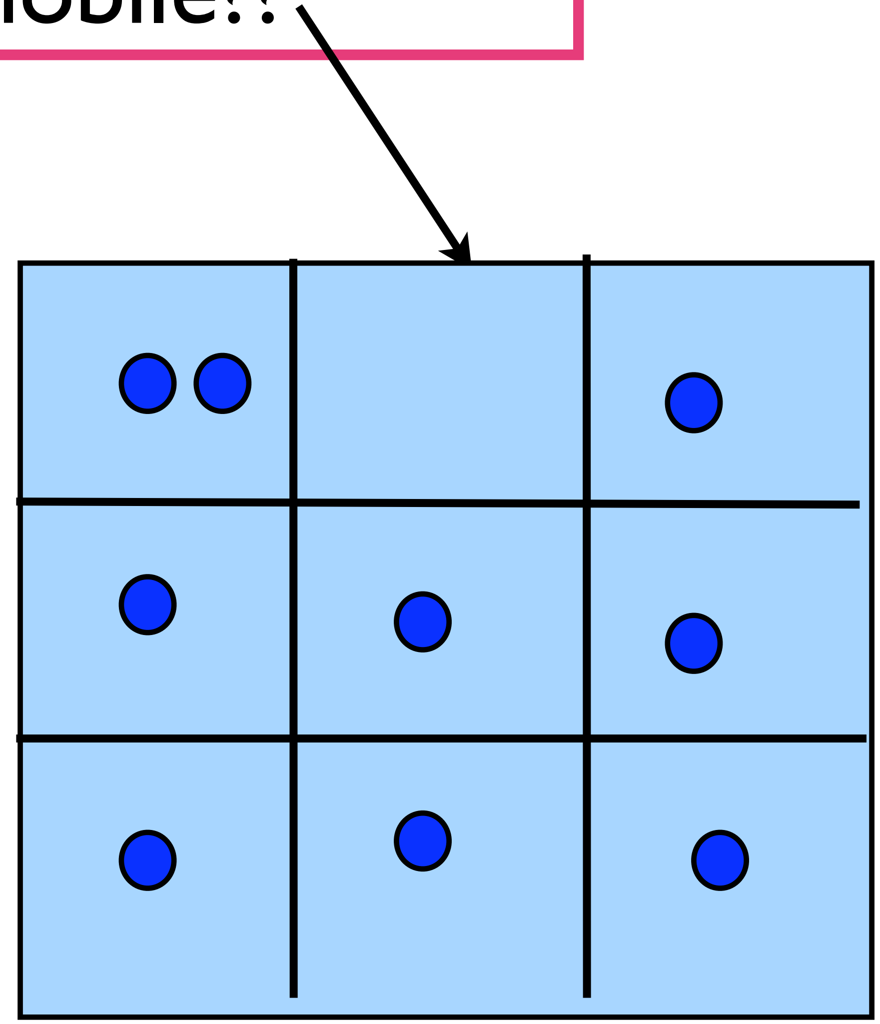

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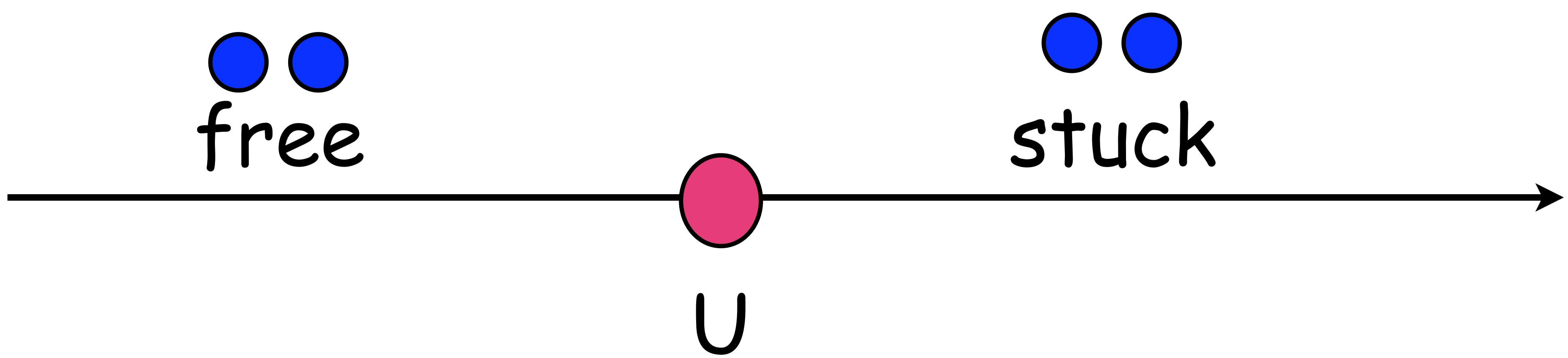
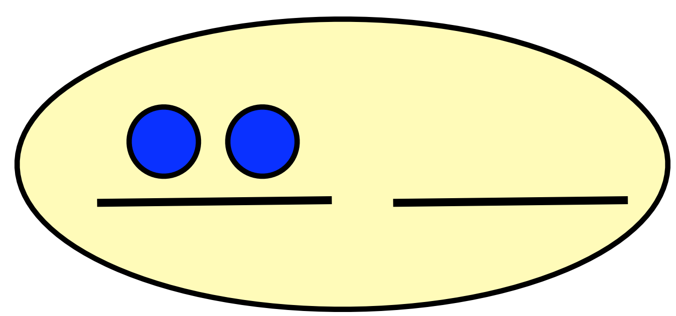
localisation criterion



Mott Problem: what is the dynamical degree of freedom that makes this happen?

new bound states

Kohn, Mott, Castellani, others



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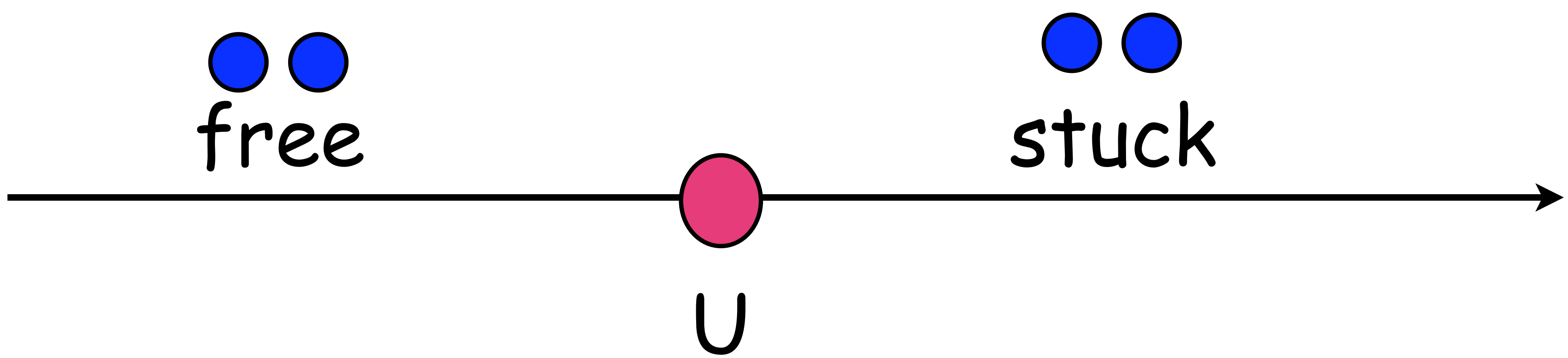

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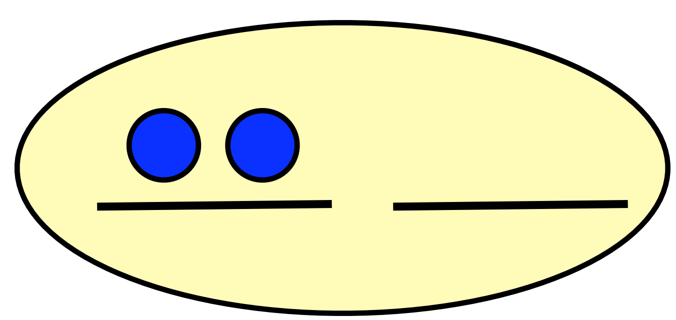
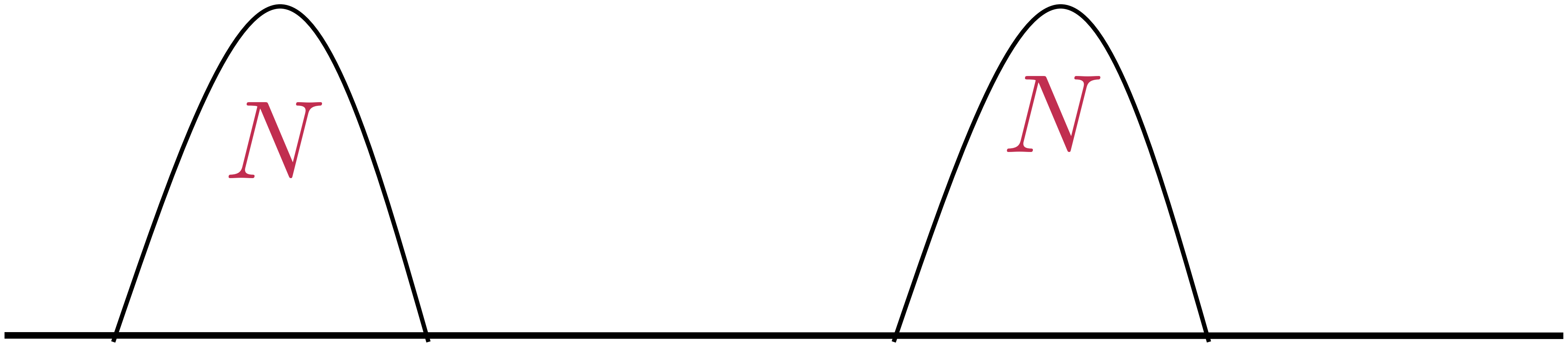


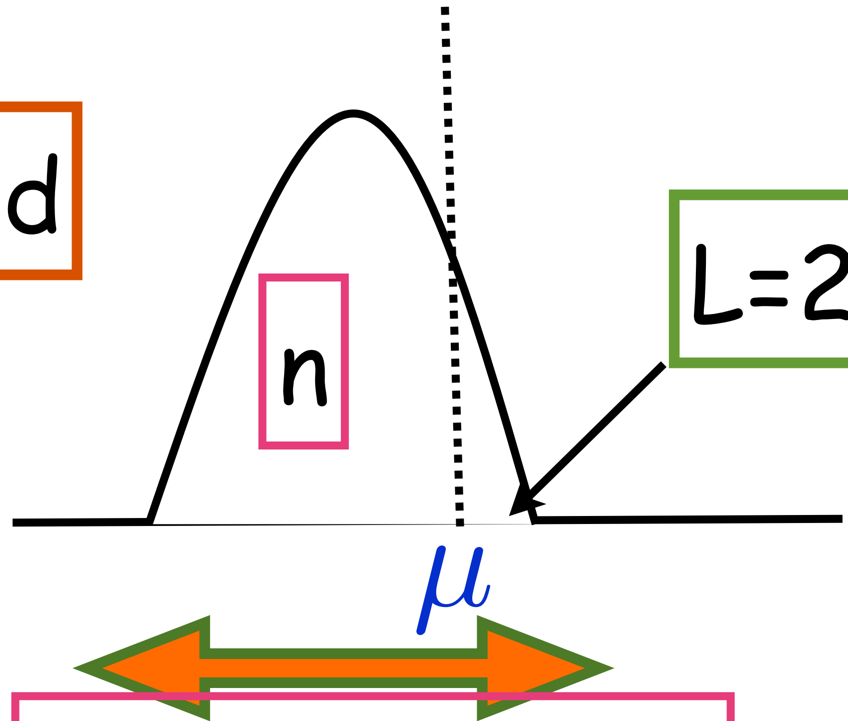
No proof exists? Mottness is ill-defined

Second Problem: spectral weight transfer



the weight of each band depends on the filling!

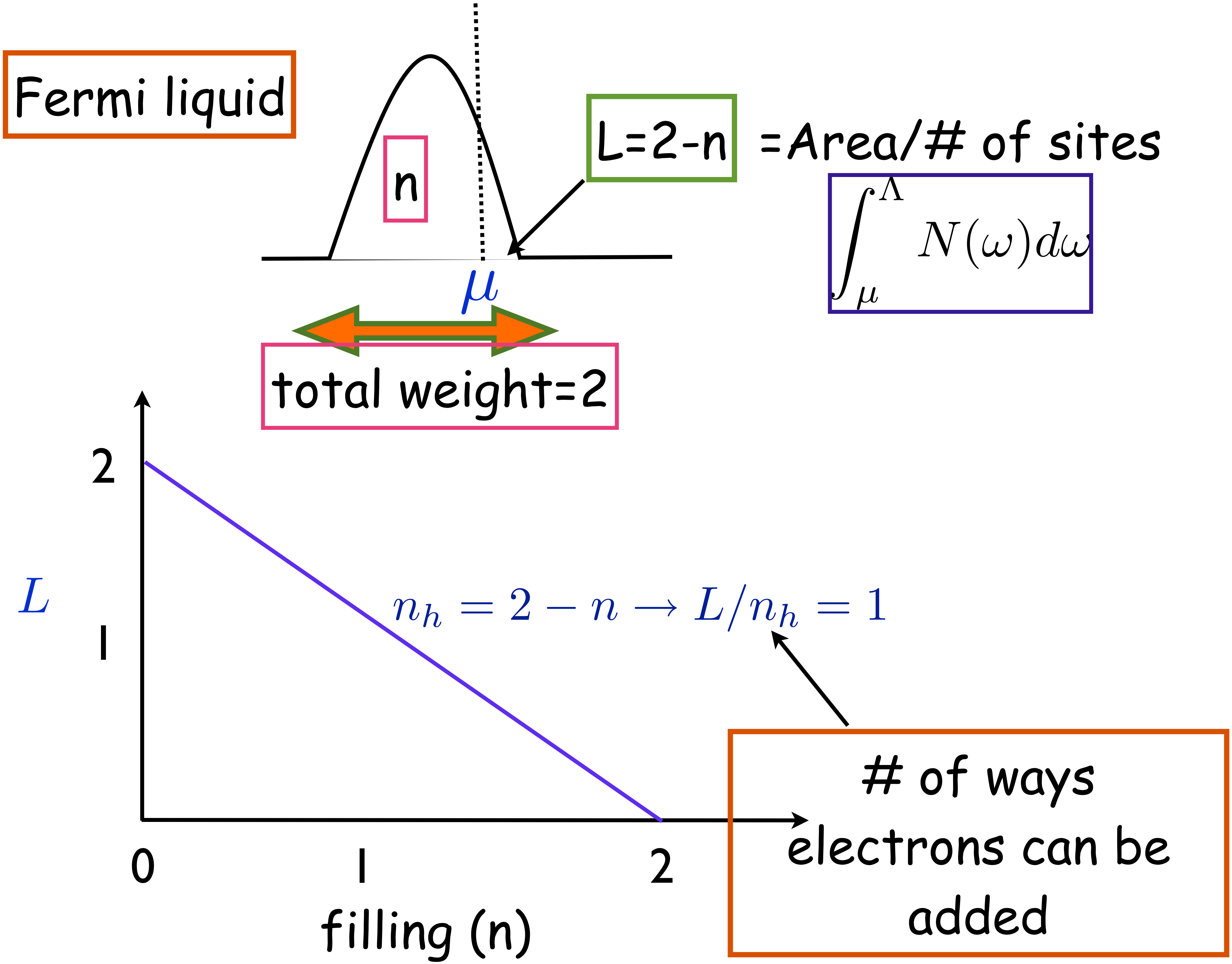
Fermi liquid



total weight=2

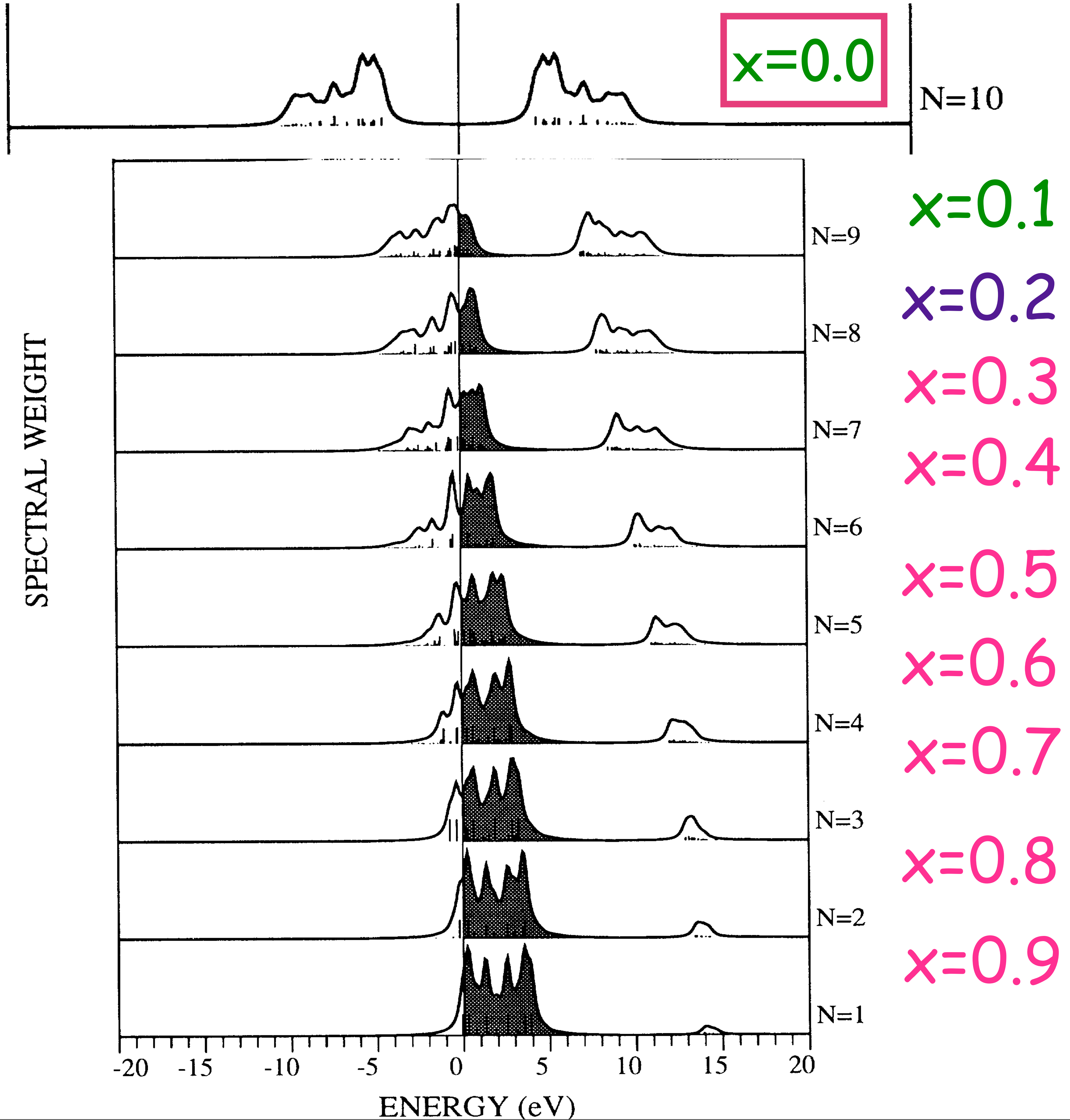
L=2-n =Area/# of sites

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

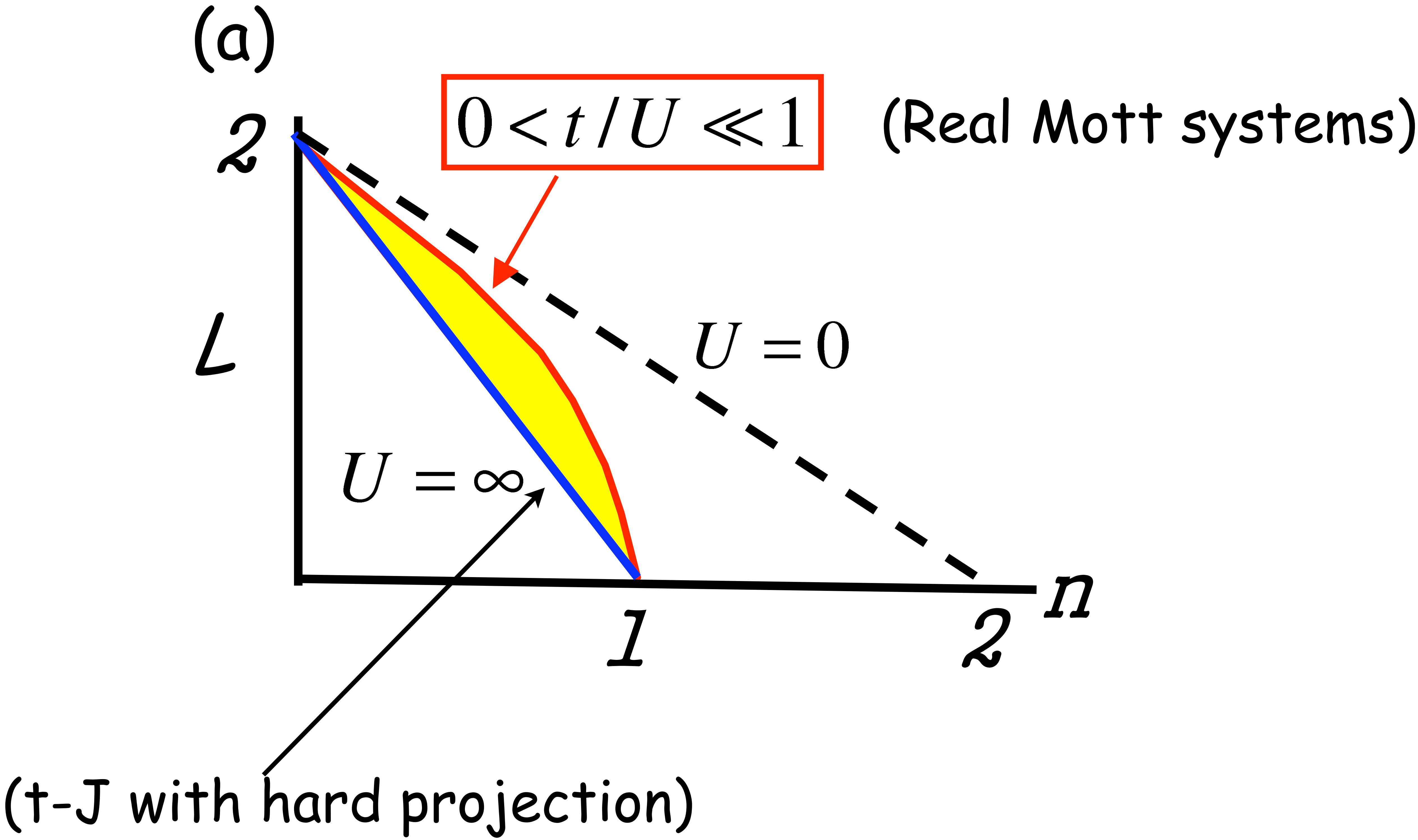


Fermi liquid
n
L=2-n
=Area/# of sites
$\int_{\mu}^{\Lambda} N(\omega)d\omega$
μ
total weight=2
2
1
L
$n_h = 2 - n \rightarrow L/n_h = 1$
0
1
2
filling (n)
# of ways electrons can be added

Mott gap

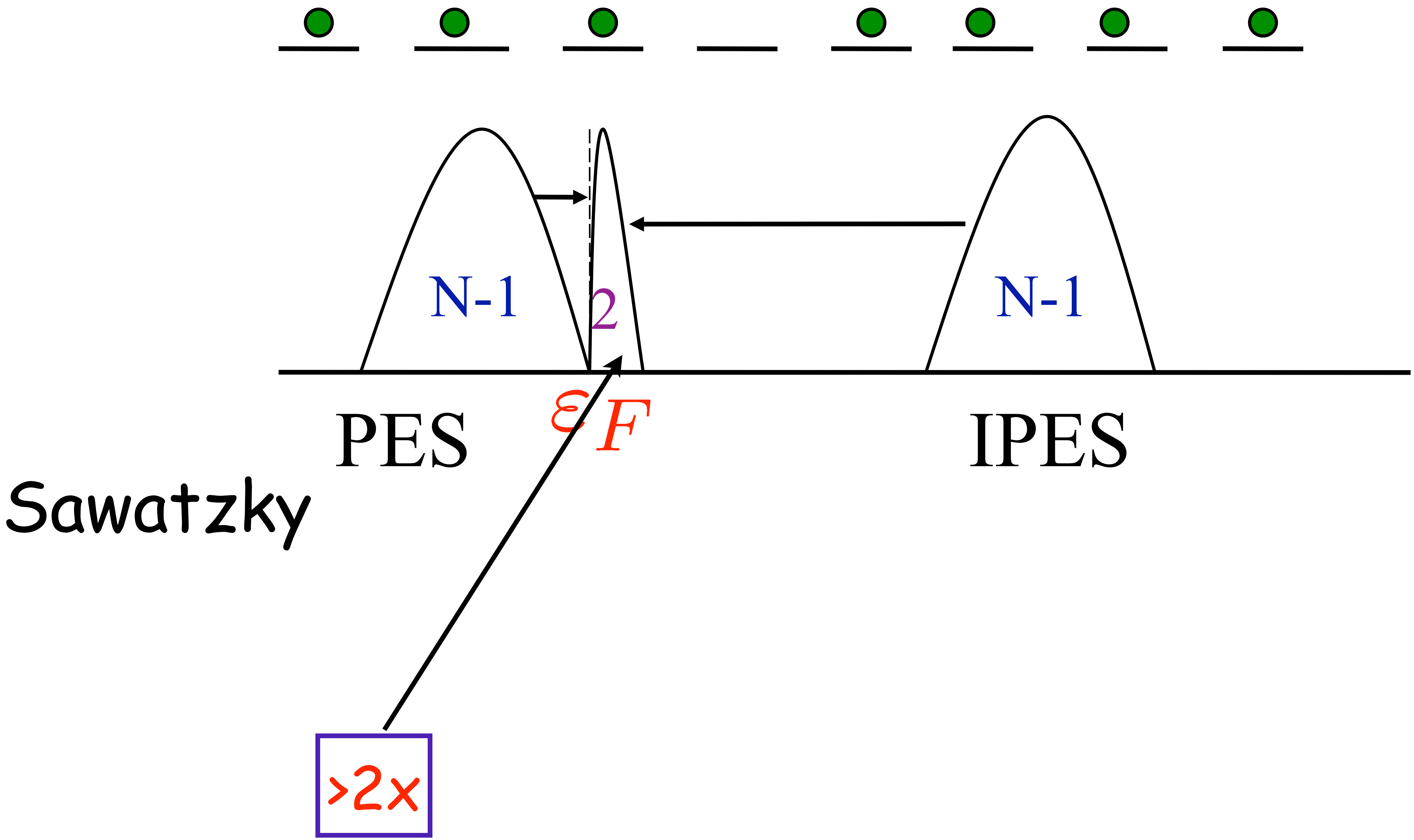


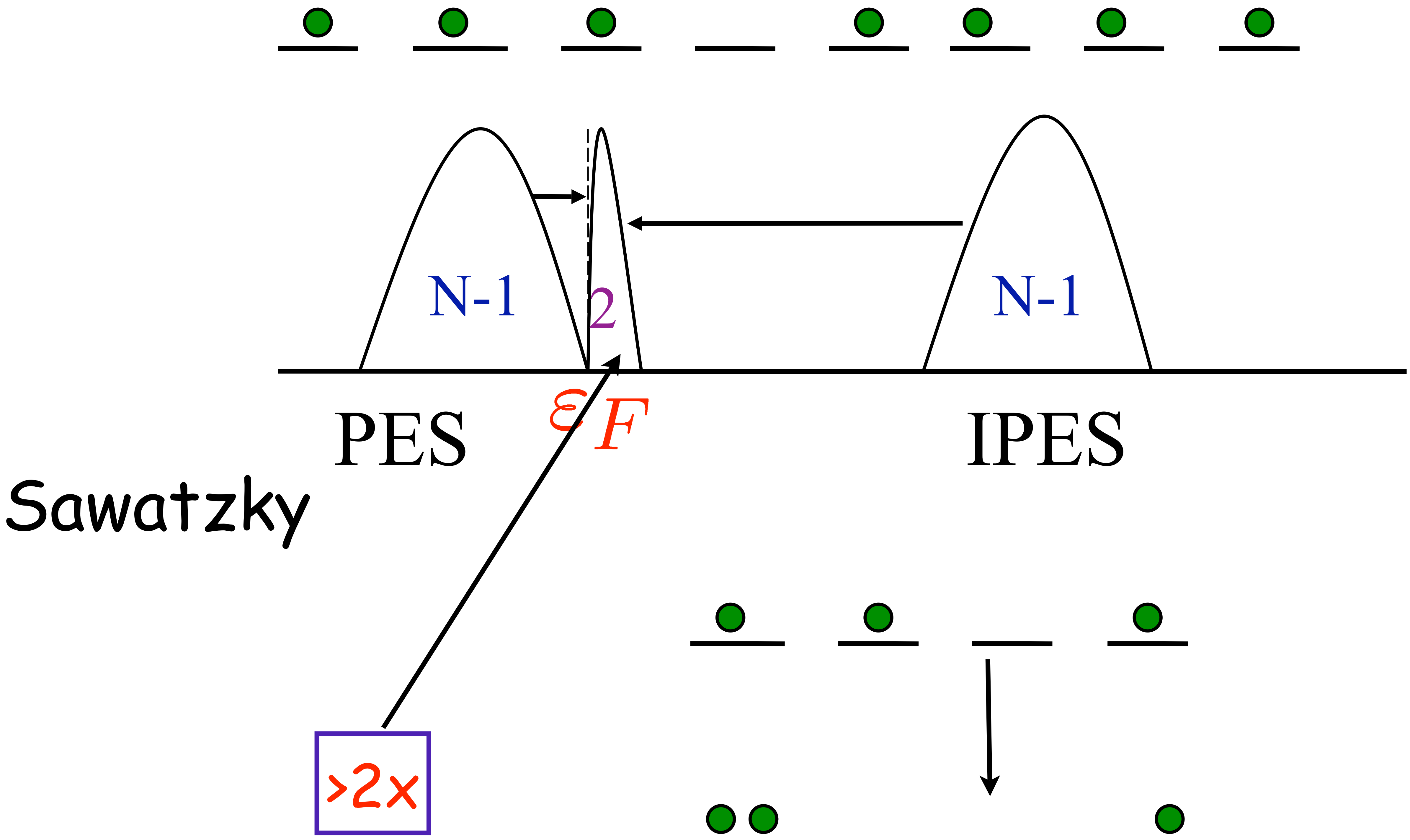
x=0.0
N=10
x=0.1
x=0.2
x=0.3
x=0.4
x=0.5
x=0.6
x=0.7
x=0.8
x=0.9
N=9
N=8
N=7
N=6
N=5
N=4
N=3
N=2
N=1
SPECTRAL WEIGHT
-20 -15 -10 -5 0 5 10 15 20
ENERGY (eV)



(a)
$0 < t/U \ll 1$
(Real Mott systems)
2
L
$U = 0$
$U = \infty$
1
2
n
(t-J with hard projection)

Why?


N-1
2
N-1
PES
ε_F
IPES
Sawatzky
>2x


N-1
2
N-1
ε_F
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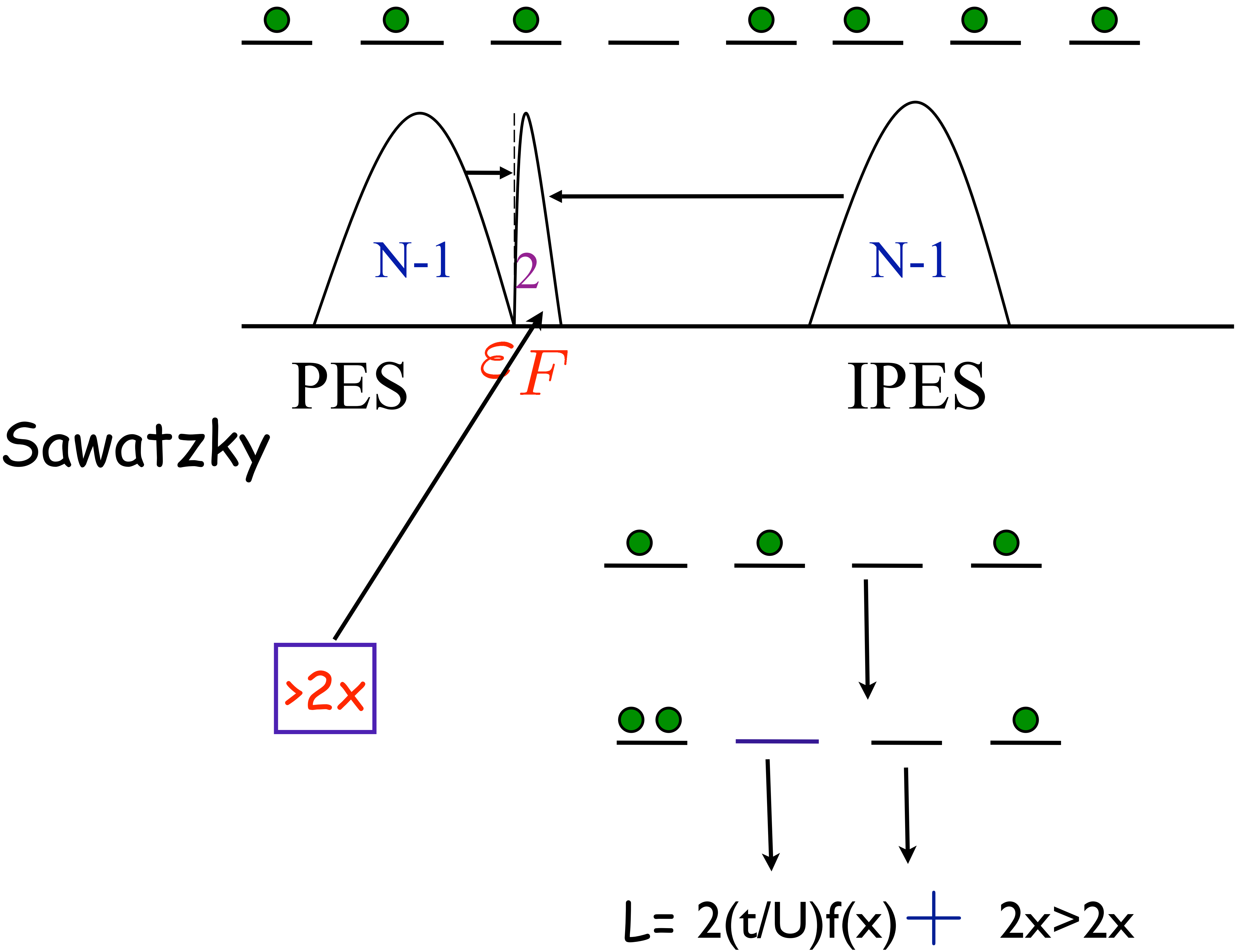


N-1
2
N-1
PES
εF
IPES
Sawatzky
>2x
L= 2(t/U)f(x) + 2x>2x

Number of low energy states per electron per spin > 1

Mottness

L-2x of the states are orthogonal to electron addition

new degree of freedom is relevant

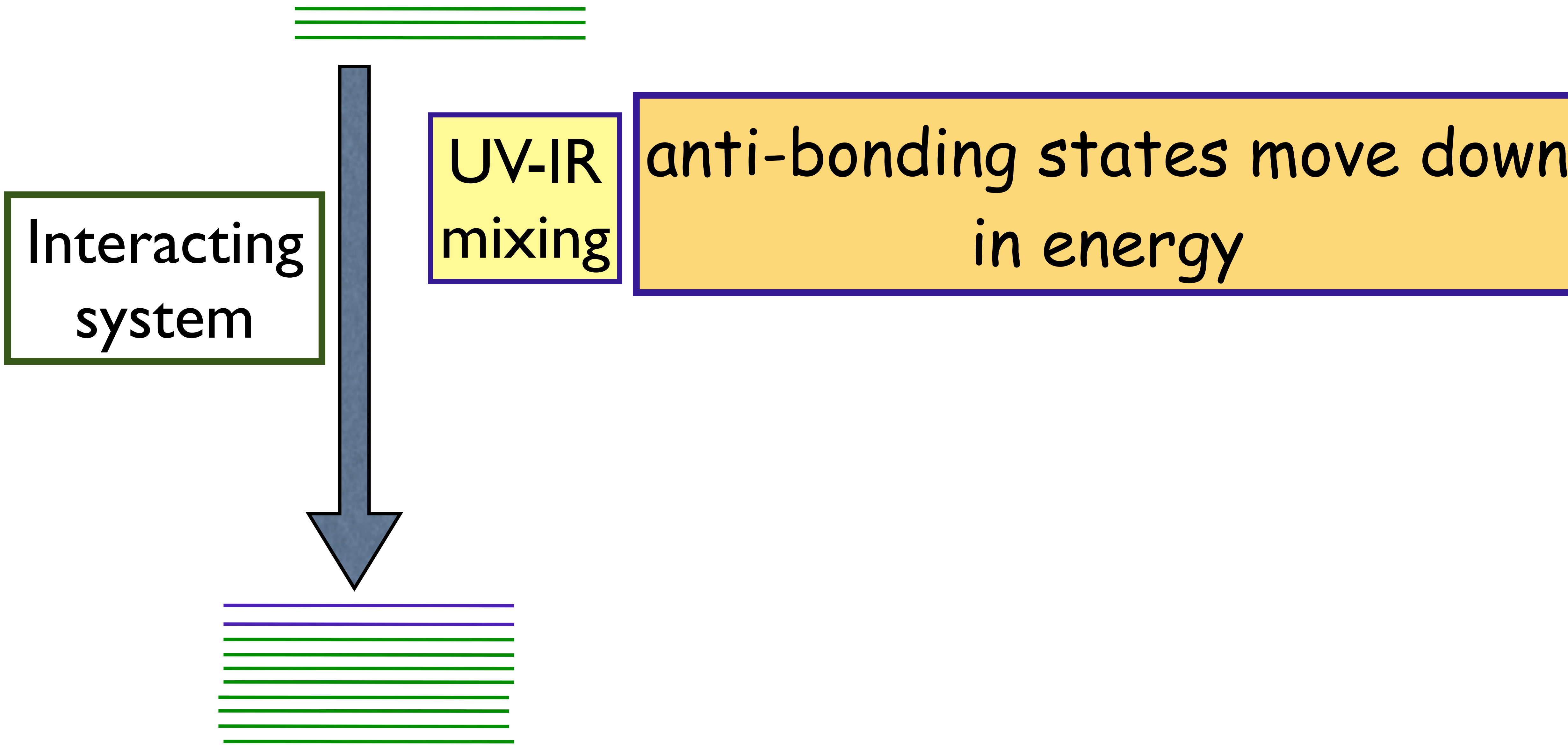
Number of low energy states per electron per spin > 1

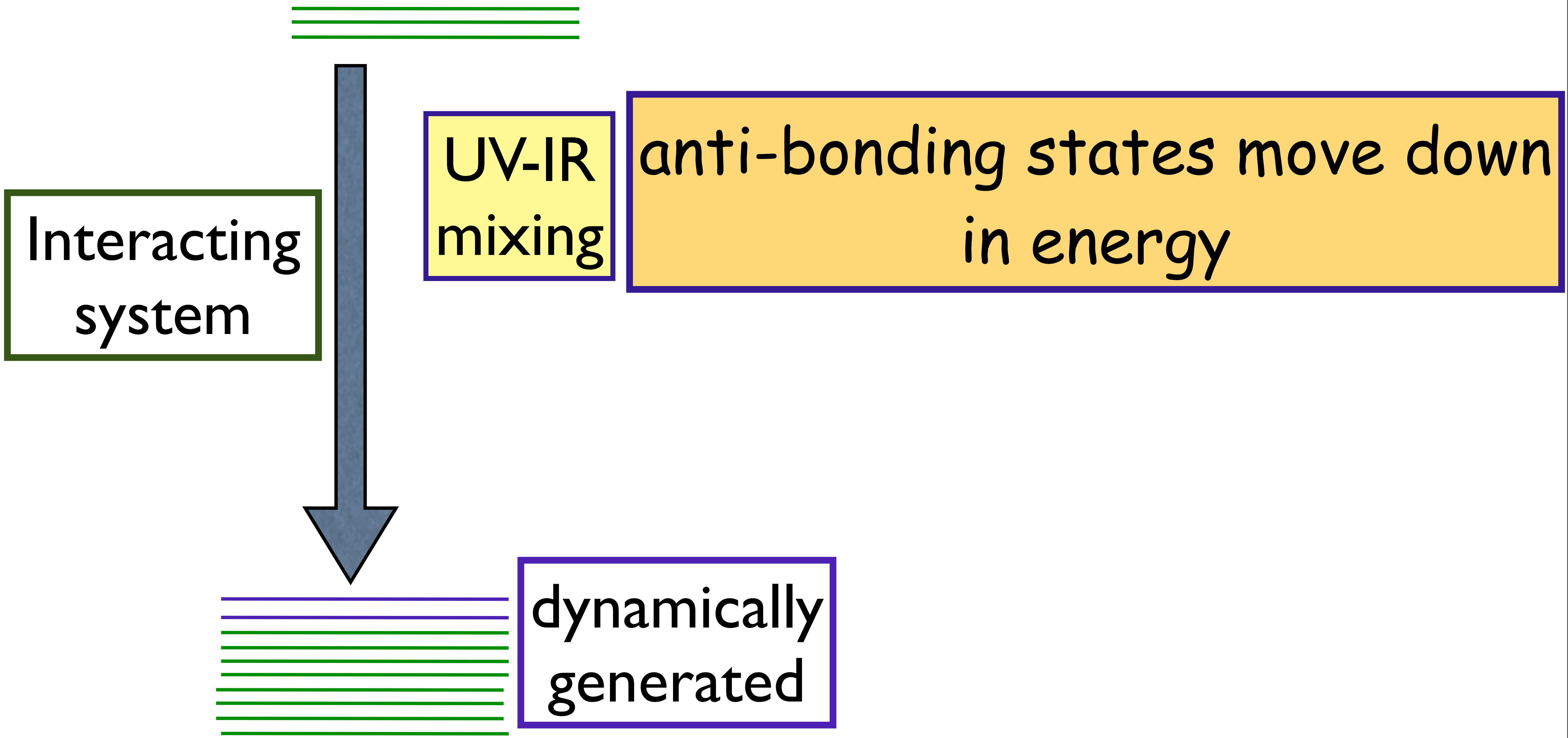
Mottness

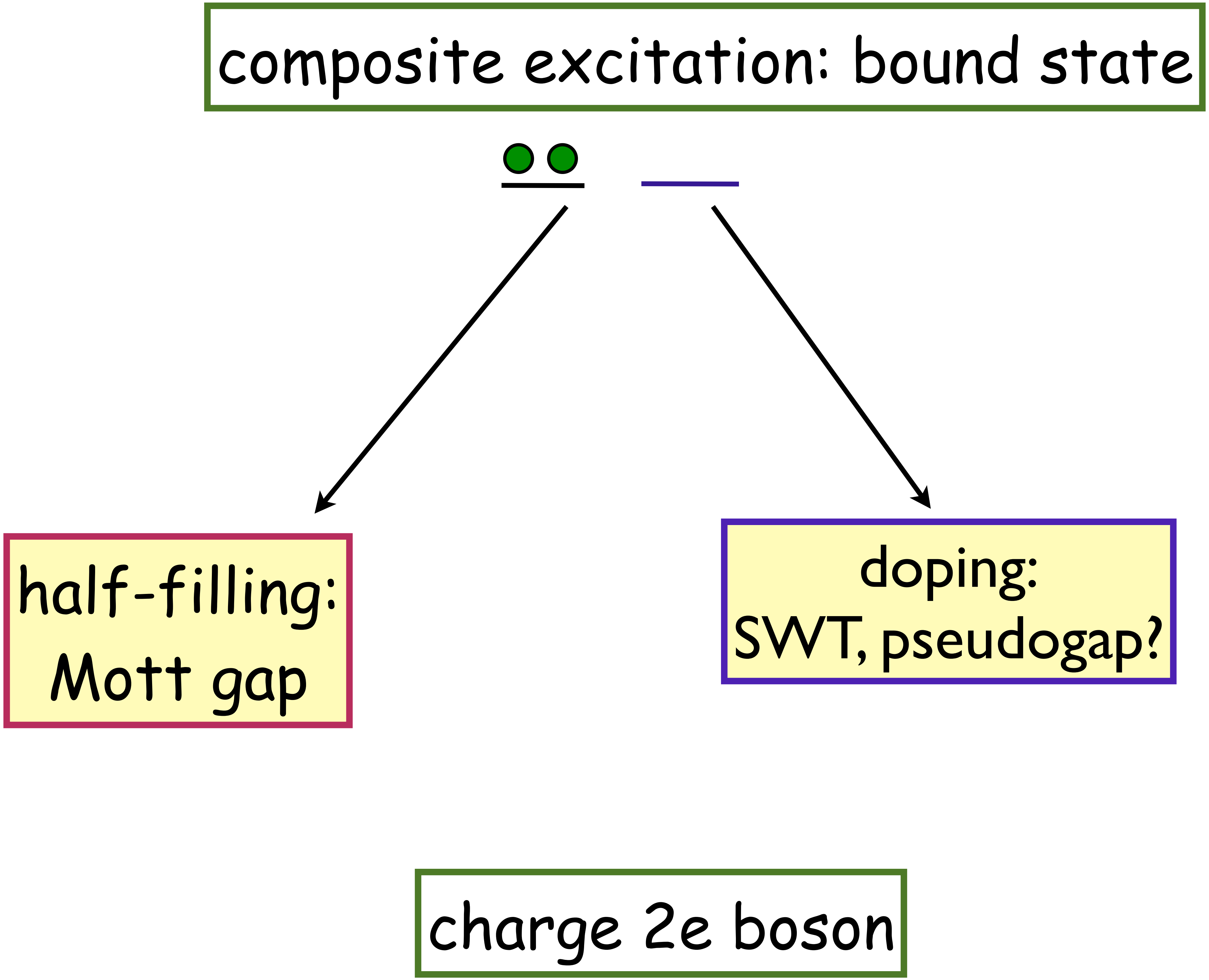
L-2x of the states are orthogonal to electron addition

pseudogap

new degree of freedom is relevant


Interacting system
UV-IR mixing
anti-bonding states move down in energy


Interacting system
UV-IR mixing
anti-bonding states move down in energy
dynamically generated


composite excitation: bound state
half-filling:
Mott gap
doping:
SWT, pseudogap?
charge 2e boson

identifying the propagating degrees of freedom

Effective Theories:

$S(\phi)$ at half-filling

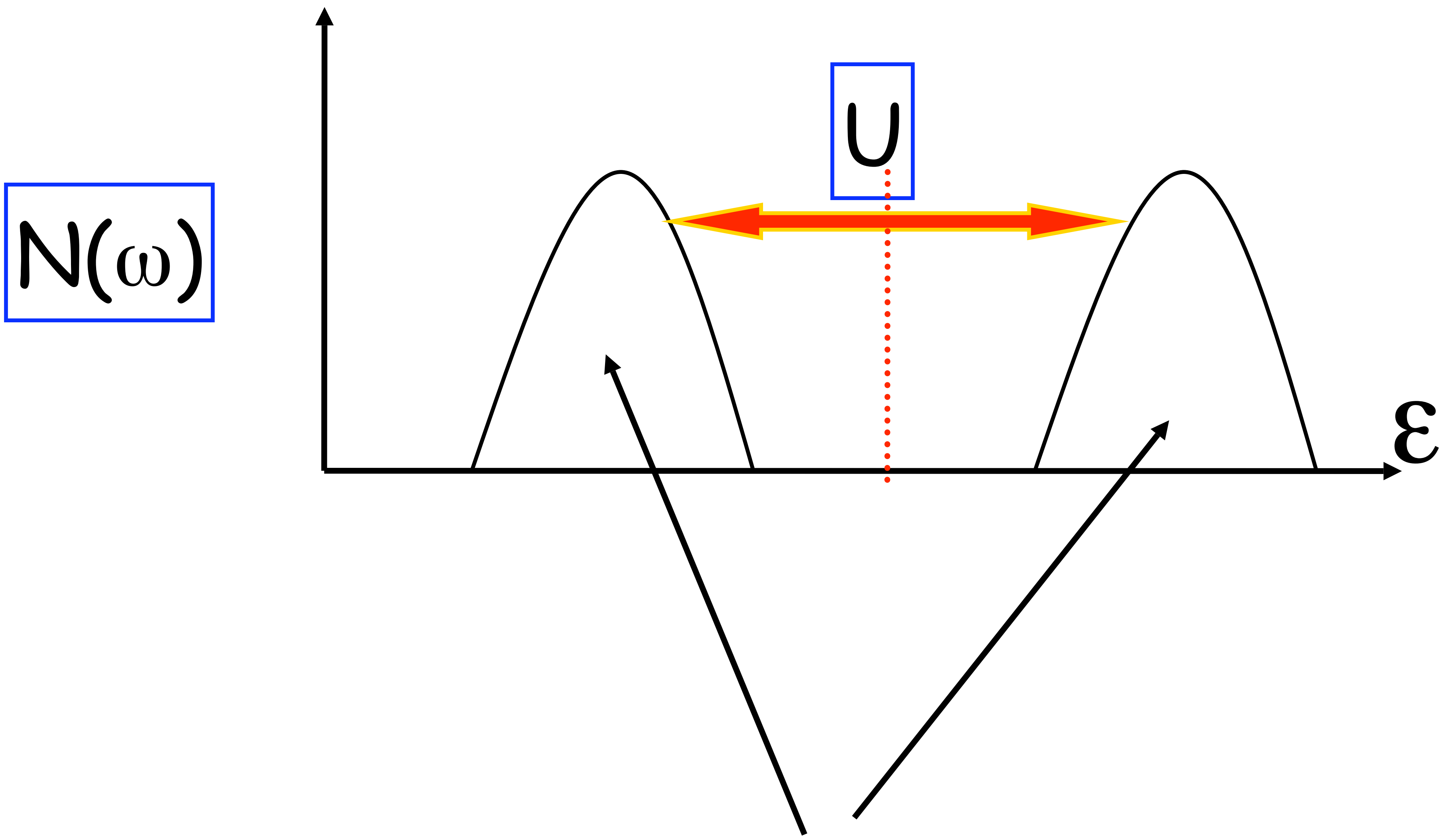
Integrate Out high Energy fields

$\phi=\phi_L+\phi_H$

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

Low-energy theory of M I

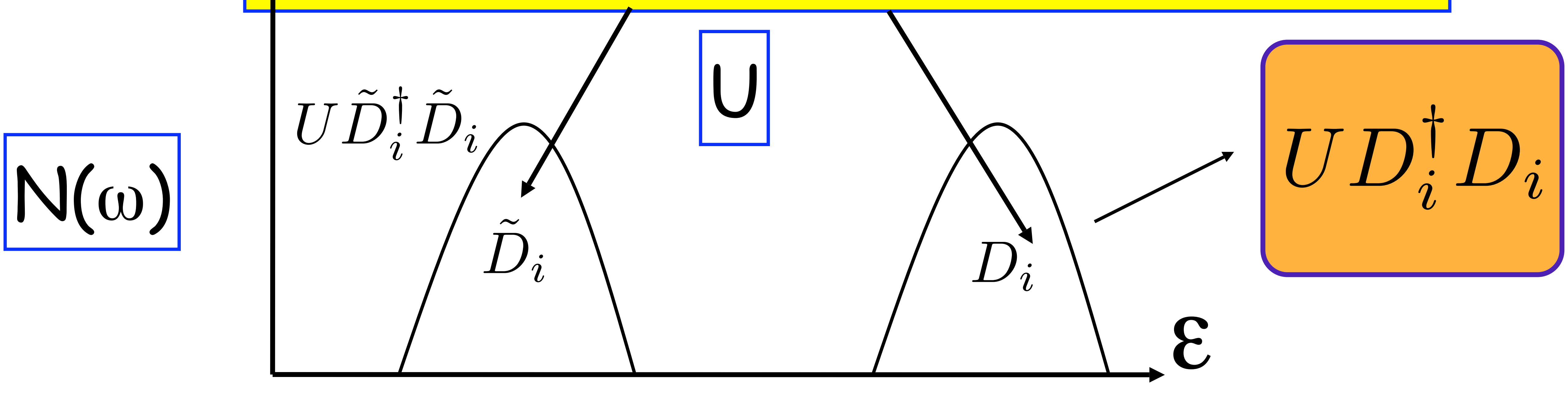
Half-filling



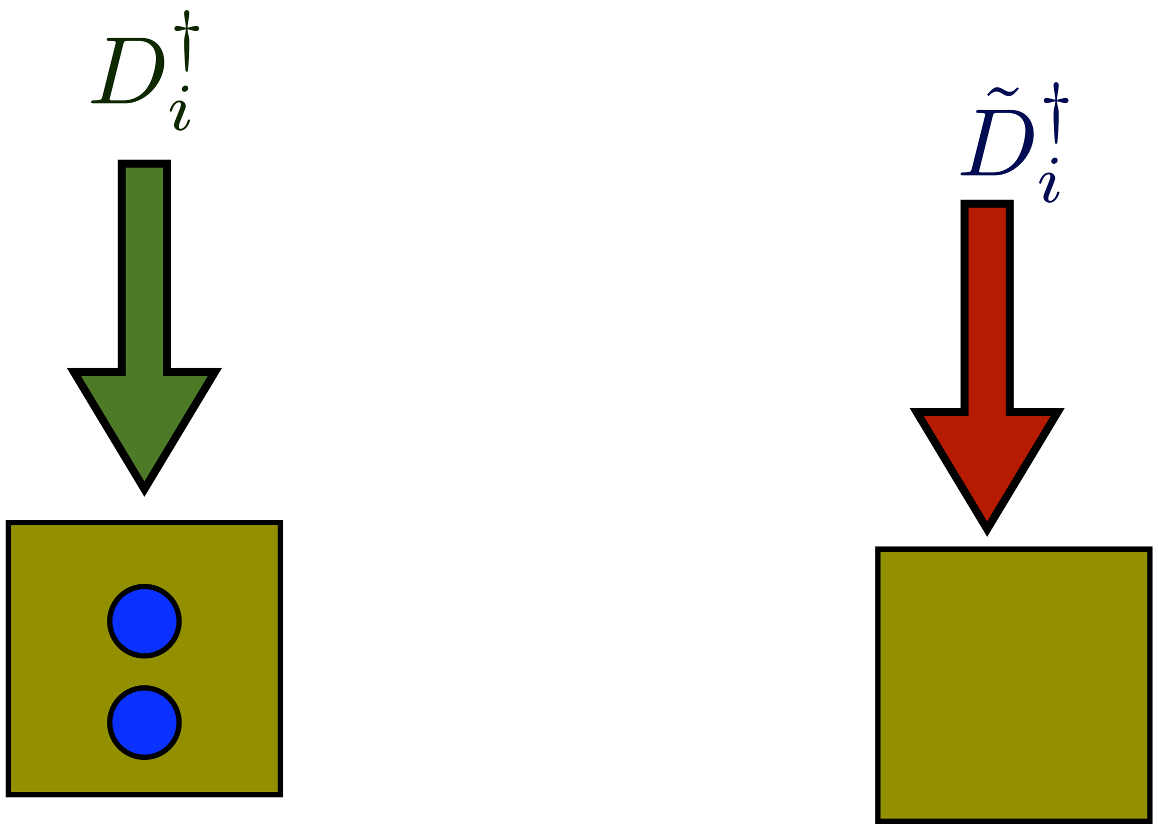
Integrate out both

Key idea: similar to Bohm/Pines

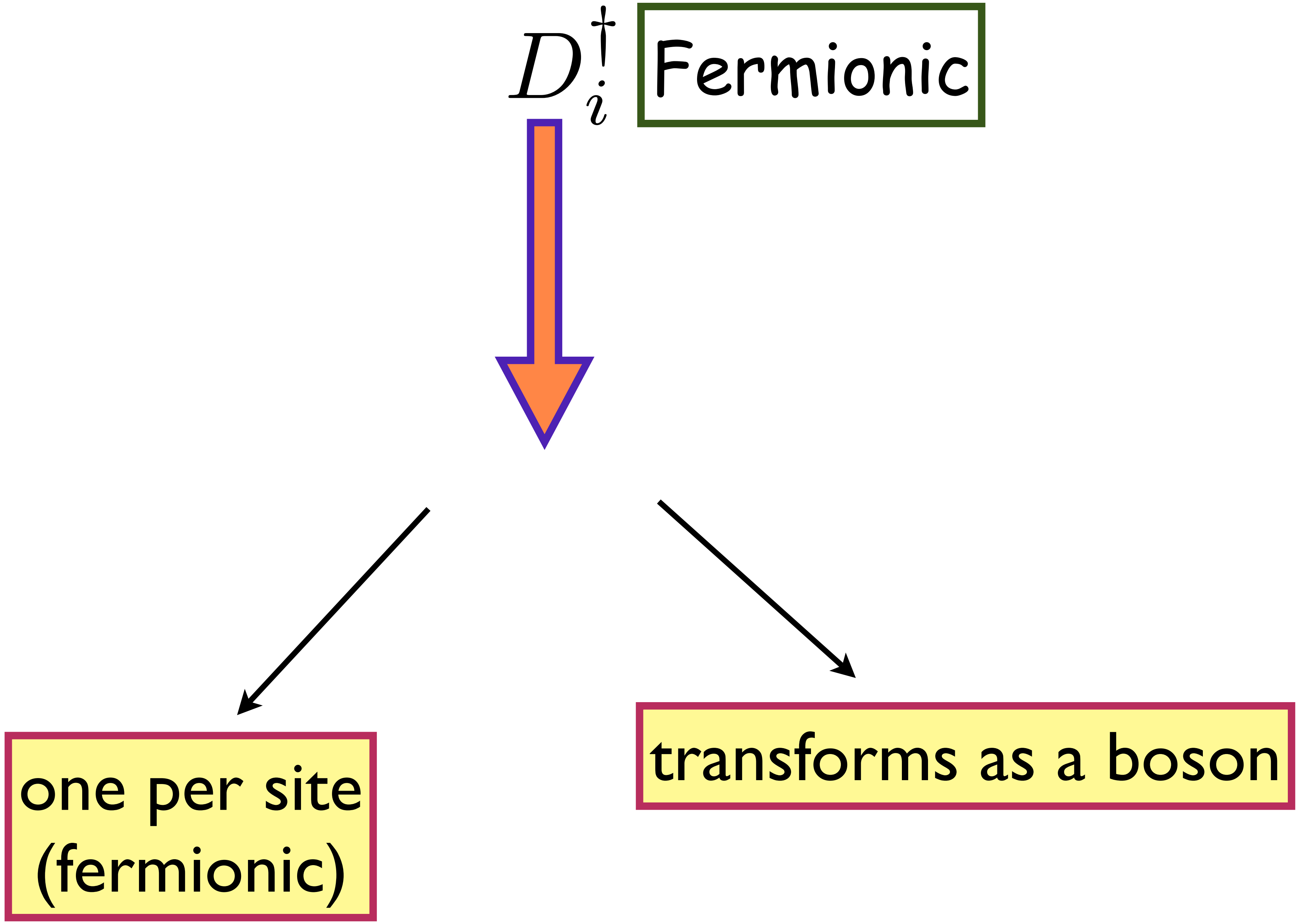
Extend the Hilbert space:
Associate with U-scale new
Fermionic oscillators

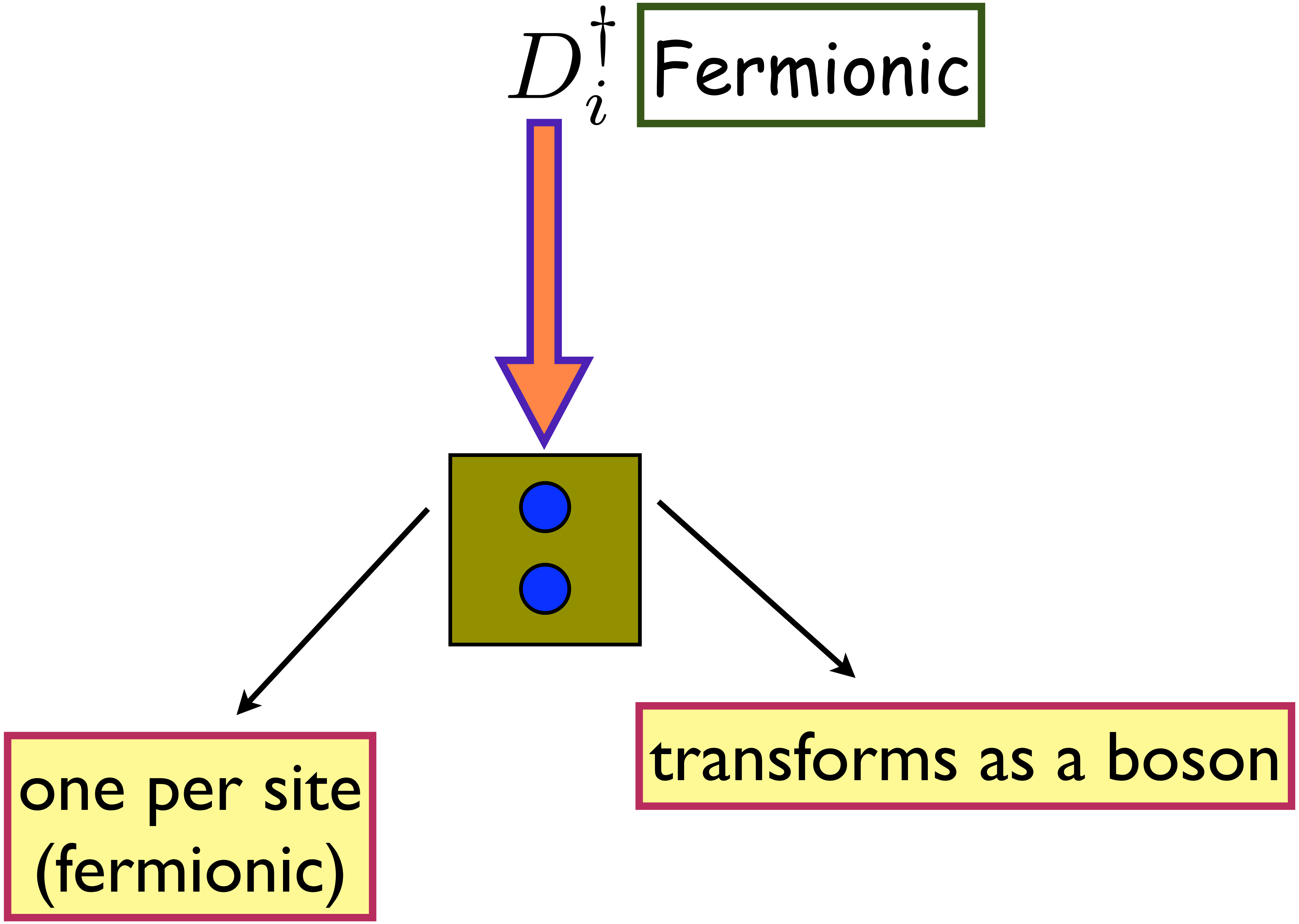


Impose Constraint:



How is this possible with Fermions?


$D_i^\dagger$
Fermionic
one per site
(fermionic)
transforms as a boson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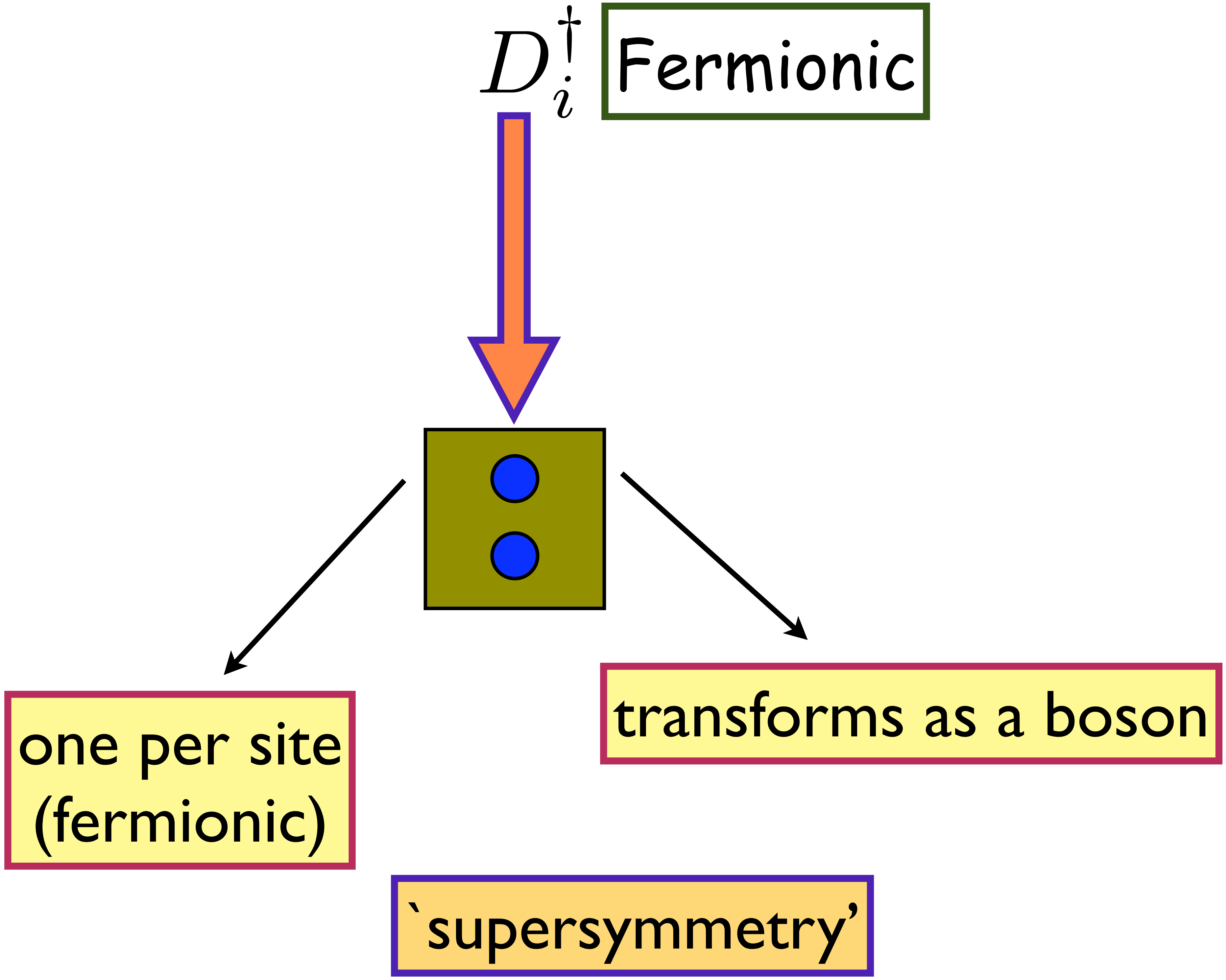
$D_i^\dagger$
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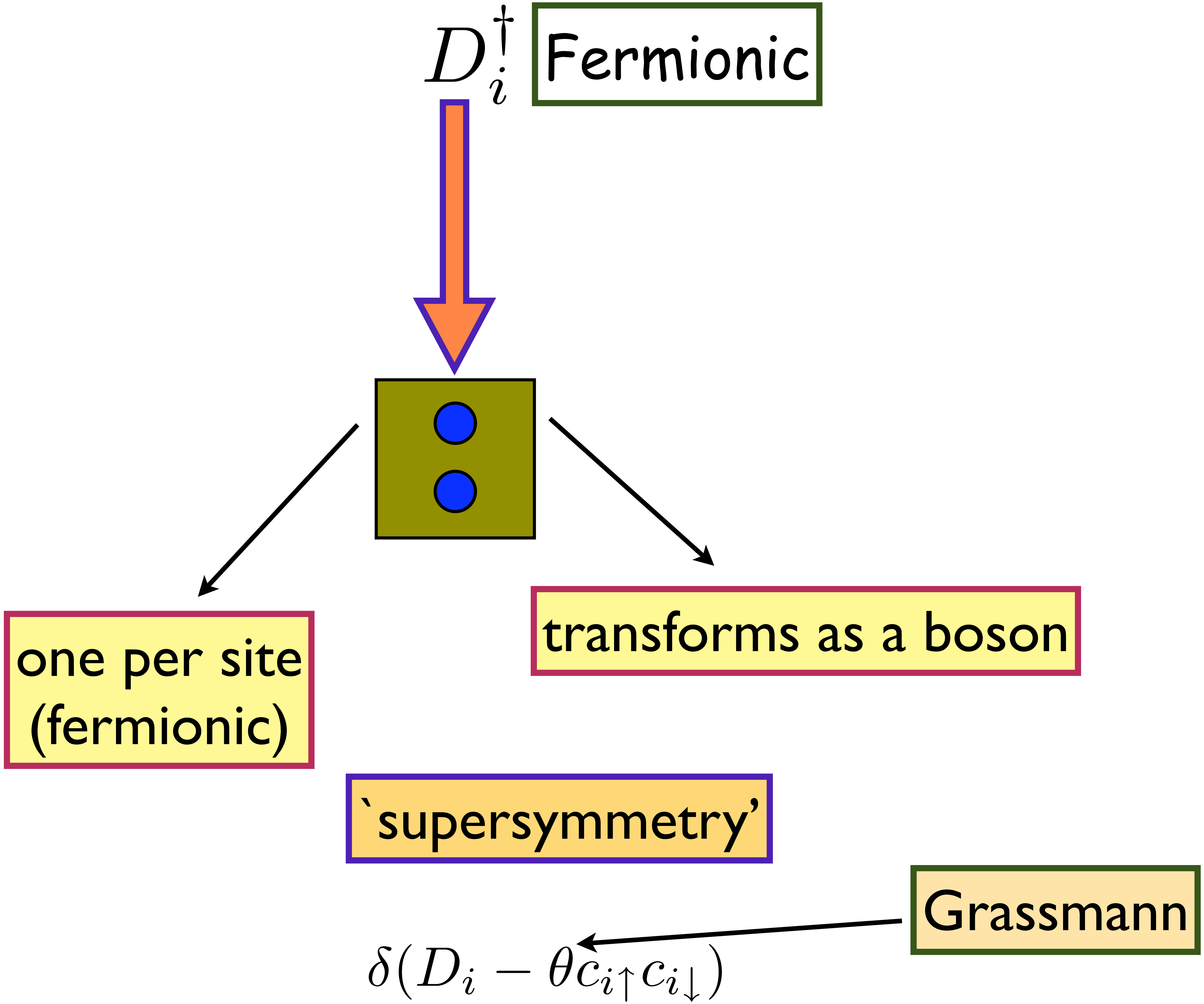
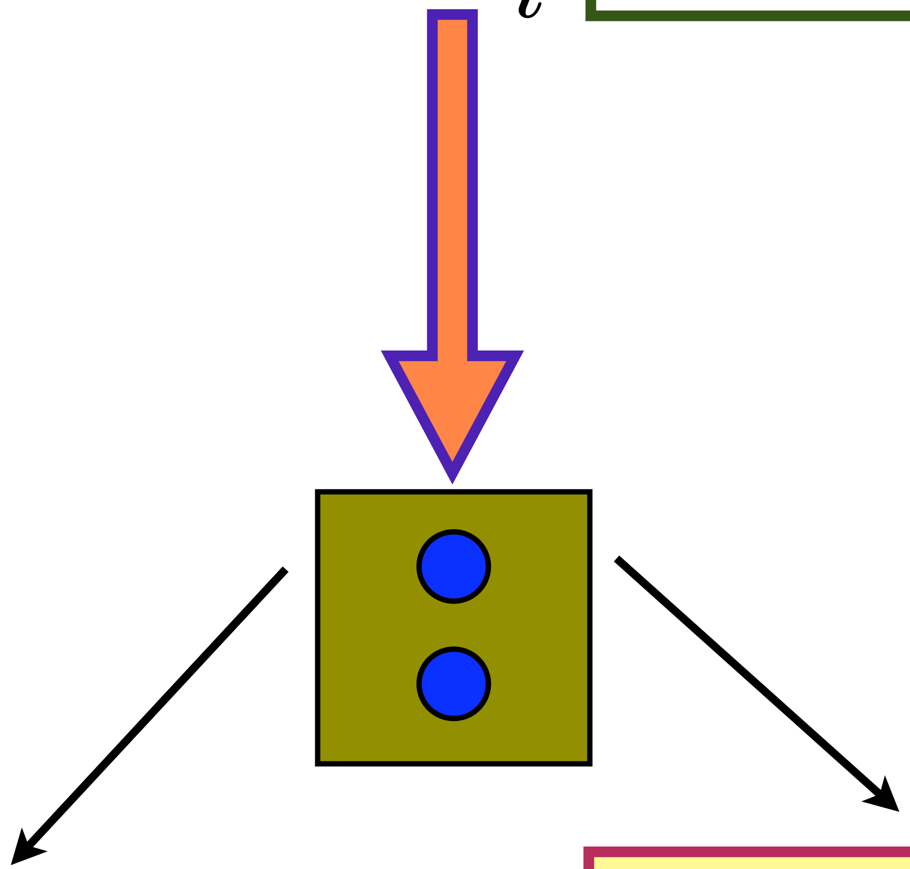
`supersymmetry'


$D_i^\dagger$
Fermionic
one per site (fermionic)
transforms as a boson
`supersymmetry'
Grassmann
$\delta(D_i - \theta c_{i\uparrow} c_{i\downarrow})$

$D_i^\dagger$ Fermionic



one per site (fermionic)

transforms as a boson

\`supersymmetry'

Grassmann

$$\delta(D_i - \theta c_{i\uparrow} c_{i\downarrow})$$

super field: $X^\mu(\sigma, \theta) = X^\mu(\sigma) + \theta \gamma^\mu(\sigma)$ (Ramond)

$$
\begin{aligned}
L_{\mathrm{UV}}^{\mathrm{hf}} &= \int d^2\theta \Bigg[iD^\dagger \dot{D} - i\dot{\tilde{D}}^\dagger \tilde{D} - \frac{U}{2}(D^\dagger D - \tilde{D}\tilde{D}^\dagger) \\
&+ \frac{t}{2} D^\dagger \theta b + \frac{t}{2}\bar{\theta} b \tilde{D} + h.c. + s\bar{\theta}\varphi^\dagger (D - \theta c_\uparrow c_\downarrow) \\
&+ \tilde{s}\bar{\theta}\tilde{\varphi}^\dagger (\tilde{D} - \theta c_\uparrow^\dagger c_\downarrow^\dagger) + h.c. \Bigg], \qquad (1)
\end{aligned}
$$

$$
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+ \; & \left. \tilde{s}\bar{\theta}\tilde{\varphi}^\dagger (\tilde{D} - \theta c_\uparrow^\dagger c_\downarrow^\dagger) + h.c. \right], \qquad (1)
\end{aligned}
$$

$$b_i = \sum_j g_{ij}(c_{i\uparrow}c_{j\downarrow} - c_{i\downarrow}c_{j\uparrow})$$

$$|b_i|^2 \propto S_i \cdot S_j$$

$$
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charge |2e| boson

$$
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+\;& \frac{t}{2} D^\dagger \theta b + \frac{t}{2}\bar{\theta} b \tilde{D} + h.c. + s\bar{\theta}\varphi^\dagger (D - \theta c_\uparrow c_\downarrow) \\
+\;& \tilde{s}\bar{\theta}\tilde{\varphi}^\dagger (\tilde{D} - \theta c_\uparrow^\dagger c_\downarrow^\dagger) + h.c. \Big], \qquad (1)
\end{aligned}
$$

$$b_i = \sum_j g_{ij}(c_{i\uparrow}c_{j\downarrow} - c_{i\downarrow}c_{j\uparrow})$$

$$|b_i|^2 \propto S_i \cdot S_j$$

charge |2e| boson

solve constraint

$$\int d^2\theta\ \bar{\theta}\theta L_{\mathrm{Hubb}} = \sum_{i,\sigma} c^\dagger_{i,\sigma}\dot{c}_{i,\sigma} + H_{\mathrm{Hubb}},$$

Exact low-energy Lagrangian

$$L \quad = \quad \# L_{\rm bare}(\text{electrons}) + \#\mathrm{L}_{\rm bare}(\text{bosons})$$

$$+f(\omega) L_{\rm int}(c, \varphi) \; + \tilde{f}(\omega) L_{\rm int}(c, \tilde{\varphi})$$

$f(\omega) = 0$

dispersion
of propagating
modes

composite excitations

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

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

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

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

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

$$S = \Psi^\dagger \Psi$$ local SU(2)

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

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

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

Exact IR Lagrangian

bare fields have no dynamics

$$L_{\rm IR}^{\rm hf} \rightarrow 2\frac{|s|^2}{U}|\varphi_\omega|^2 + 2\frac{|\tilde{s}|^2}{U}|\tilde{\varphi}_{-\omega}|^2 + \frac{t^2}{U}|b_\omega|^2$$

$$\left\{ \begin{array}{l} +s\gamma_{\vec{p}}^{(\vec{k})}(\omega)\varphi^\dagger_{\omega,\vec{k}} c_{\vec{k}/2+\vec{p},\omega/2+\omega',\uparrow} c_{\vec{k}/2-\vec{p},\omega/2-\omega',\downarrow} \\ +\tilde{s}^*\tilde{\gamma}_{\vec{p}}^{(\vec{k})}(\omega)\tilde{\varphi}_{-\omega,\vec{k}} c_{\vec{k}/2+\vec{p},\omega/2+\omega',\uparrow} c_{\vec{k}/2-\vec{p},\omega/2-\omega',\downarrow} + h.c. \end{array} \right.$$

bosons
and fermions
are strongly coupled

$$\gamma_{\vec{p}}^{(\vec{k})}(\omega) = \frac{U - t\varepsilon_{\vec{p}}^{(\vec{k})} - 2\omega}{U}\sqrt{1+2\omega/U}$$

$$\tilde{\gamma}_{\vec{p}}^{(\vec{k})}(\omega) = \frac{U + t\varepsilon_{\vec{p}}^{(\vec{k})} + 2\omega}{U}\sqrt{1-2\omega/U}.$$

$$\varepsilon_{\vec{p}}^{(\vec{k})} = 4\sum_\mu \cos(k_\mu a/2)\cos(p_\mu a)$$

turn-on of spectral weight governed by composite excitations (CEXONS)

$$L \quad = \quad \#L_{\rm bare}(\text{electrons}) + \#\mathrm{L}_{\rm bare}(\text{bosons})$$

$$+f(\omega)L_{\rm int}(c,\varphi) \;\; +\tilde{f}(\omega)L_{\rm int}(c,\tilde{\varphi})$$

$$\downarrow \qquad\qquad\qquad\qquad \downarrow$$

$$\Psi^\dagger\Psi \qquad\qquad\qquad\qquad \tilde{\Psi}^\dagger\tilde{\Psi}$$

quadratic form:
composite or bound
excitations of

$$\varphi^\dagger c_{i\sigma}$$

composite excitations determine spectral density

$$\gamma_{\vec{p}}^{(\vec{k})}(\omega) = \frac{U - t\varepsilon_{\vec{p}}^{(\vec{k})} - 2\omega}{U}\sqrt{1 + 2\omega/U}$$

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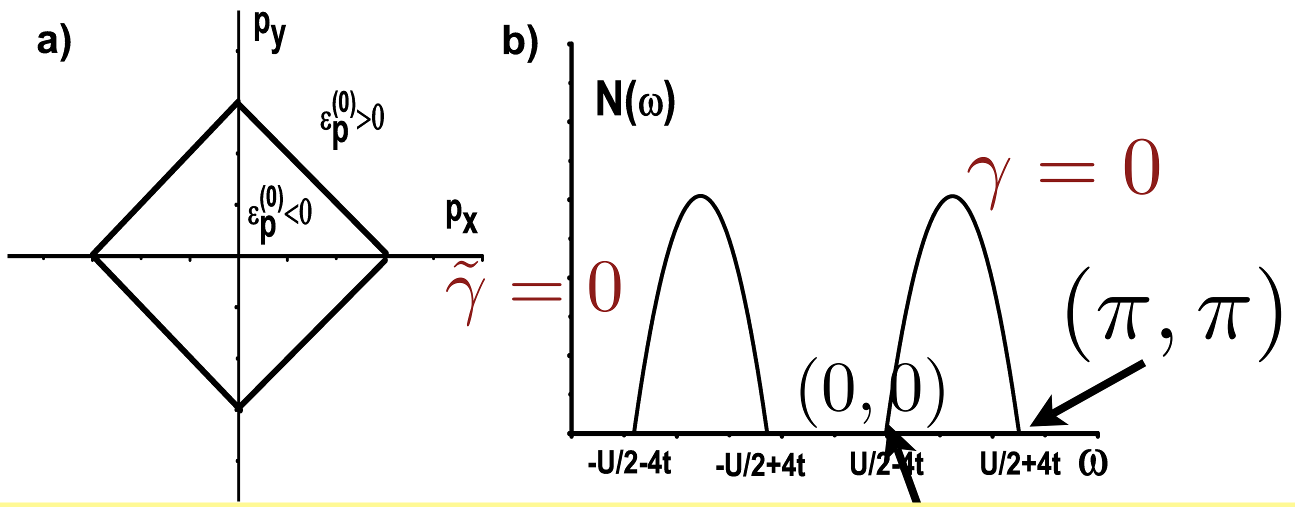

each momentum has SD at two distinct energies

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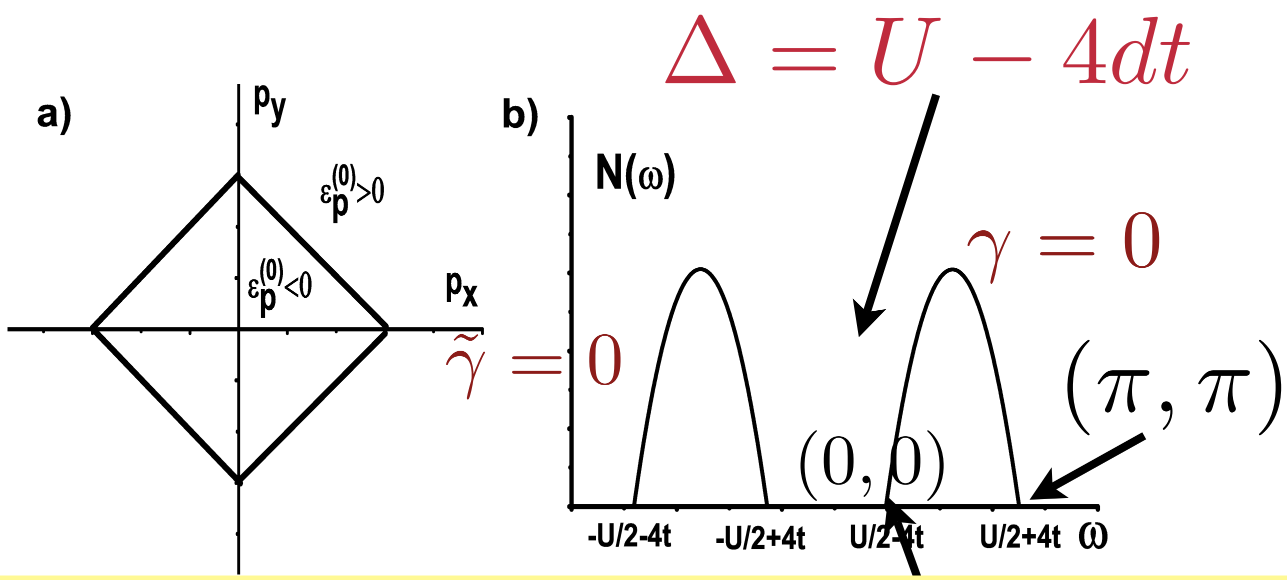


each momentum has SD at two distinct energies

electron transform at low energies

$$L_{\rm UV}^{\rm hf} \to L_{\rm UV}^{\rm hf} + \int d^2\theta J_{i,\sigma}\left[V_\sigma D_i^\dagger c_{i,-\sigma}\theta + V_\sigma \bar\theta c_{i,-\sigma}\tilde D_i\right] + h.c.$$

UV

IR

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

$$c_{i,\sigma}^\dagger \to \tilde c_{i,\sigma}^\dagger \quad \equiv \quad -V_\sigma \frac{t}{U}\left(c_{i,-\sigma}b_i^\dagger + b_i^\dagger c_{i,-\sigma}\right) + V_\sigma \frac{2}{U}\left(s\varphi_i^\dagger + \tilde s\tilde\varphi_i\right)c_{i,-\sigma}$$

spin-fluctuations

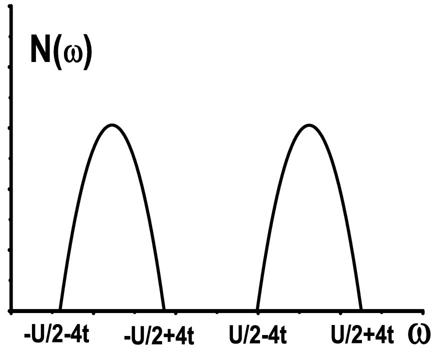
CEXON

UV-IR mixing: spectral weight transfer

electron overlap with composite excitations?

$$O = |\langle c^\dagger | \tilde{c}^\dagger \rangle \langle \tilde{c}^\dagger | \Psi \rangle|^2 P_\Psi$$

destructive interference at low energy



$$\Delta_{\rm electron} > \Delta_{\rm composites}$$

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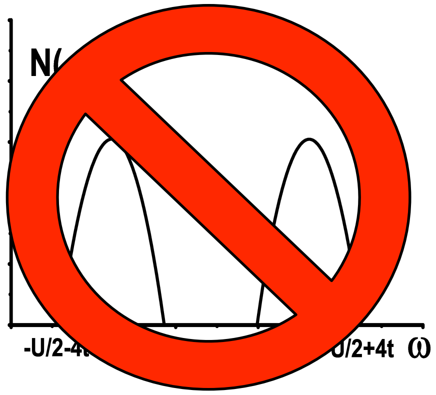


$$\Delta_{\mathrm{electron}} > \Delta_{\mathrm{composites}}$$

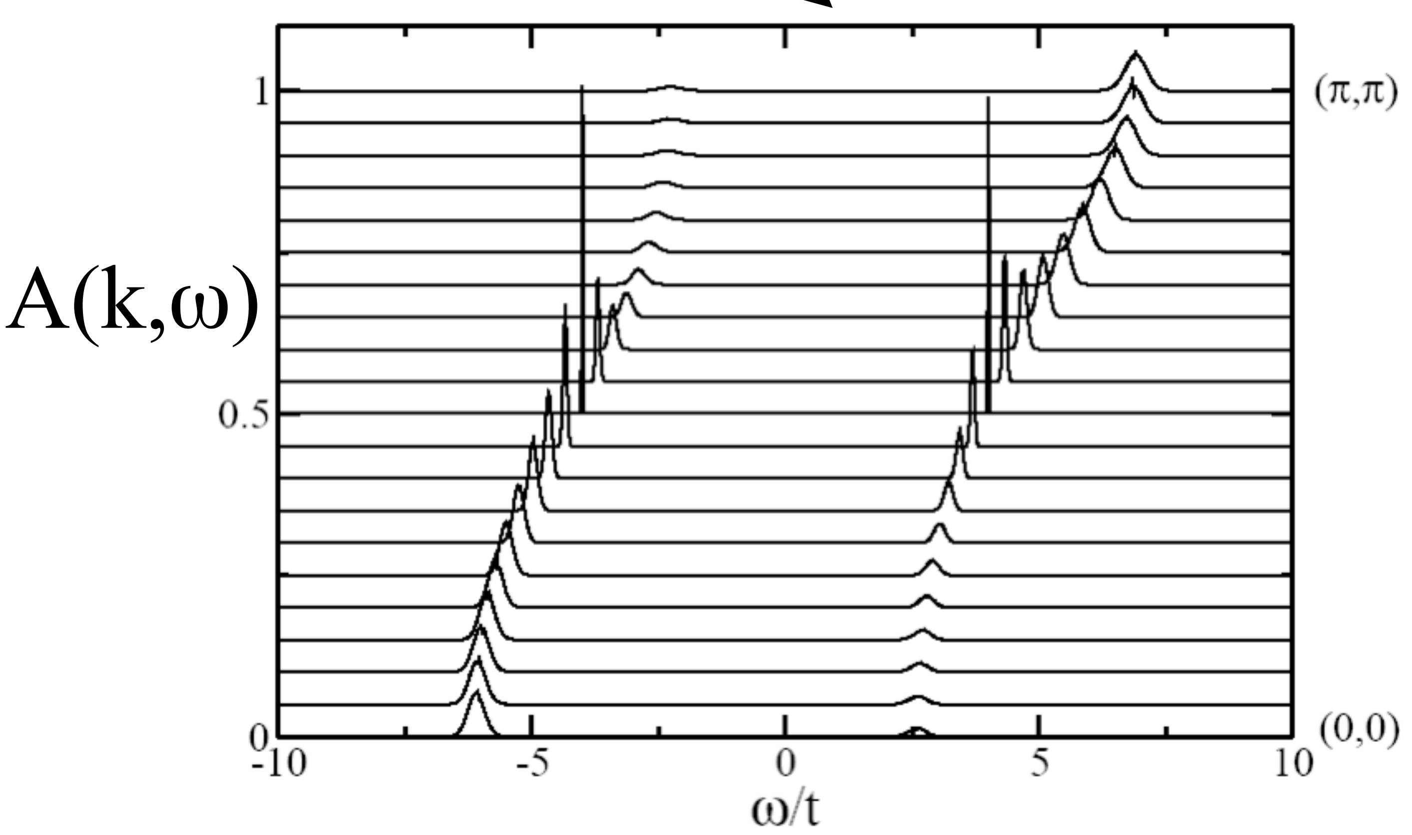
$$H(\varphi, \tilde{\varphi}, c, c^\dagger)$$

1.) no derivative couplings with respect to bosonic field

2.) spatially uniform

3.) spin-spin sub-dominant (non-dispersive)

consistent with exact argument



bosonic field contains all the Mott physics (numerically verified that spatial variation of bosonic field does nothing) spin part irrelevant

Strong-coupling antiferromagnet

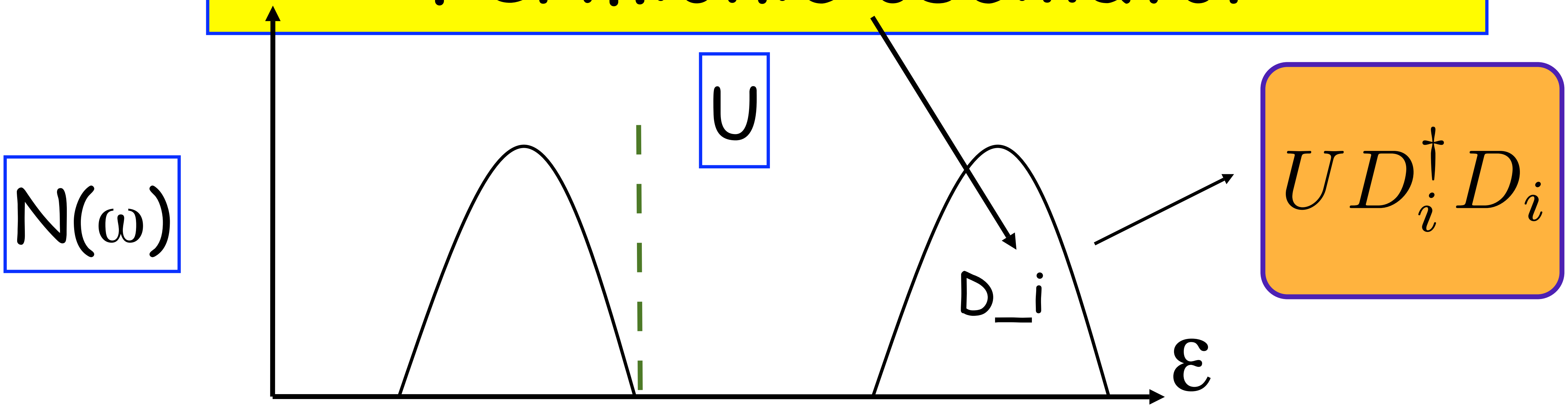
$$B_{ij} = \langle g_{ij} \varphi_i^\dagger c_{i,\uparrow} c_{j,\downarrow} \rangle.$$

No adiabatic connection with weak-coupling AF

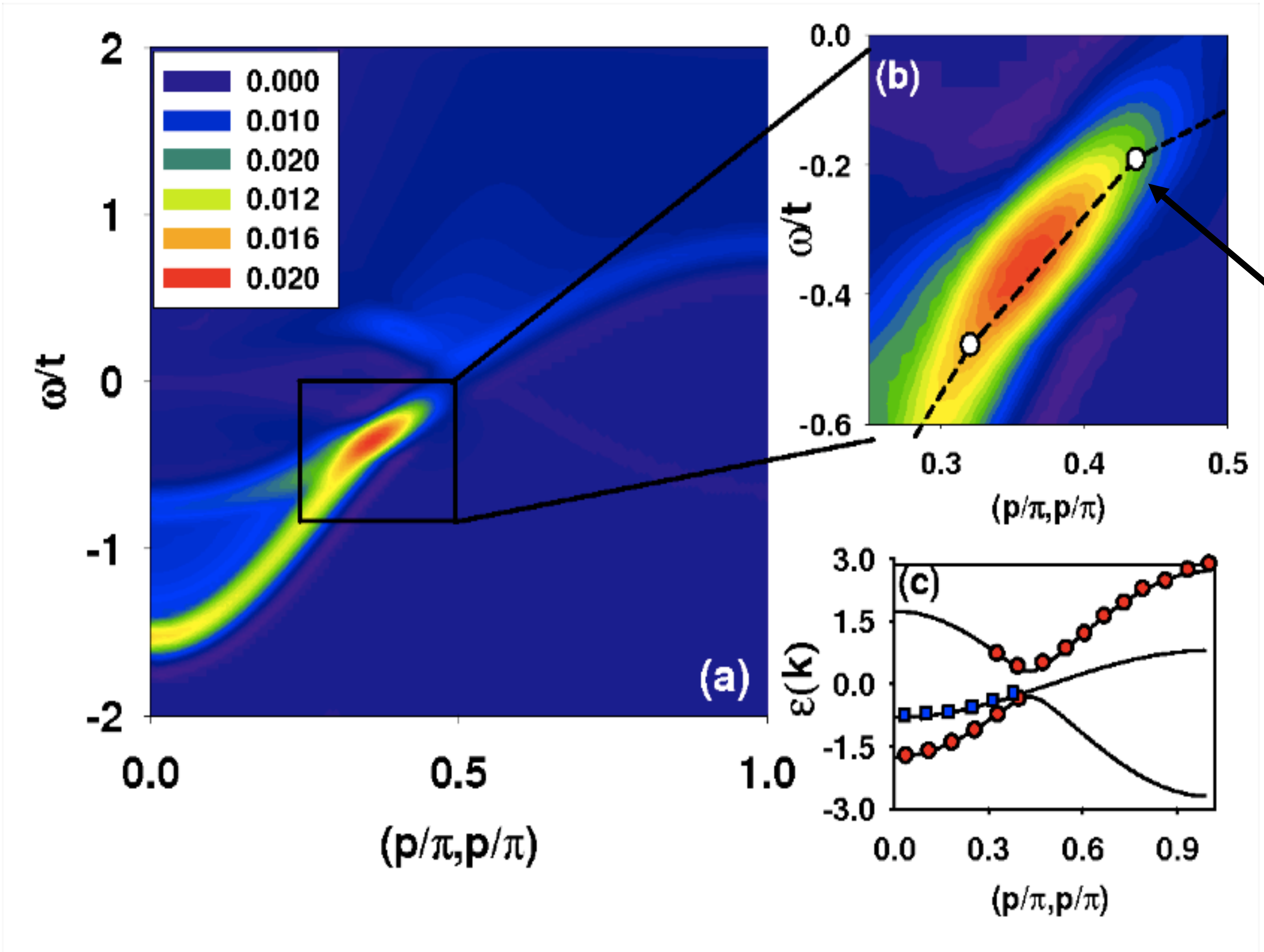
bound states of the boson
mediate the Mott gap:
mechanism of localization of double occupancy

hole-doping

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

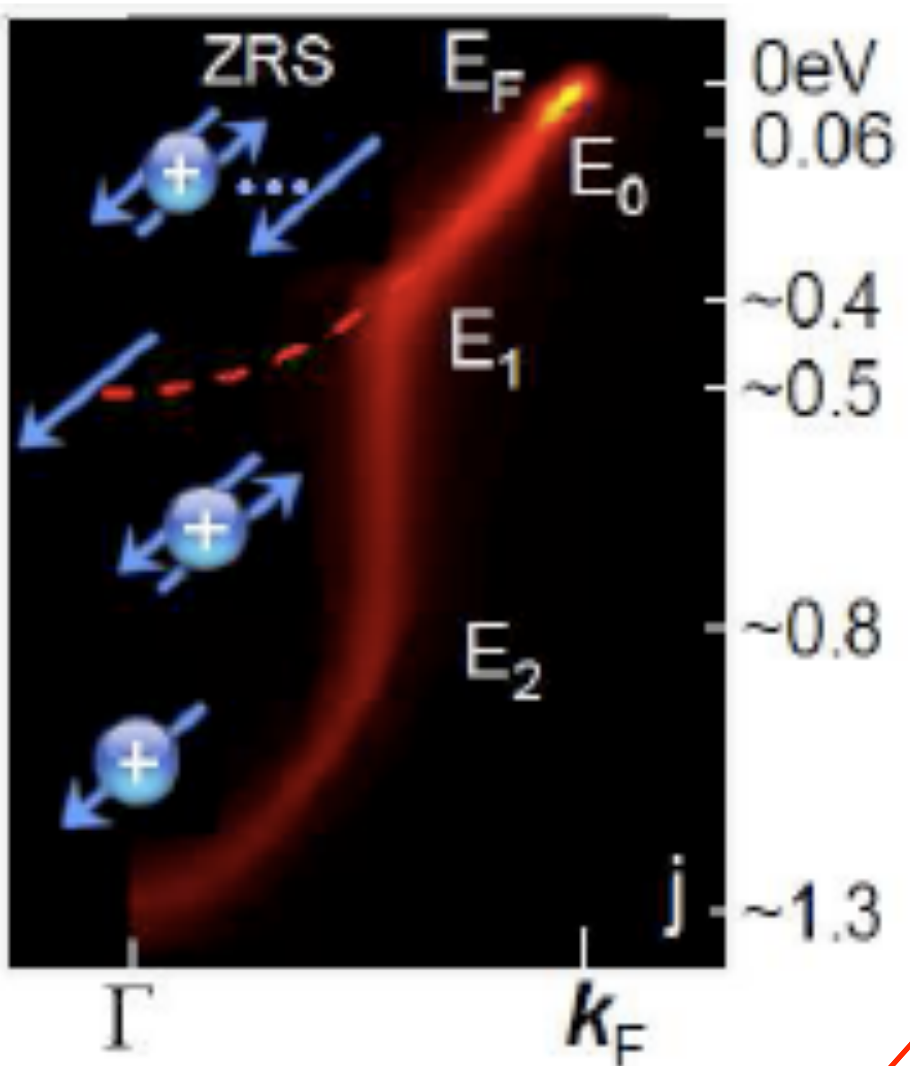


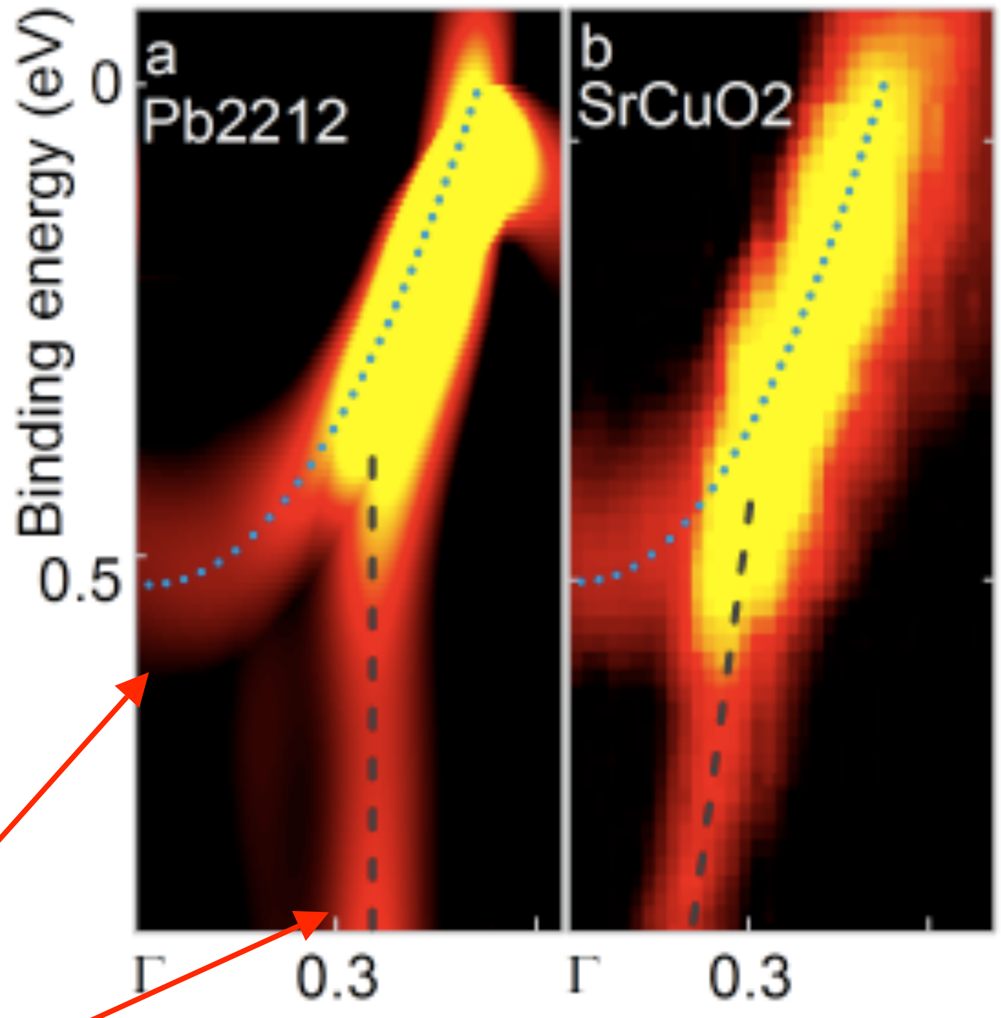
Electron spectral function



$t^2/U \sim 60meV$

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





Two bands!!

Spin-charge separation?

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

Origin of two bands

Two charge e excitations

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

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

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φ_i is confined (no kinetic energy)

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

New bound state

Pseudogap

two types of charges

'free'

bound

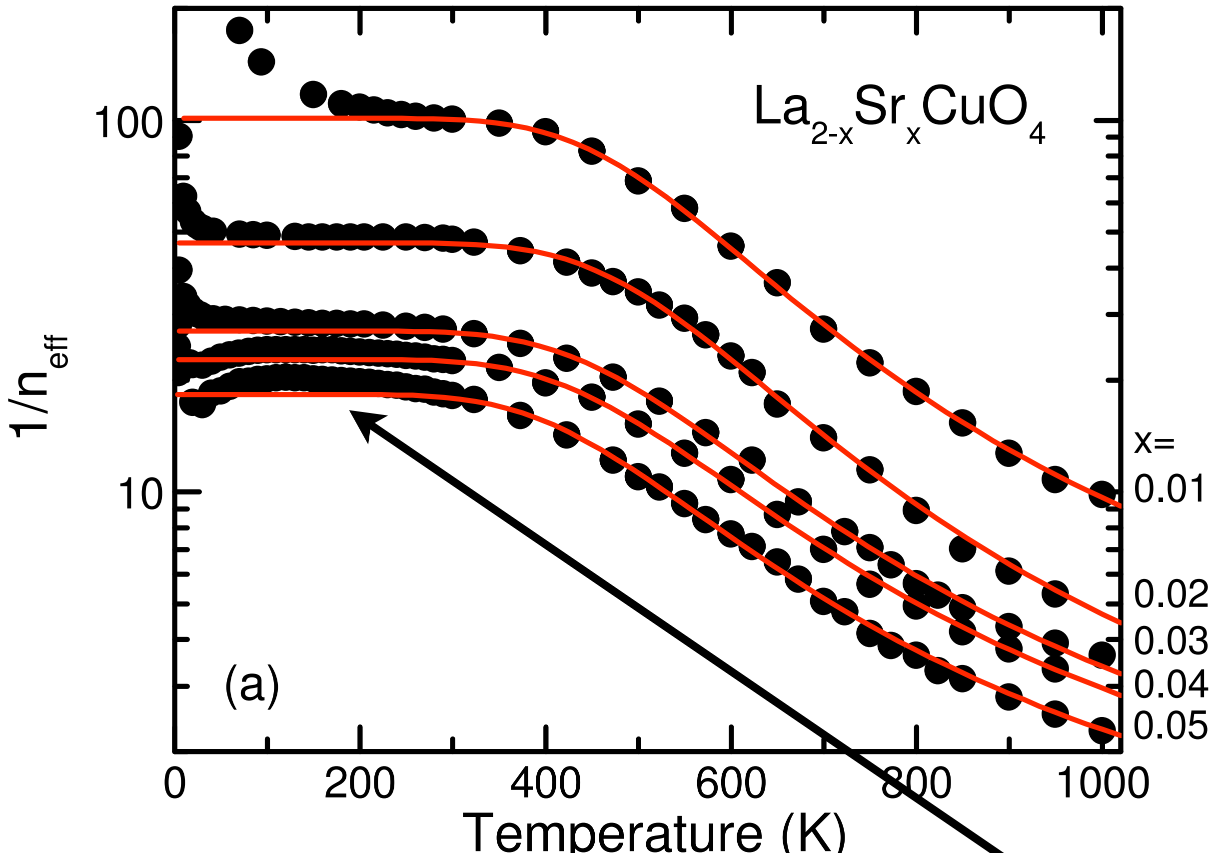
direct evidence

direct evidence

charge carrier density:

direct evidence

charge carrier density:

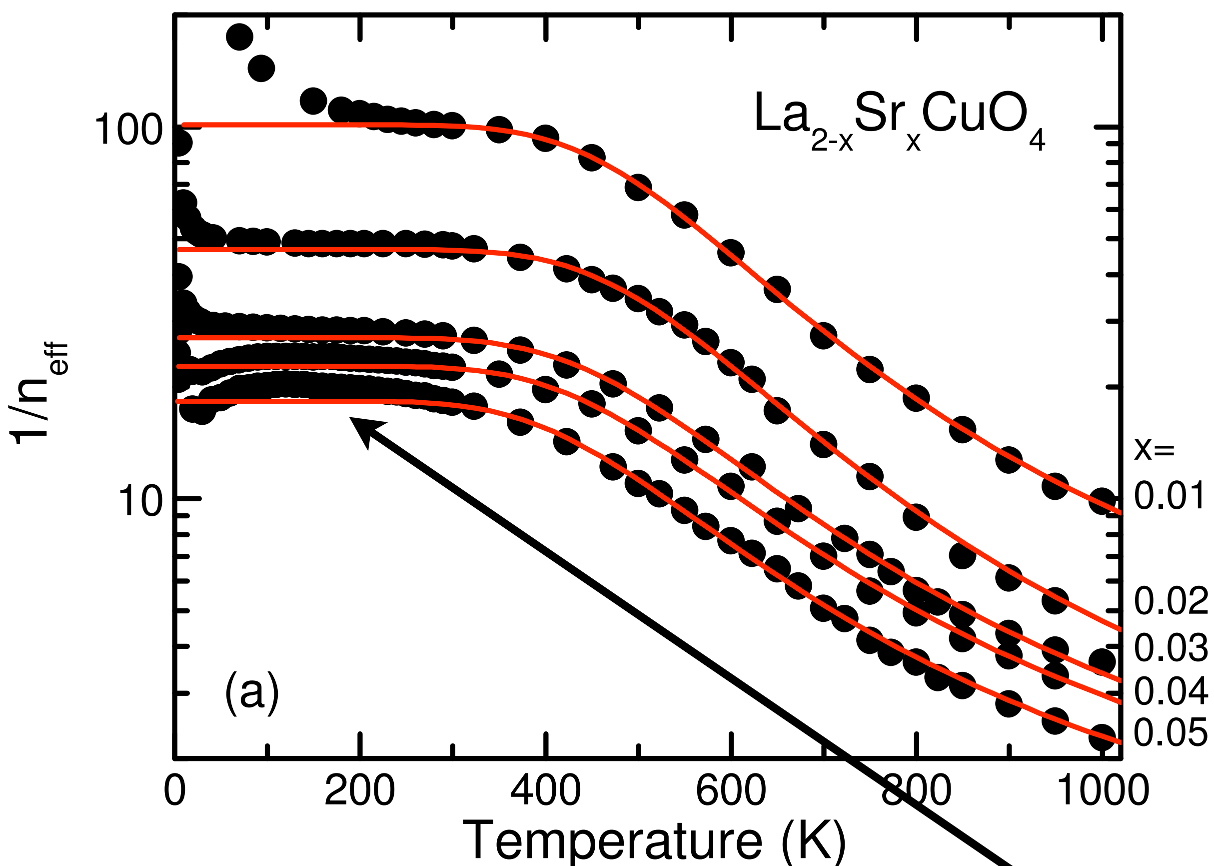


Ono, et al., Phys. Rev. B 75, 024515 (2007)

$$n_{\mathrm{Hall}}(x,T) = n_0(x) + n_1(x)\exp(-\Delta(x)/T),$$ PRL, vol. 97, 247003 (2006).

direct evidence

charge carrier density:



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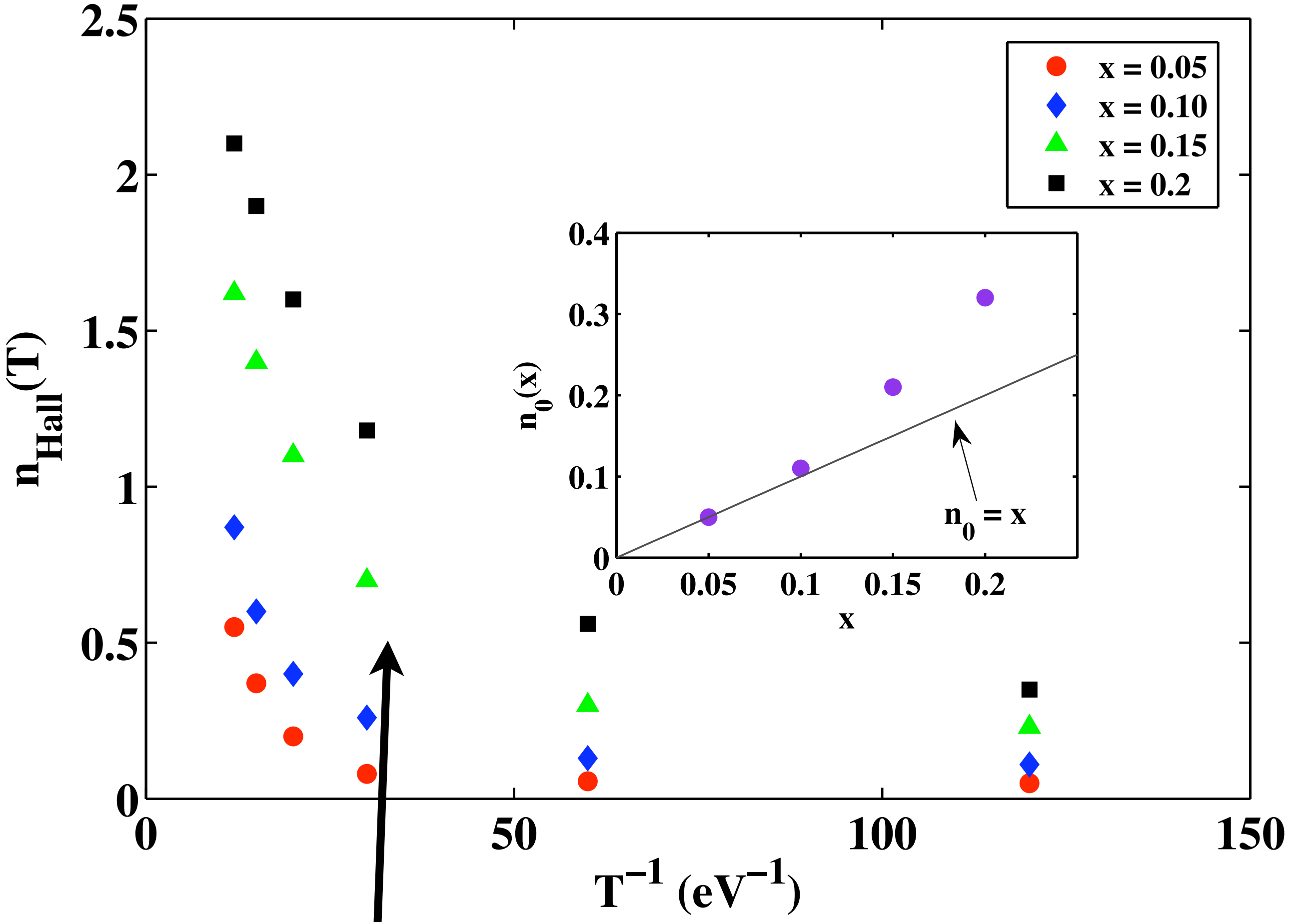
$$n_{\text{Hall}}(x,T) = n_0(x) + n_1(x)\exp(-\Delta(x)/T),$$ PRL, vol. 97, 247003 (2006).

exponentially suppressed: confinement

Our Theory

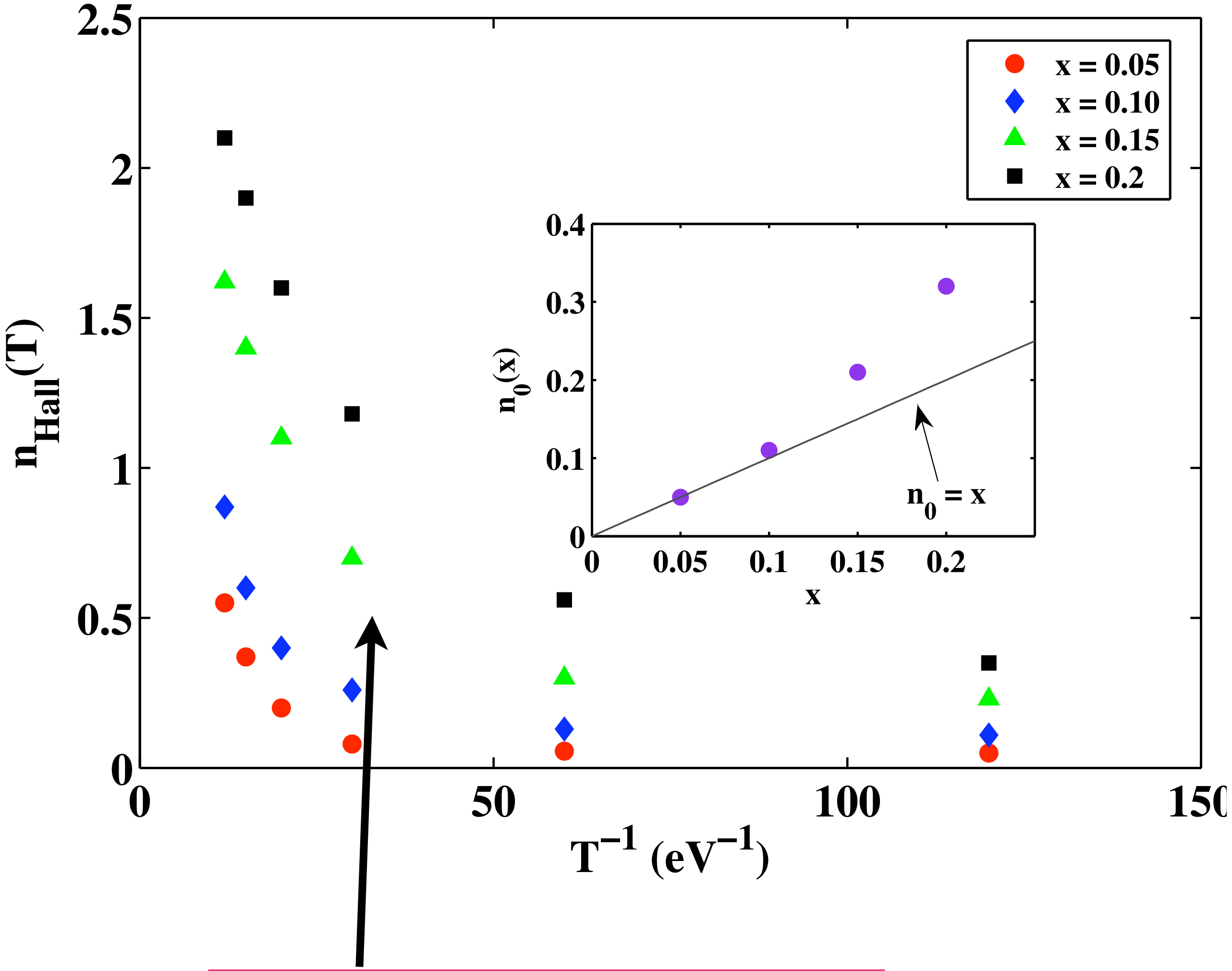


exponential T-dependence

no model-dependent free parameters: just t/U

Our Theory

gap



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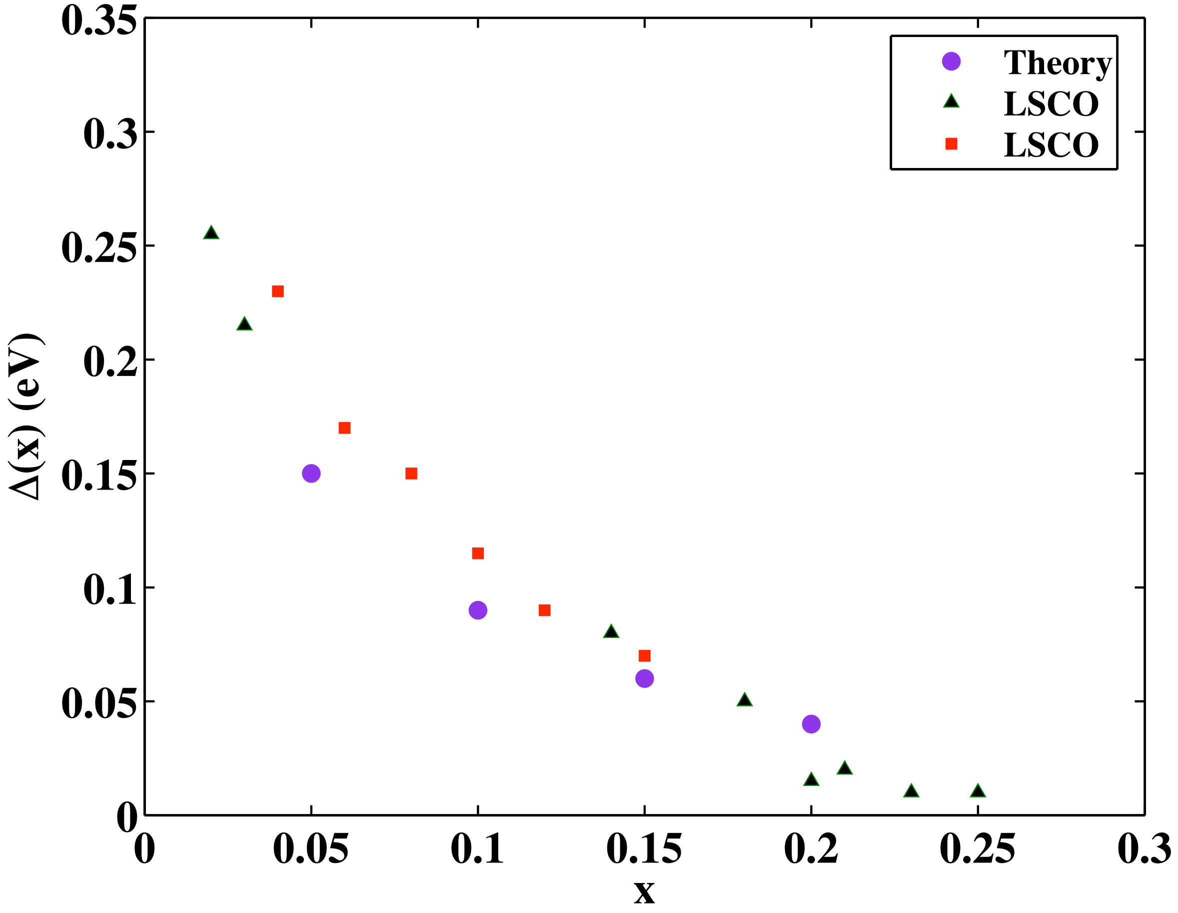
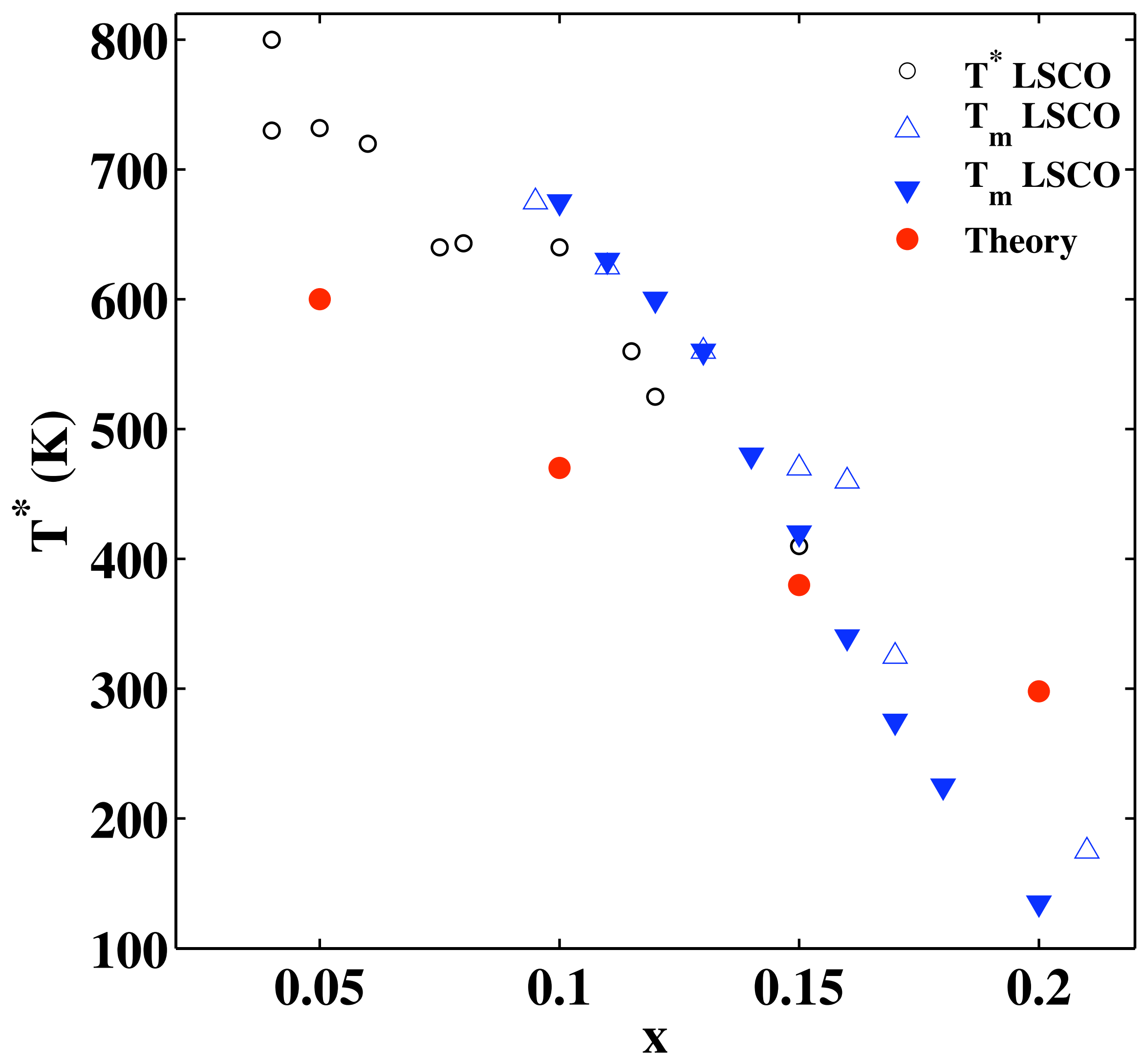


no model-dependent free parameters: just t/U

Like Mott gap,
Pseudogap is a bound-state problem with new IR modes

strange metal: breakup (`deconfinement') of bound states



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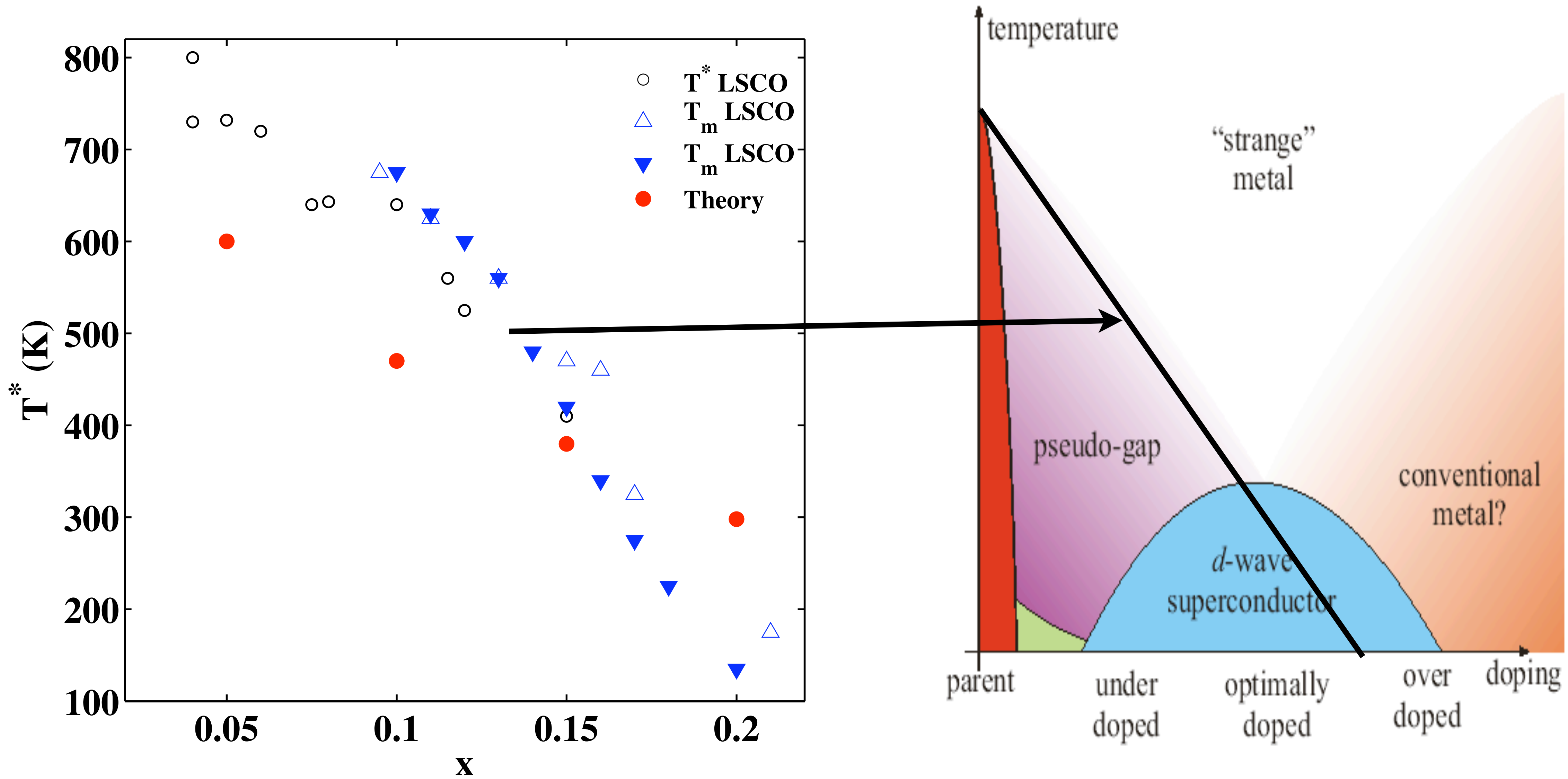
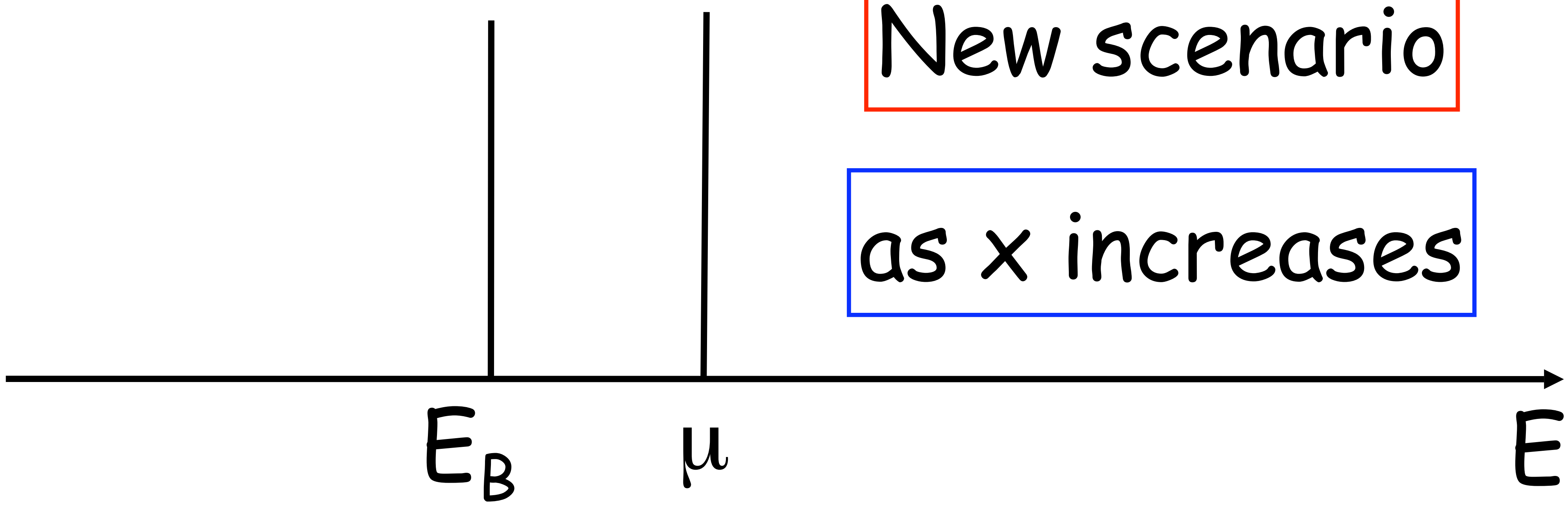
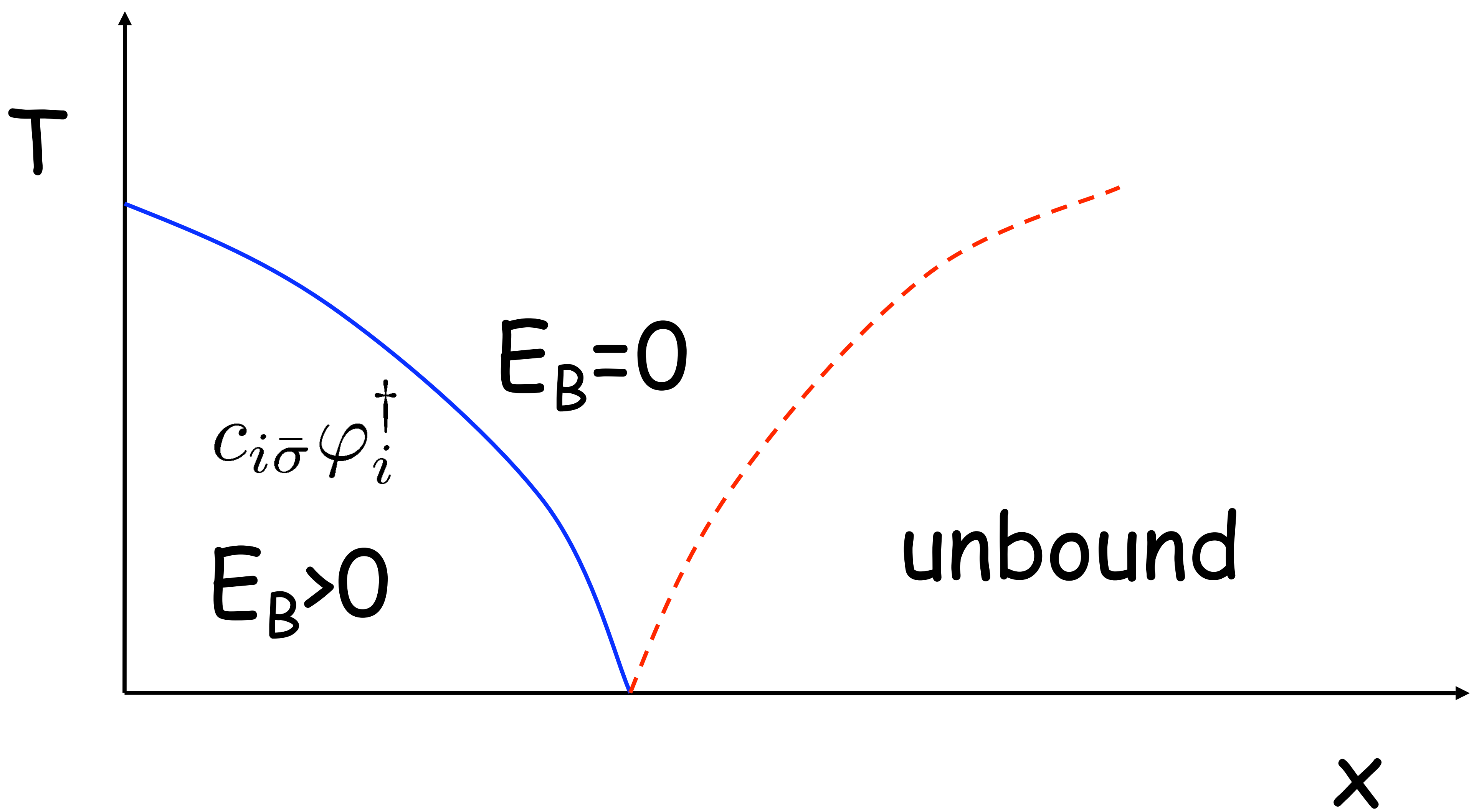


T-linear resistivity

New scenario

as x increases





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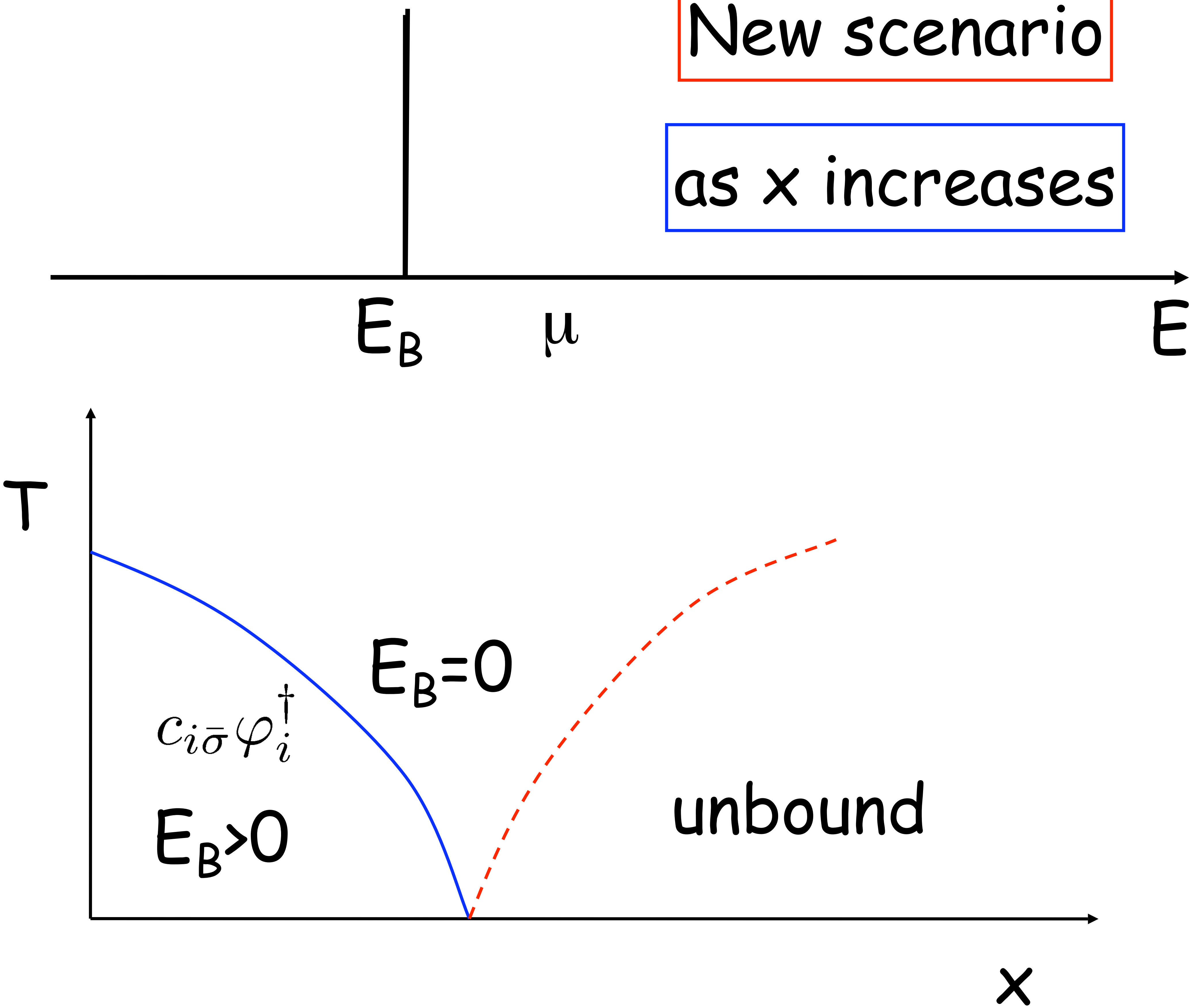

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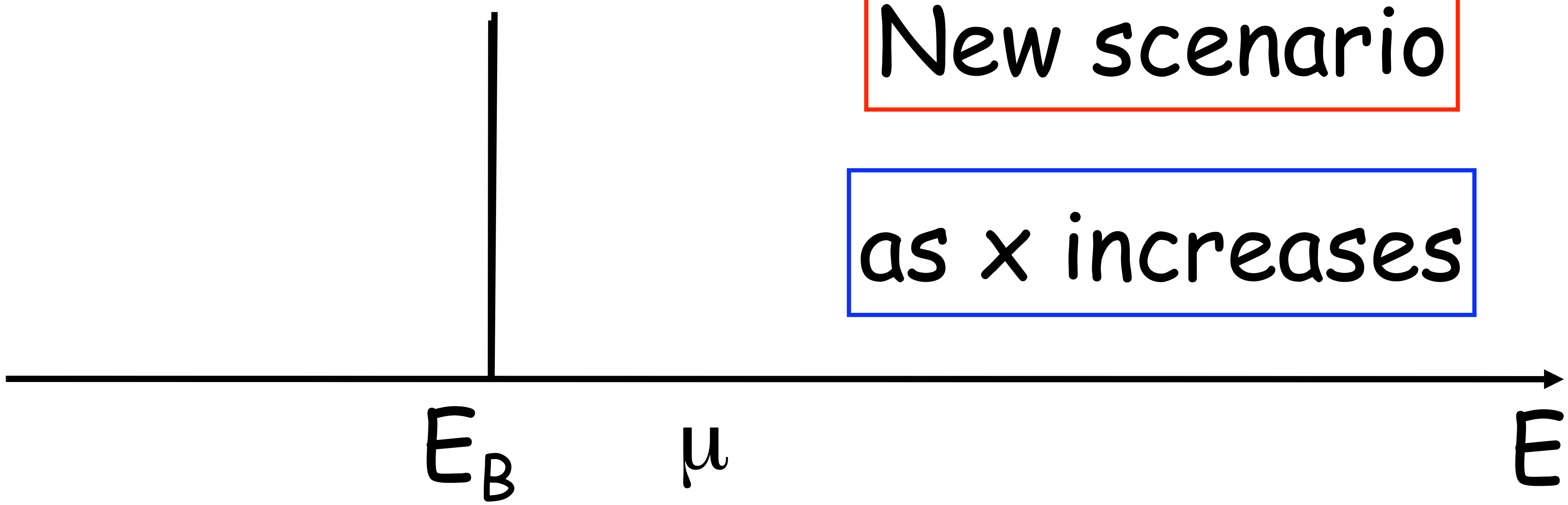
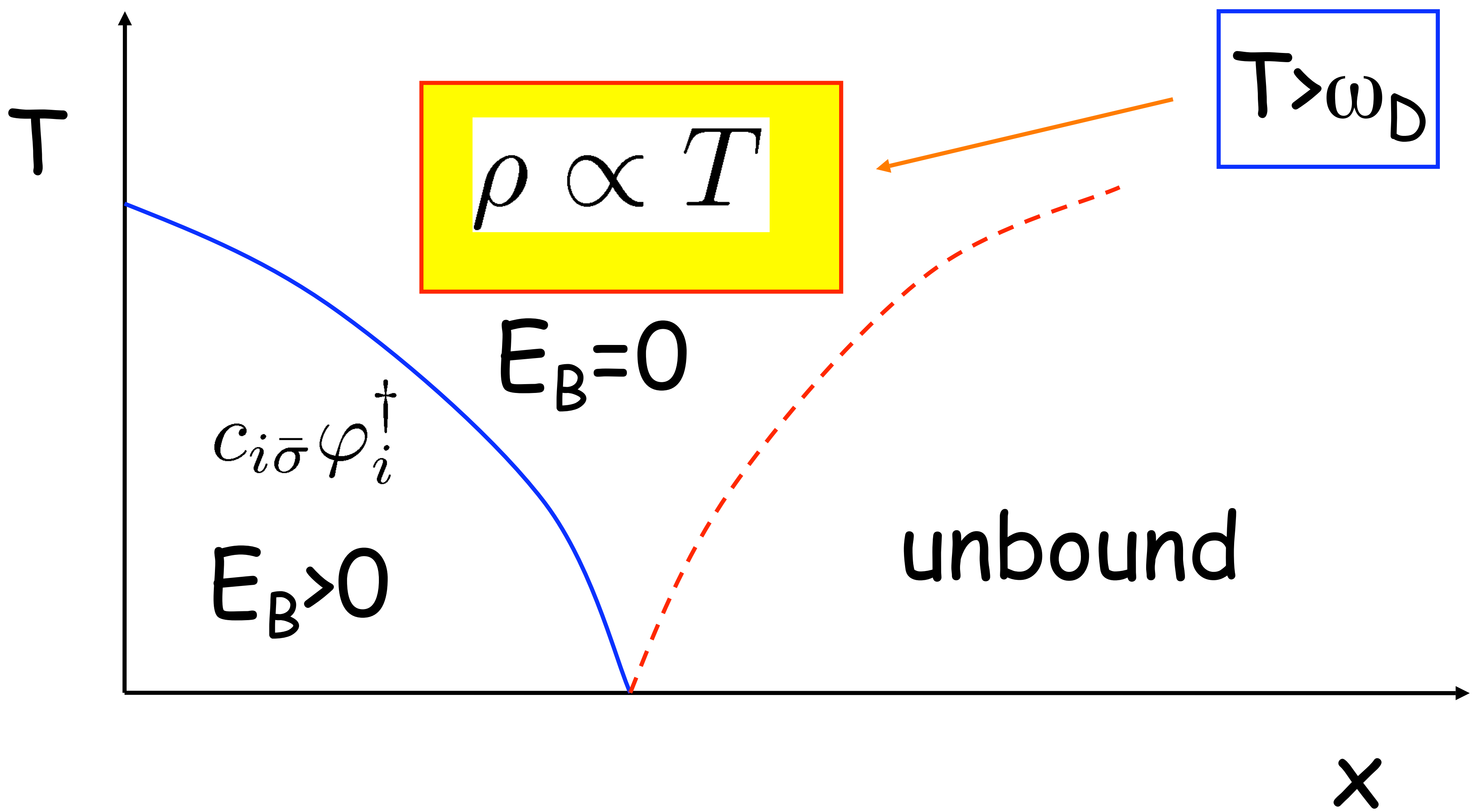




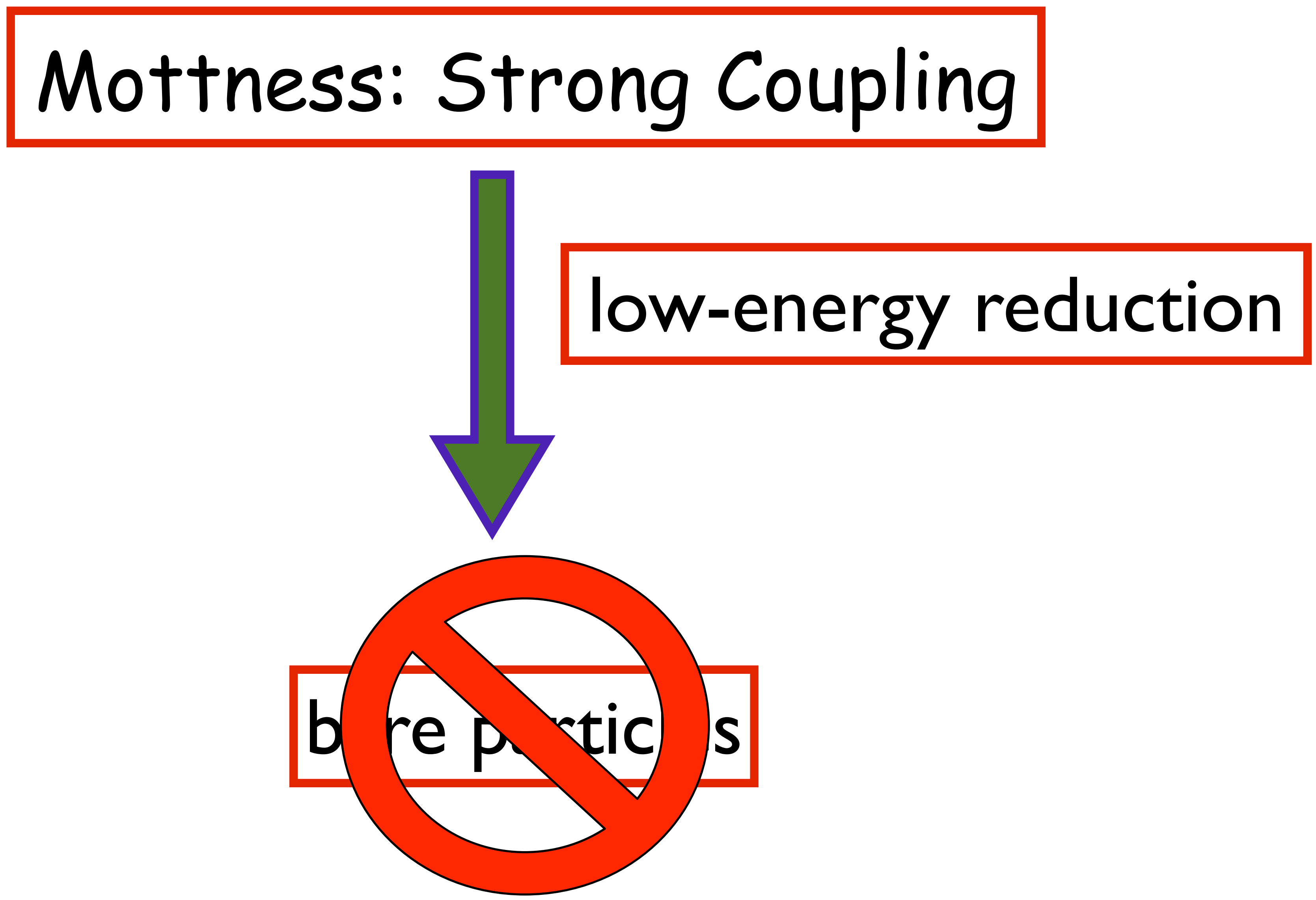
Mottness: Strong Coupling

low-energy reduction

Mottness: Strong Coupling

low-energy reduction

bare particles


Mottness: Strong Coupling
low-energy reduction
b re p rtic s

Mottness: Strong Coupling

low-energy reduction

~~bare particles~~

Pseudogap=`confinement'

Mottness: Strong Coupling

low-energy reduction

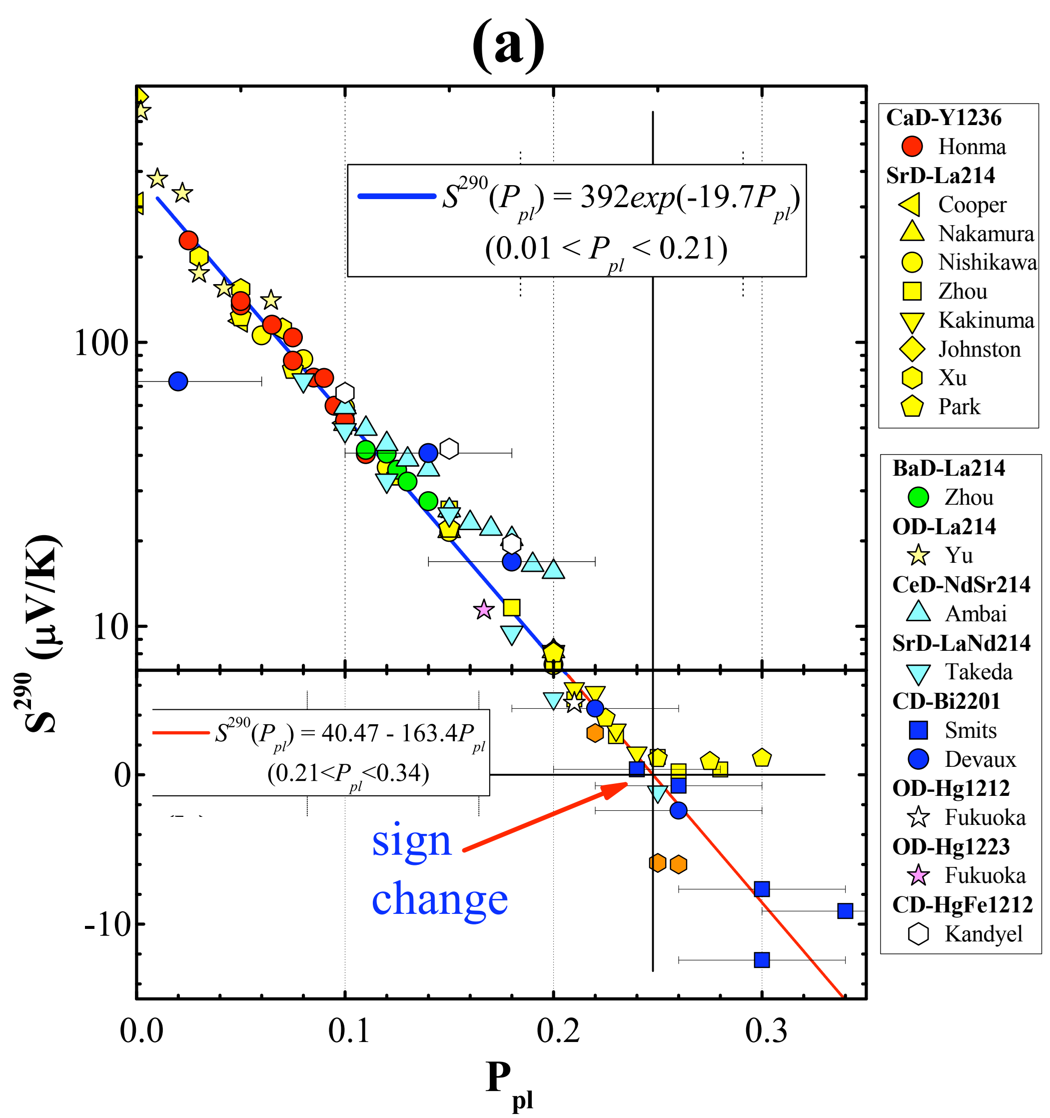
bare particles

composite or bound states not in UV theory

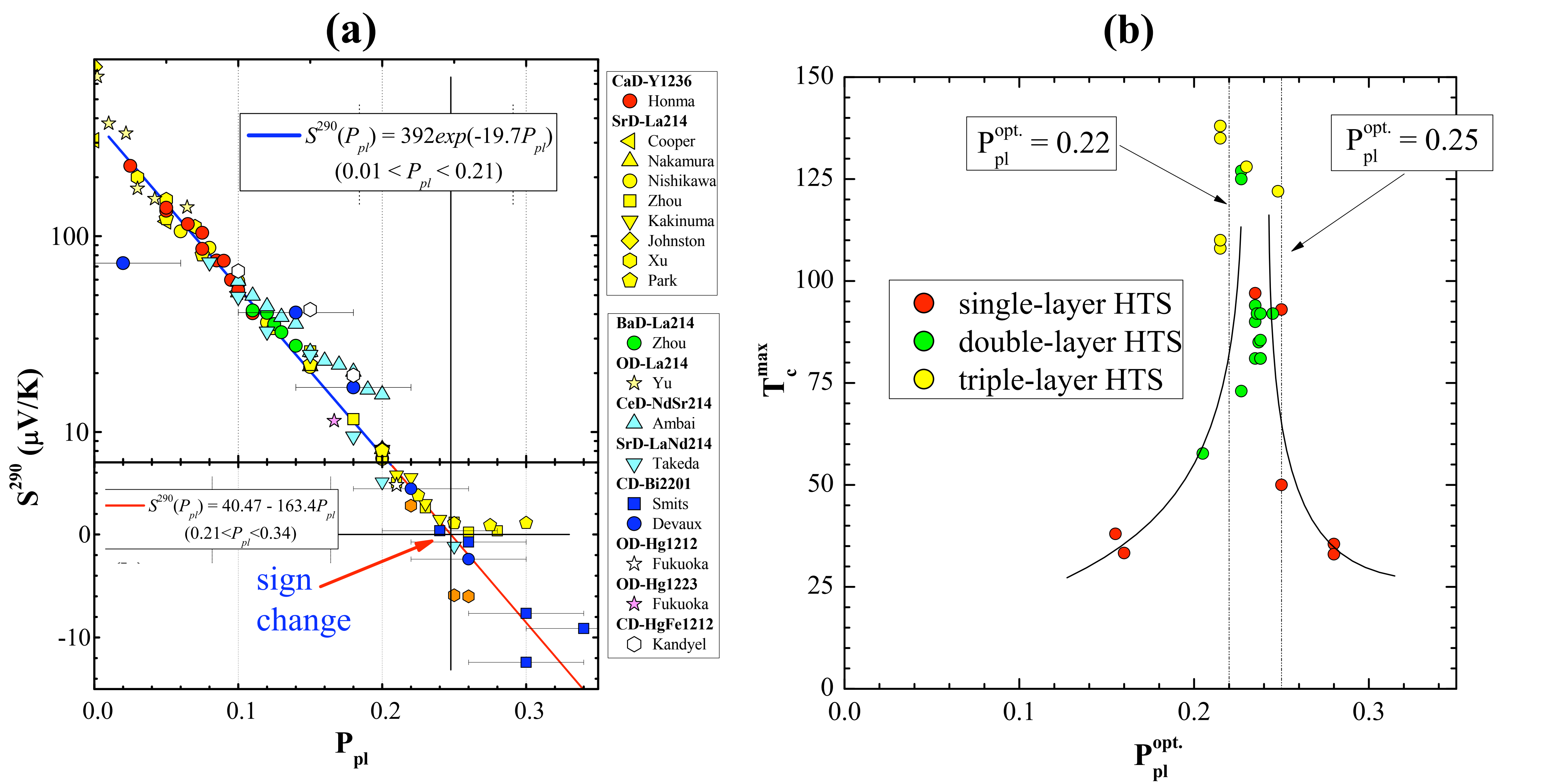
Pseudogap=`confinement'

Third Problem:
Correlate of superconductivity?

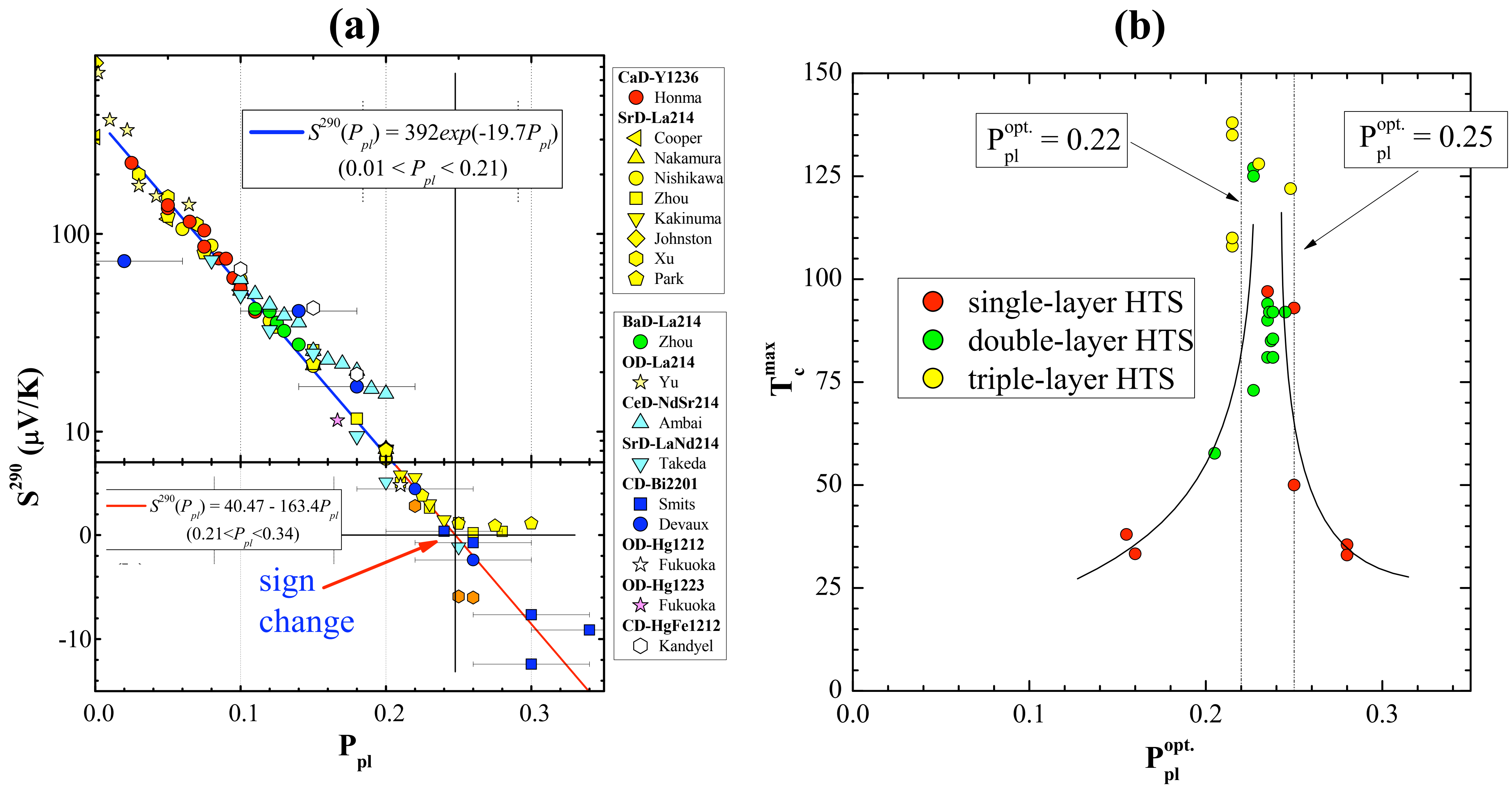
Universal sign change of thermopower



Universal sign change of thermopower

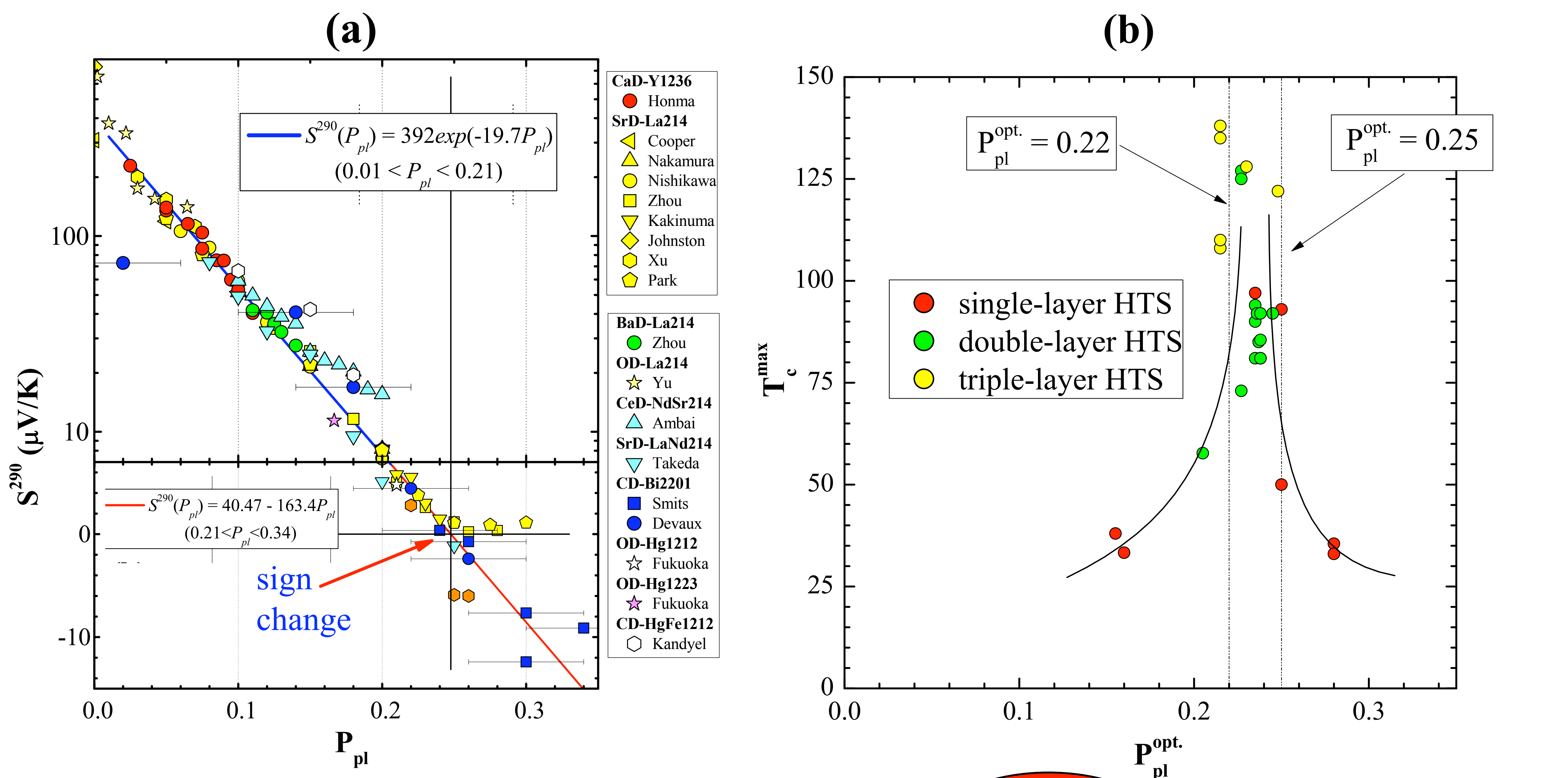


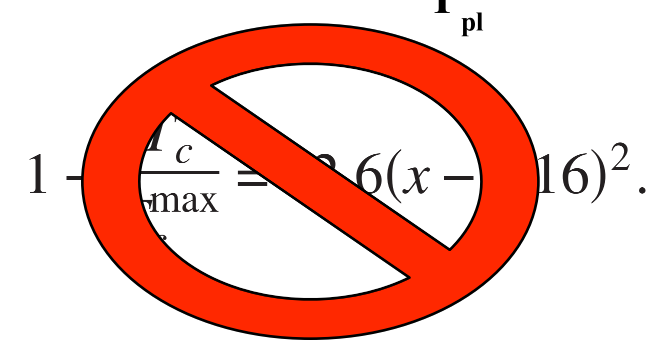
Universal sign change of thermopower



$$1 - \frac{T_c}{T_c^{\max}} = 82.6(x - 0.16)^2.$$

Universal sign change of thermopower





Why?

Mottness

G. Beni, Phys. Rev. B vol. 10, 2186 (1973).

Exact calculation of S for atomic (t=0) limit of Hubbard model

$$S = -\frac{k_B}{e} \ln \frac{2x}{1-x}$$

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band insulator (free electrons)

$$\ln \frac{x}{2-x}$$

vanishes at half-filling

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S=0 when x=1/3; WHY?

What is so special about 2x and 1-x?

Thermopower Primer

$$S = -\frac{k_B}{e}\beta\frac{L_{12}}{L_{11}}$$

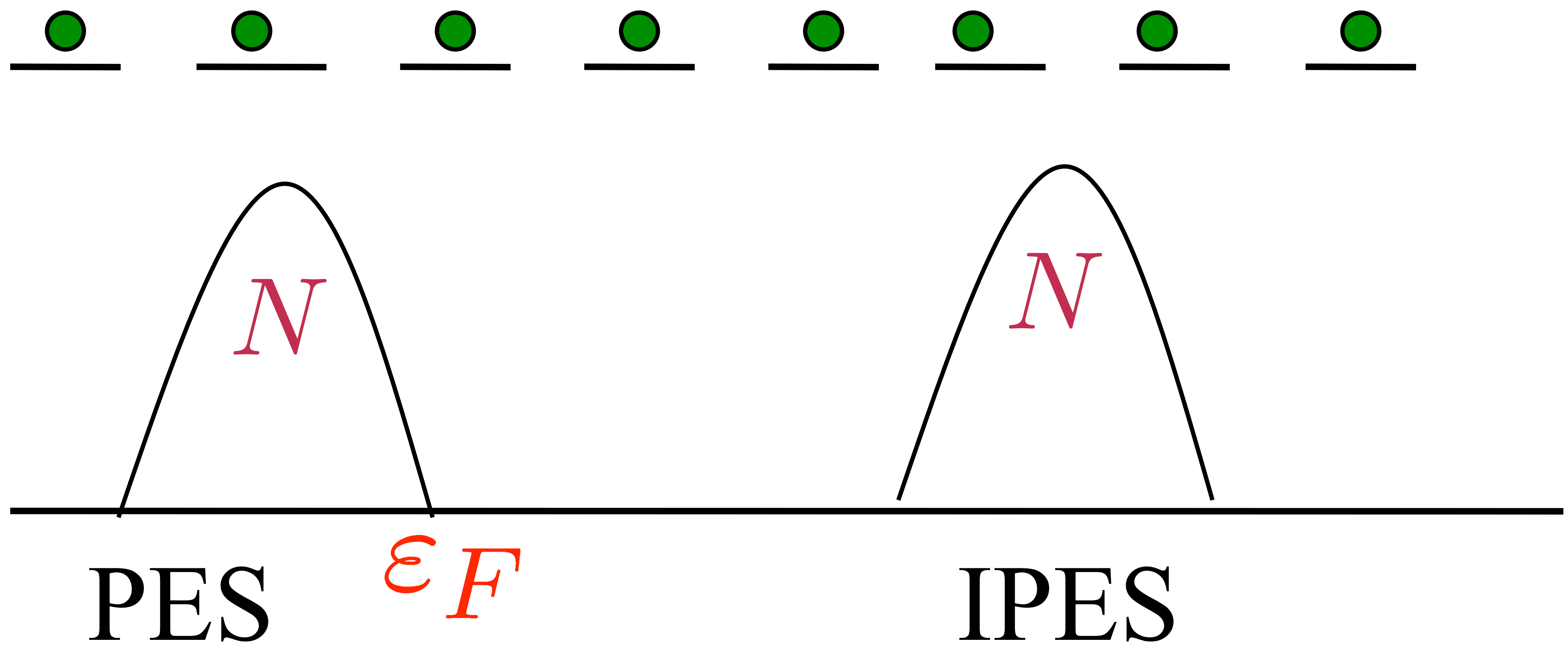
$$L_{ij} = \int_{-\infty}^{\infty} d\omega\left(-\frac{\partial f(\omega)}{\partial \omega}\right)\tau^i(\omega)\omega^{j-1}$$

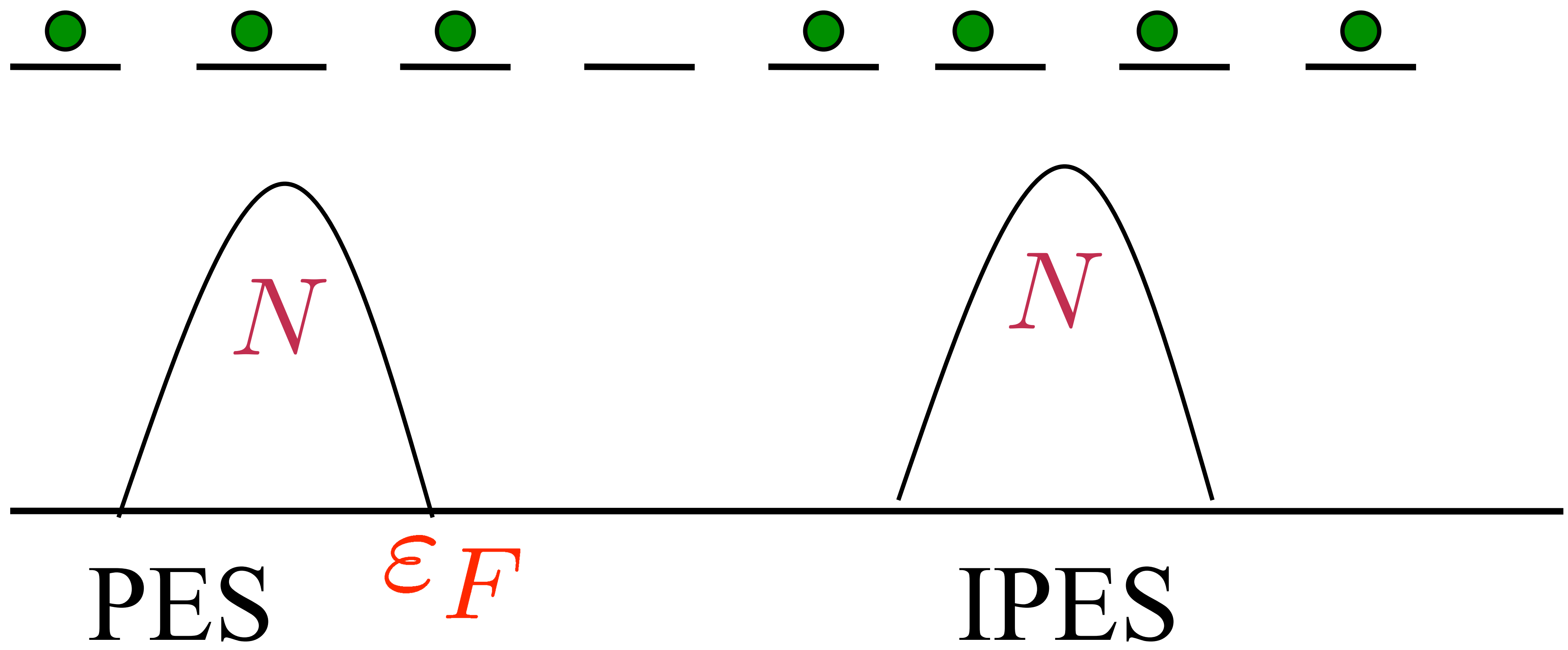
$$\tau(\omega) = \frac{1}{N}\sum_{\mathbf{k},\sigma}\left(\frac{\partial \epsilon_{\mathbf{k}}}{\partial k_x}\right)^2 A^2(\mathbf{k},\omega)$$

spectral function

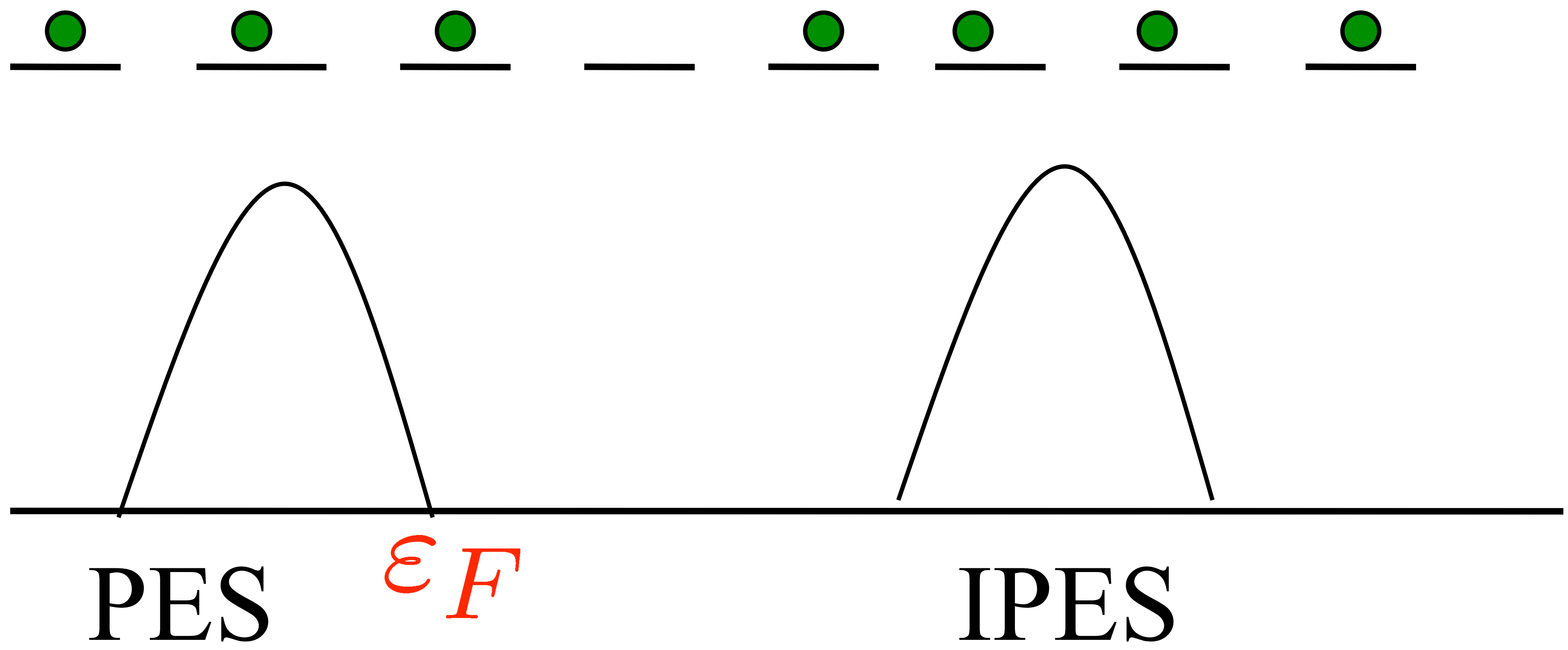
1.) τ must be symmetric about the chemical potential for S=0

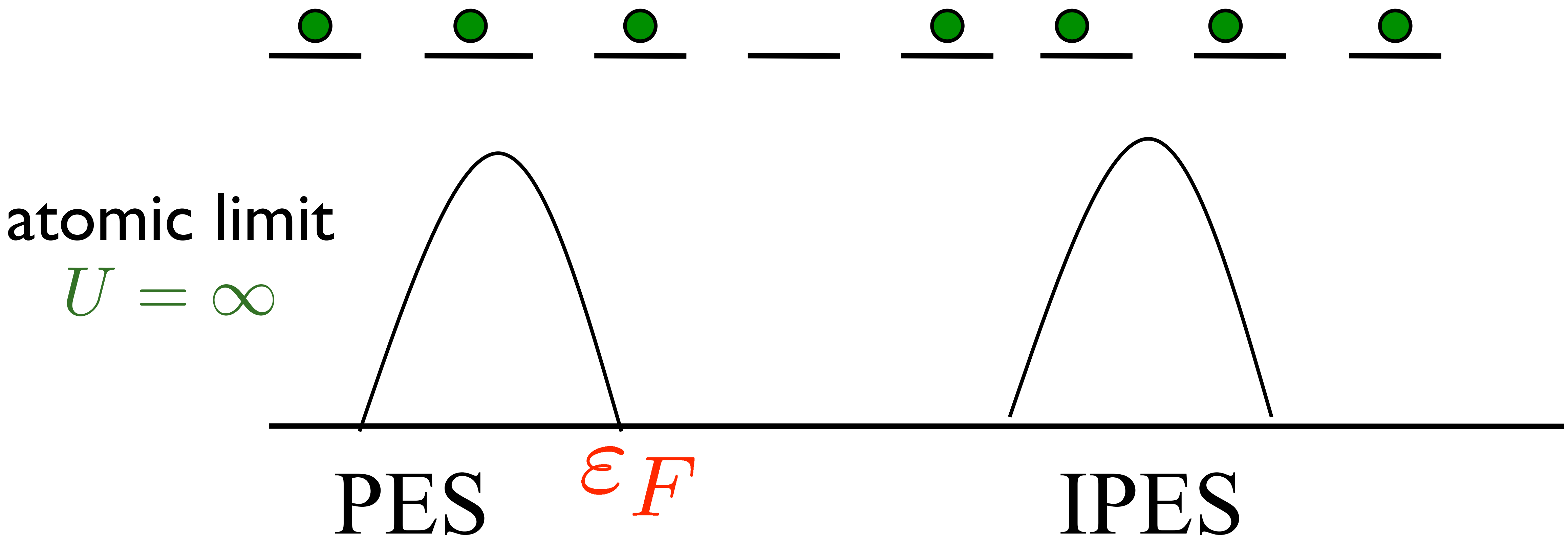
2.) but if A is momentum-independent, S=0 by particle-hole symmetry


N
N
PES
ε_F
IPES

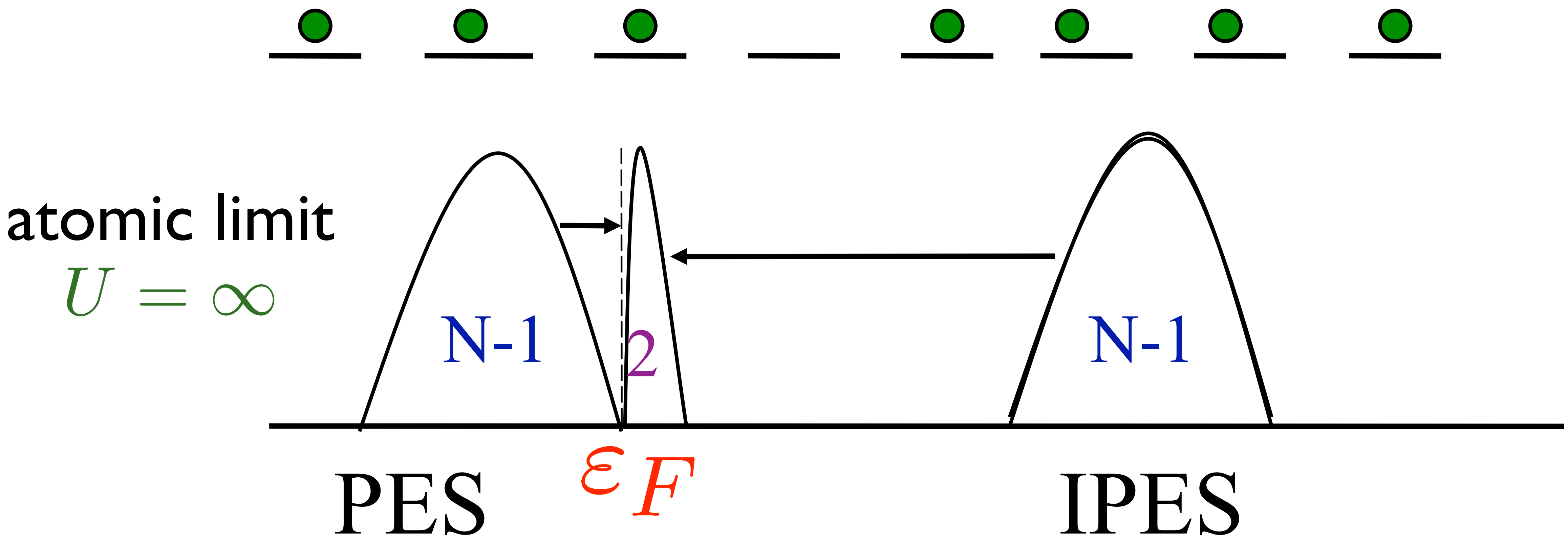


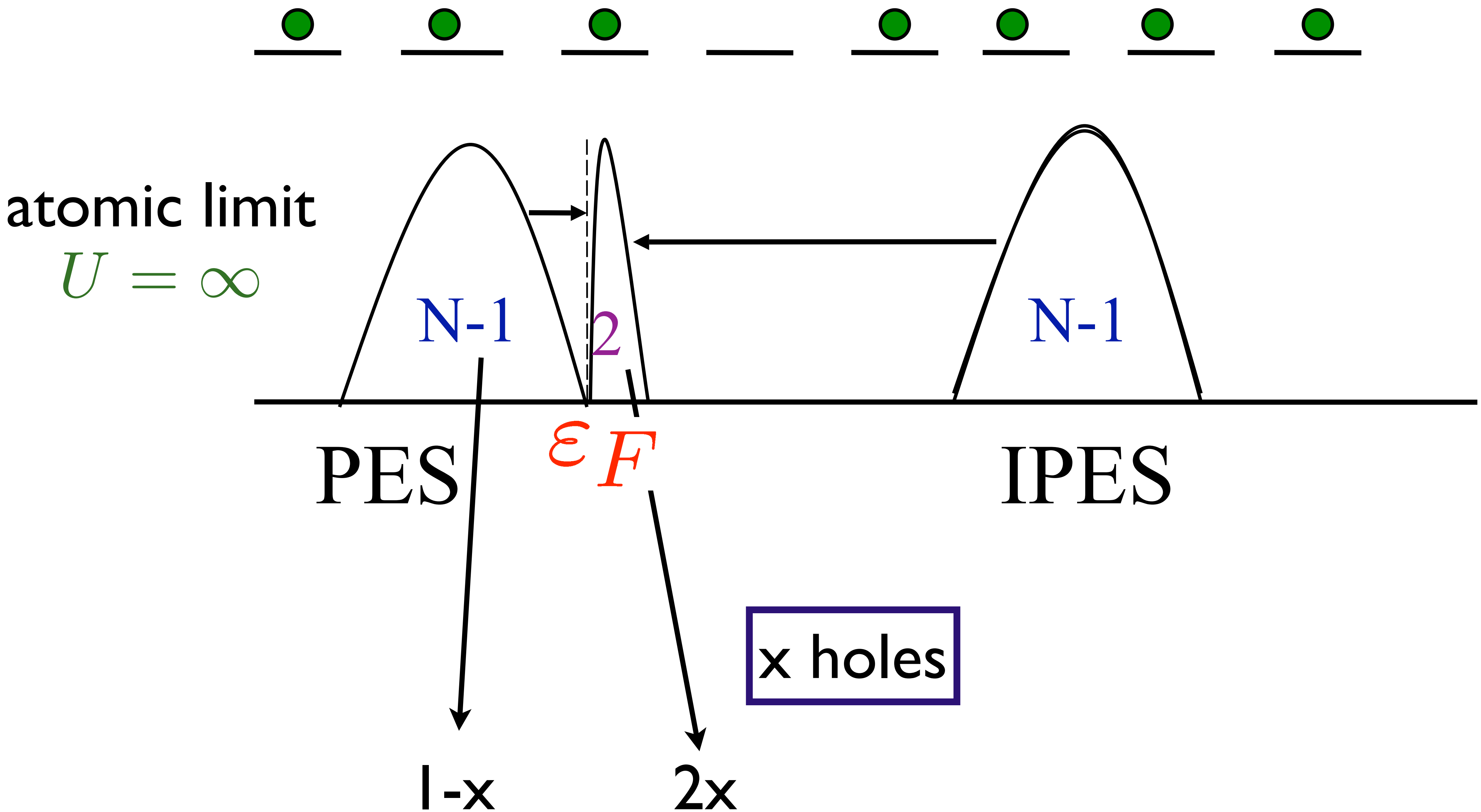
N
N
PES
ε_F
IPES


PES
ε_F
IPES

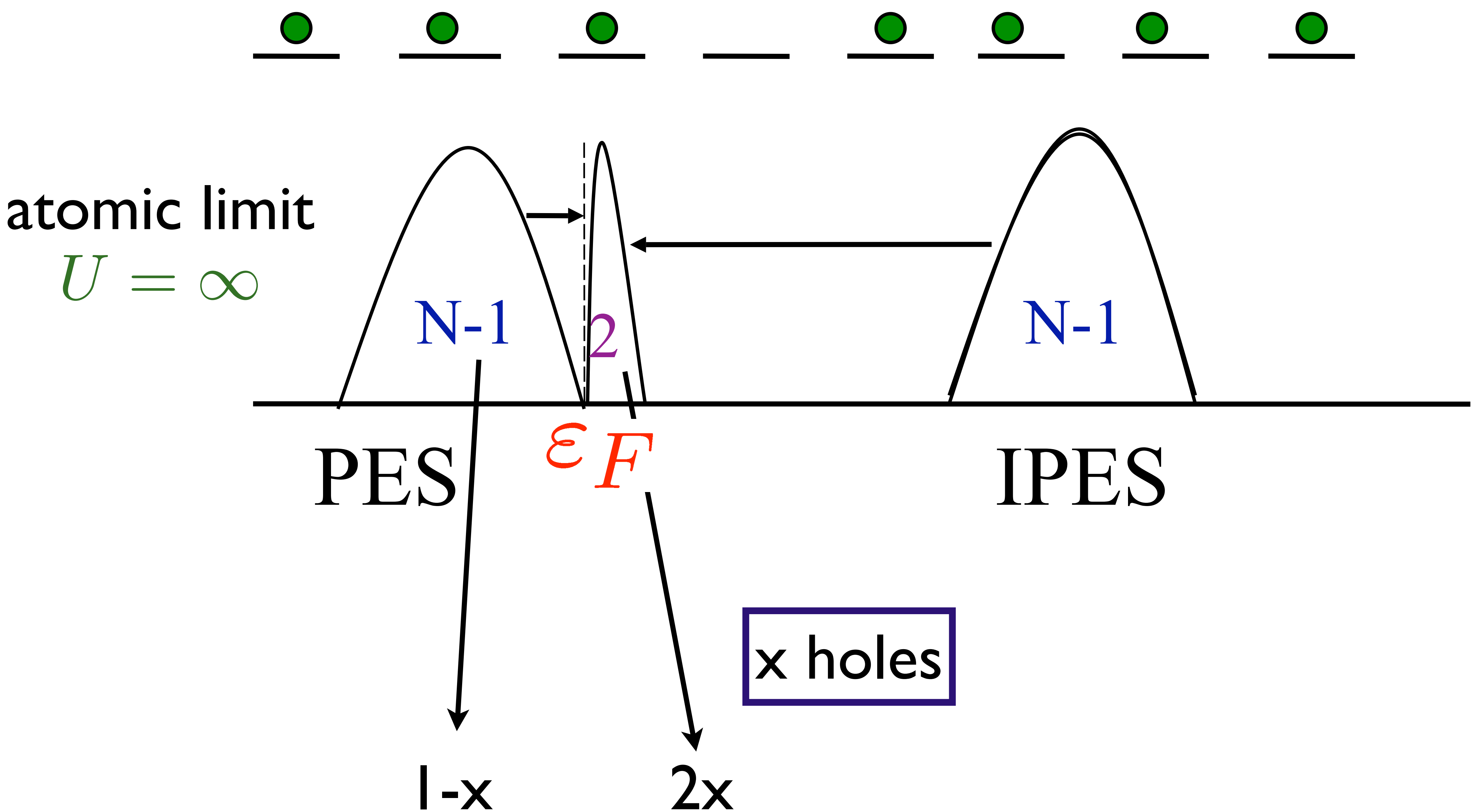


atomic limit
$U = \infty$
PES
ε_F
IPES


atomic limit
$U = \infty$
N-1
2
N-1
PES
ε_F
IPES

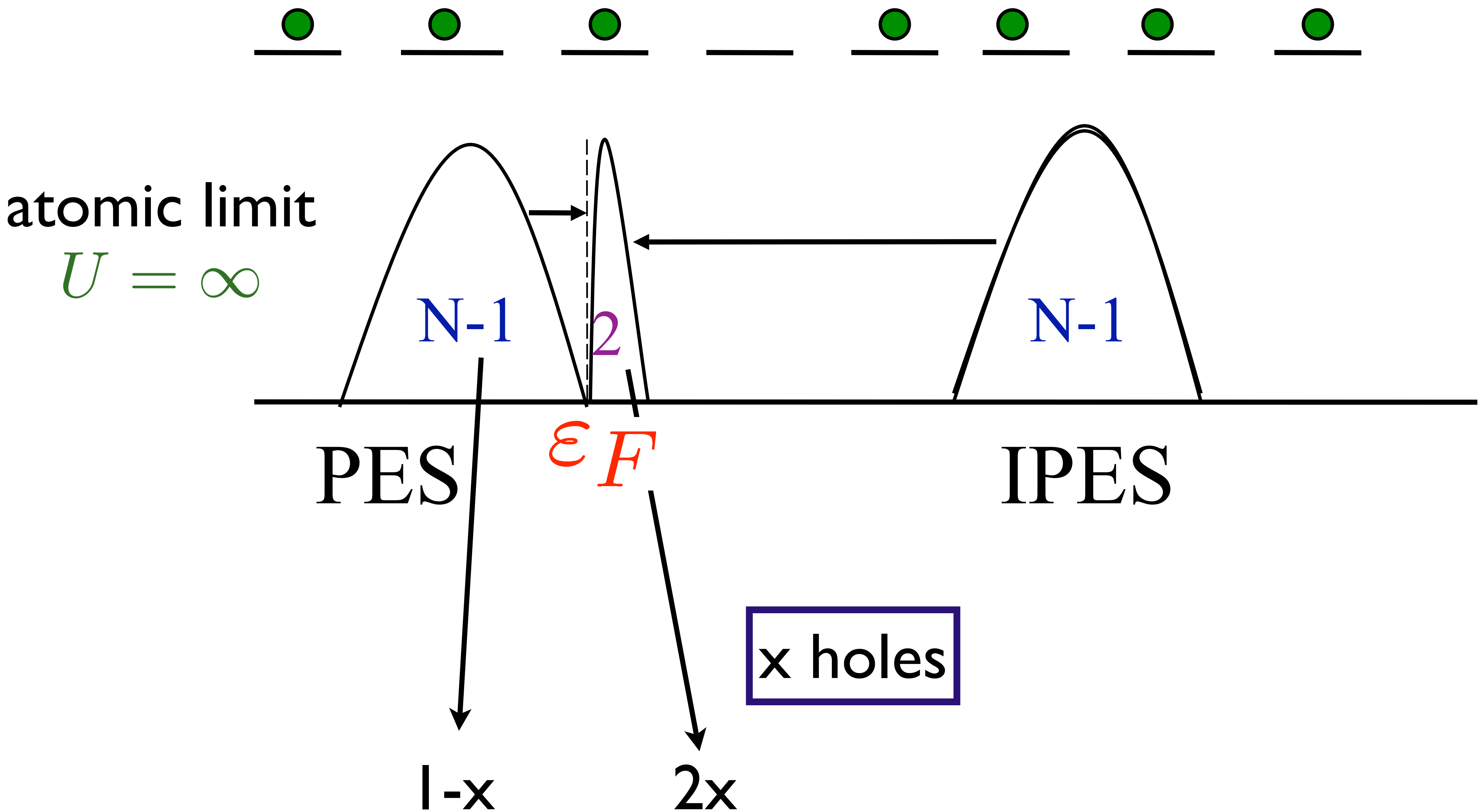


atomic limit
$U = \infty$
N-1
2
N-1
PES
ε_F
IPES
x holes
1-x
2x



criterion for vanishing of thermopower

LESW above ε_F = LESW below ε_F



criterion for vanishing of thermopower

LESW above ε_F = LESW below ε_F

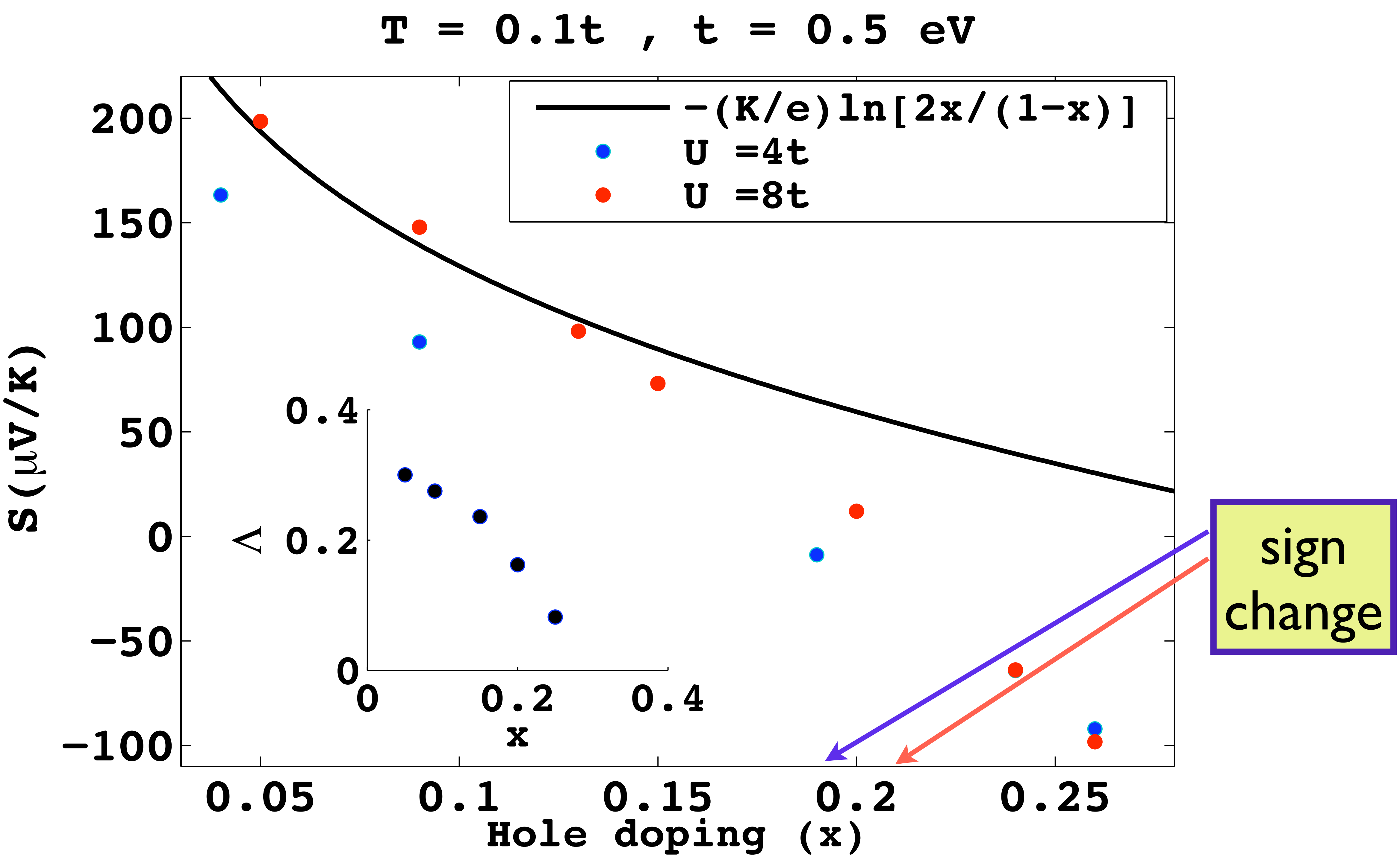
2x=1-x → x=1/3!

$$S \approx -\frac{k_B}{e} \ln \frac{\mathcal{L}}{1-x}$$

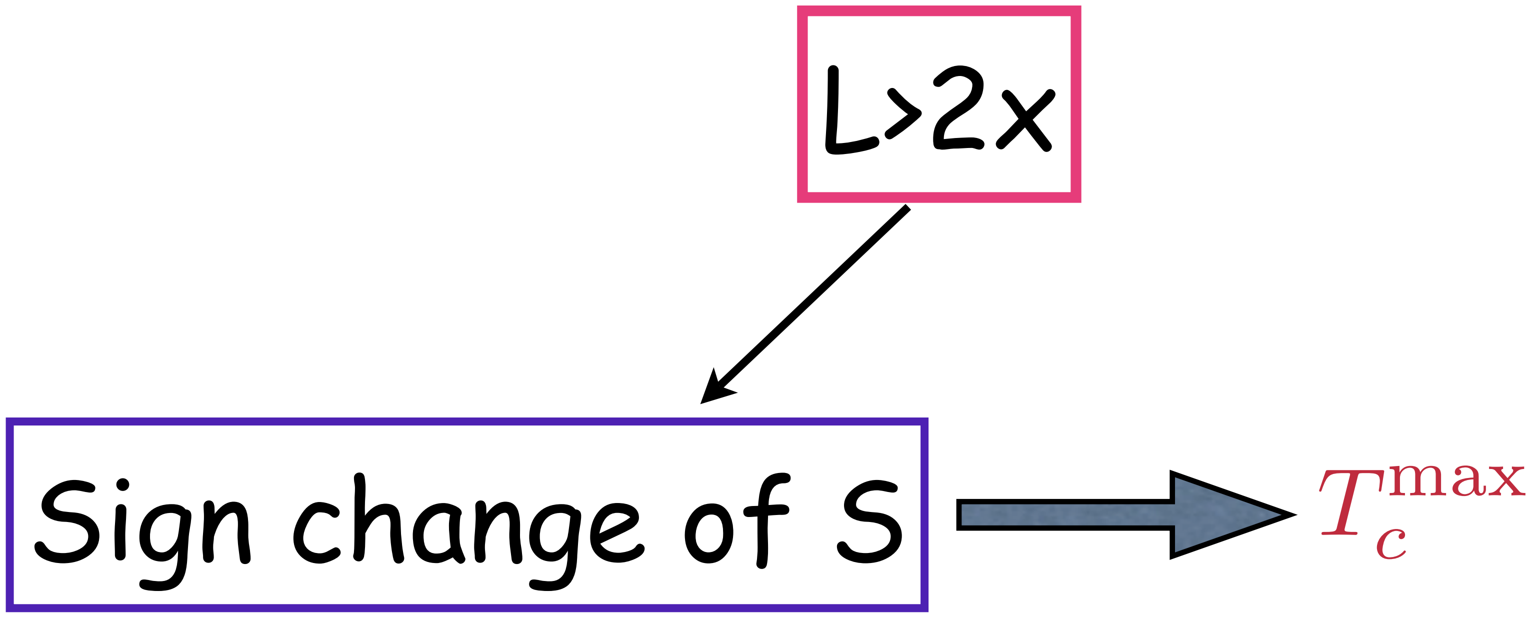
S must change sign before x=1/3
(atomic limit)

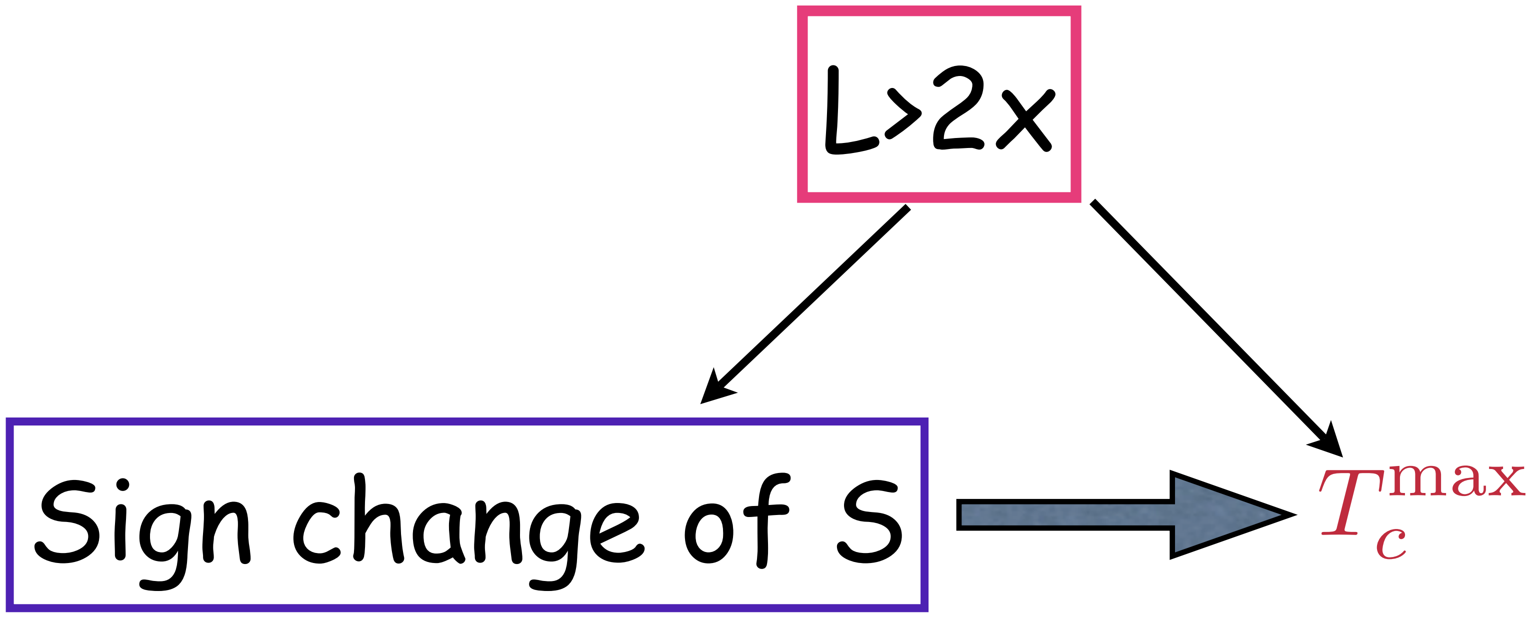
experiments: x_c=.24

Hubbard Model



arXiv:0807.2854


L>2x
Sign change of S
$T_c^{\max}$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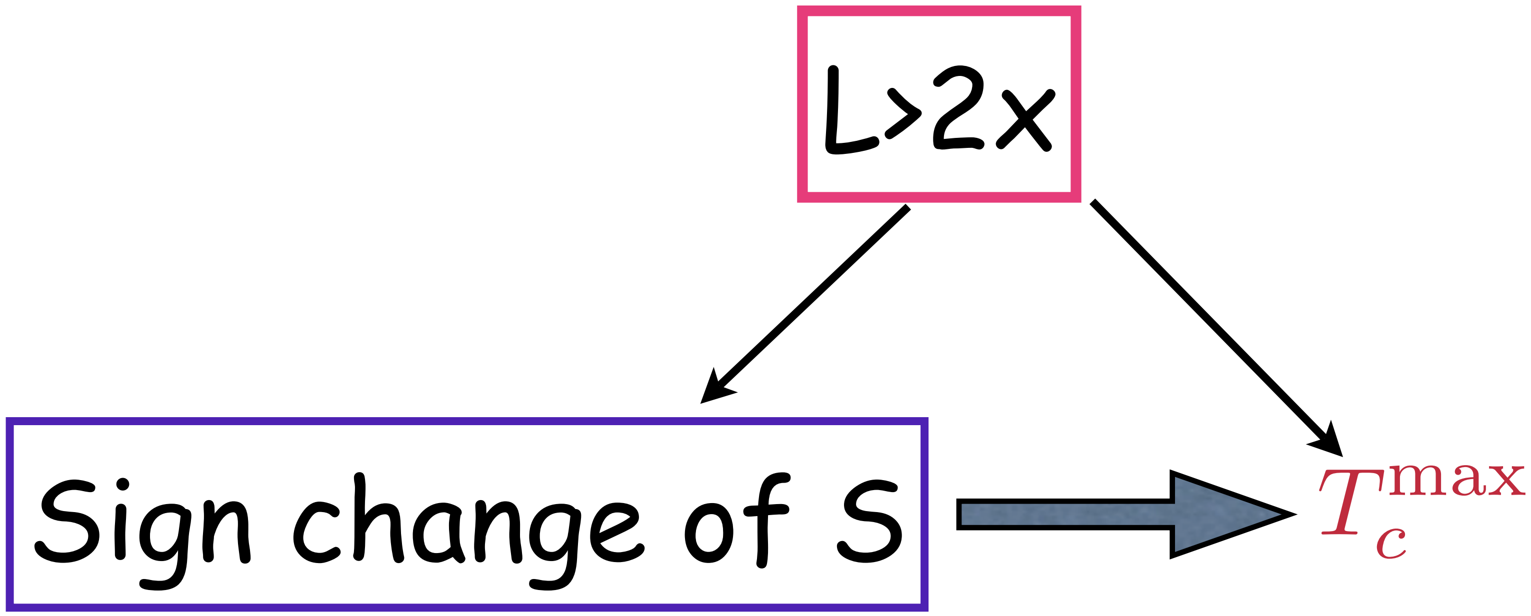

Is L>2x important qualitatively?

summary

low-energy theory: non-electron
Quantum numbers emerge---
SC boson-fermion model

Thanks to R. G. Leigh and Ting-Pong Choy, Shiladitya Chakraborty
and DMR-NSF/ACIF

summary

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summary

Boson=normal state properties of cuprates

Thanks to R. G. Leigh and Ting-Pong Choy, Shiladitya Chakraborty
and DMR-NSF/ACIF