Improved variational approach to strongly correlated systems: the RVB paradigm at work

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Outline

- The Mott transition
- Variational approach: Jastrow wave function
- The 1D Hubbard model: Luttinger liquid vs Mott insulator
- The 2D case: a novel approach for the Mott transition

M. Capello *et al.* Phys. Rev. Lett. **94**, 026406 (2005).

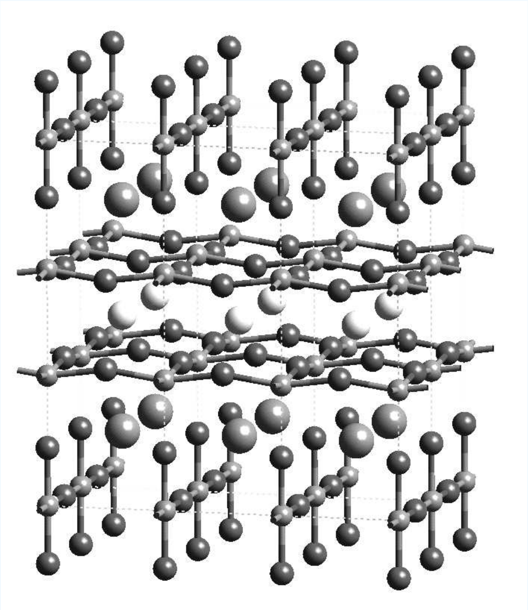
M. Capello *et al.*, Phys. Rev. B **72**, 085121 (2005).

M. Capello *et al.*, submitted (see cond-mat Sept. 2005).

The Mott transition

Band Theory + Odd number of electrons per site = Metal

but...



correlation effects may play an important role and the independent electron picture may fail

The Mott transition is a MIT induced by correlation

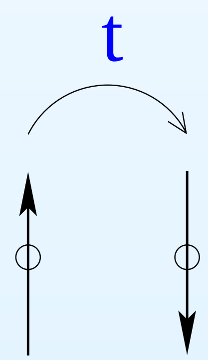
The one-band Hubbard model

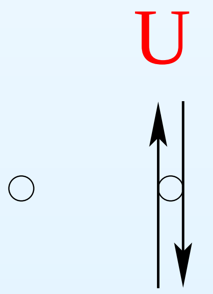
Toy model to study the Mott transition

$$H = \sum_{i,j,\sigma} t_{ij} c^{\dagger}_{i,\sigma} c_{j,\sigma} + H.c. + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$

t_{ij} is the kinetic term $\longrightarrow$ delocalizes the electrons

U is the interaction part $\longrightarrow$ localizes the electrons

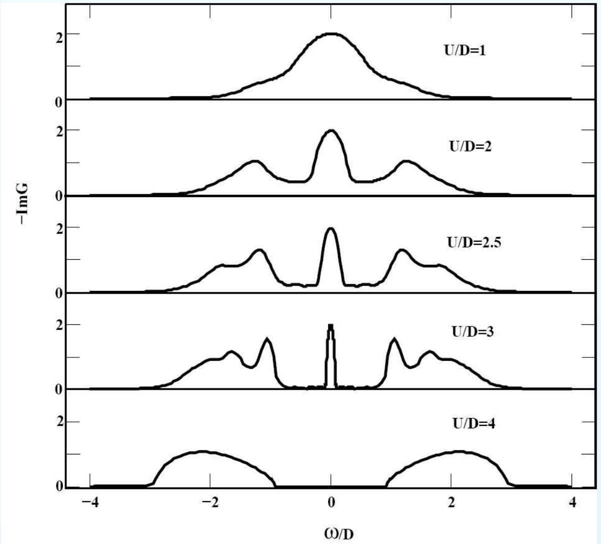


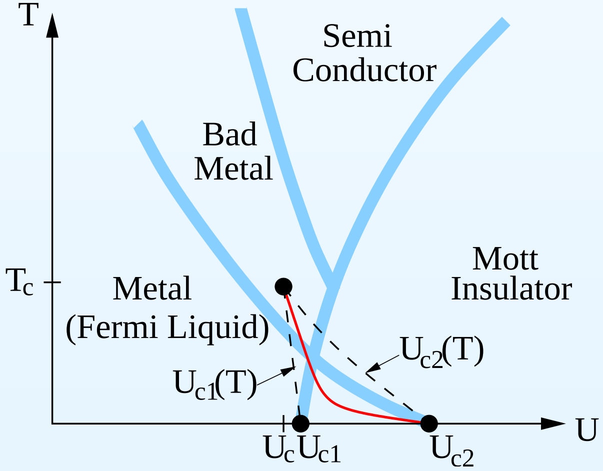


A bird's eye view on the DMFT results

Recent developments of DMFT allow us to get insight into the nature of the Mott transition in $D = \infty$

NO AF order



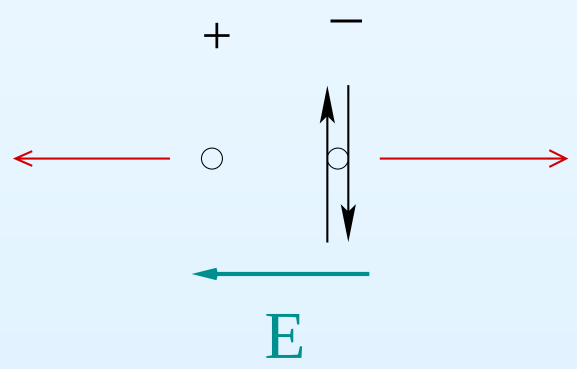


From A. Georges, "Troisieme Cycle de la Physique en Suisse Romande" (2002)

Charge fluctuations and the role of holons and doublons

Empty sites (Holons, H) and doubly occupied sites (Doublons, D) play a crucial role for the conduction

- Also in insulators there are charge fluctuations
  The case of $U = \infty$ is UNREALISTIC and TRIVIAL
- But H and D must be bound, otherwise an electric field will induce a current
- There is a spatial correlation among H and D



Jastrow wave function

$$|\Psi\rangle = \mathcal{J}|\mathcal{D}\rangle$$

$$\mathcal{J} = \exp[-\frac{1}{2}\sum_{i,j} v_{ij} n_i n_j] = \exp[-\frac{1}{2}\sum_{q} v_q n_{-q} n_q]$$

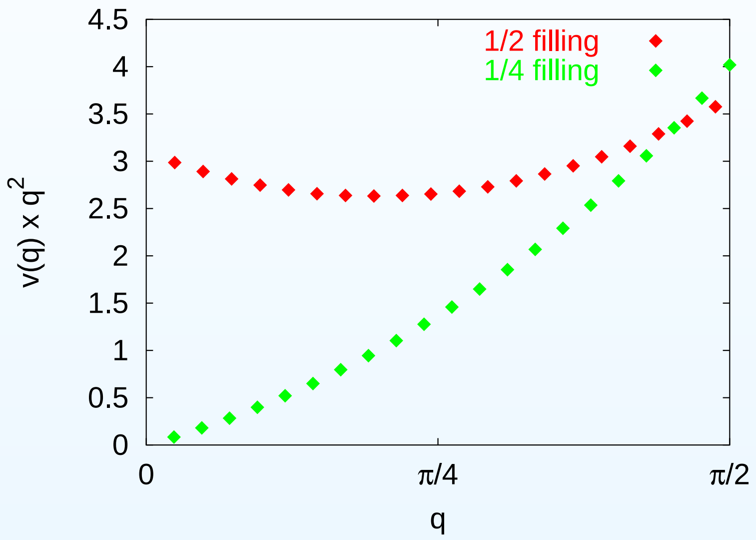
$|\mathcal{D}\rangle$ is an uncorrelated determinant: $|FS\rangle$ or $|BCS\rangle$

$$|BCS\rangle = \exp\left\{\sum_k f_k c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow}\right\} |0\rangle \qquad f_k = \frac{\Delta_k}{\epsilon_k - \mu + \sqrt{(\epsilon_k - \mu)^2 + \Delta_k^2}}$$

Find the optimal set of parameters which minimizes the energy without any apriori assumption

The one-dimensional Hubbard model

Hellberg and Mele (1991); Yokoyama and Ogata (1991); Gros and Valenti (1993)



$U/t = 10$

At finite doping $v_q \sim 1/|q|$

At half filling $v_q \sim 1/q^2$

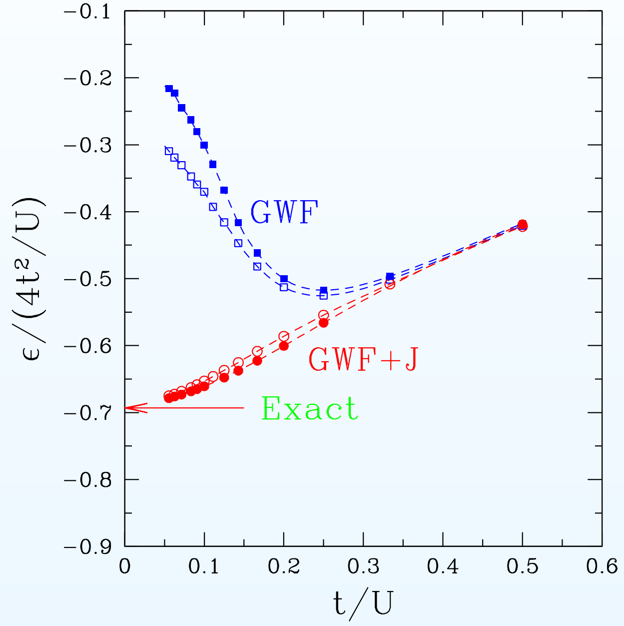
$1/q^2$ Cannot be found within the RPA for a short-range model

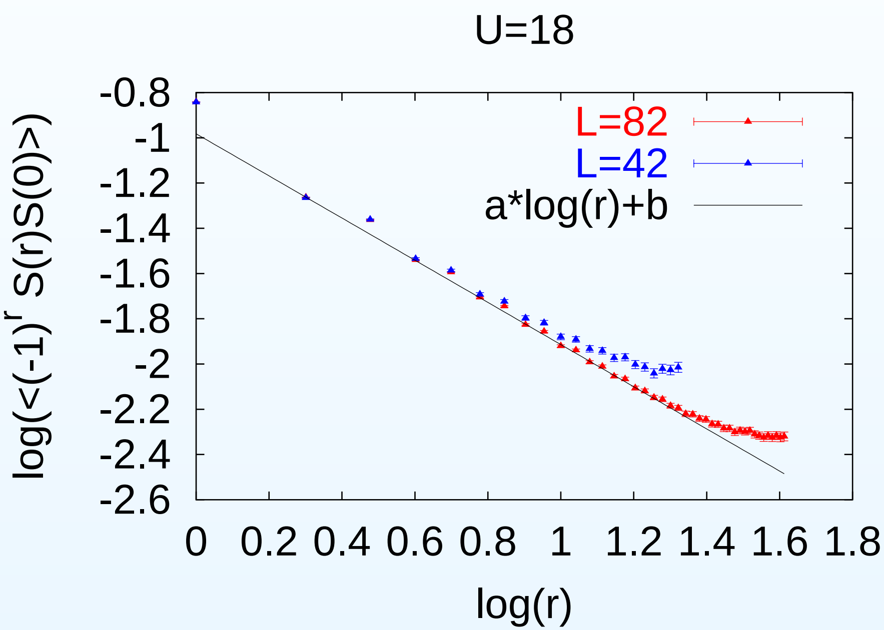
On the continuum
for free electrons
Gaskell (1961)

$$2v_q = -\frac{1}{N_0(q)} + \sqrt{\frac{1}{N_0^2(q)} + \frac{4mV(q)}{\hbar q^2}} \sim \frac{1}{|q|}$$

Correct low-energy insulating behavior

$a = -0.96 \pm 0.02 \quad b = -0.98 \pm 0.01$





$$\lim_{U/t\to\infty} \frac{\langle GWF|H|GWF\rangle}{\langle GWF|GWF\rangle} \to 0$$

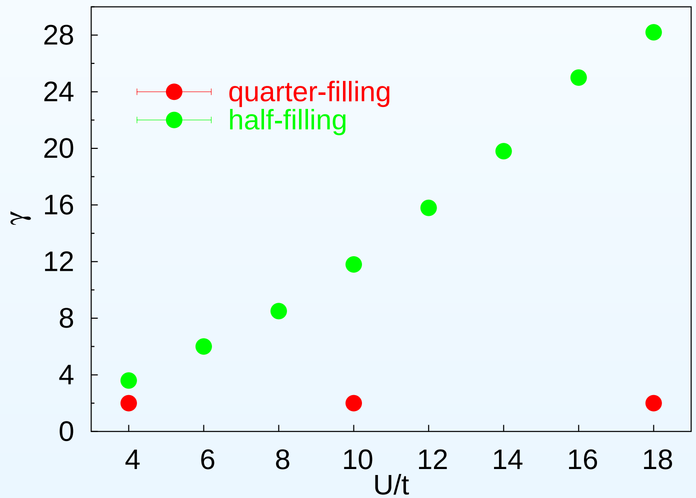
$$\frac{\langle GWF|H_{tJ}|GWF\rangle}{\langle GWF|GWF\rangle} \sim \frac{\langle GWF|e^{-iS}He^{iS}|GWF\rangle}{\langle GWF|GWF\rangle} \sim J \sim \frac{4t^2}{U}$$

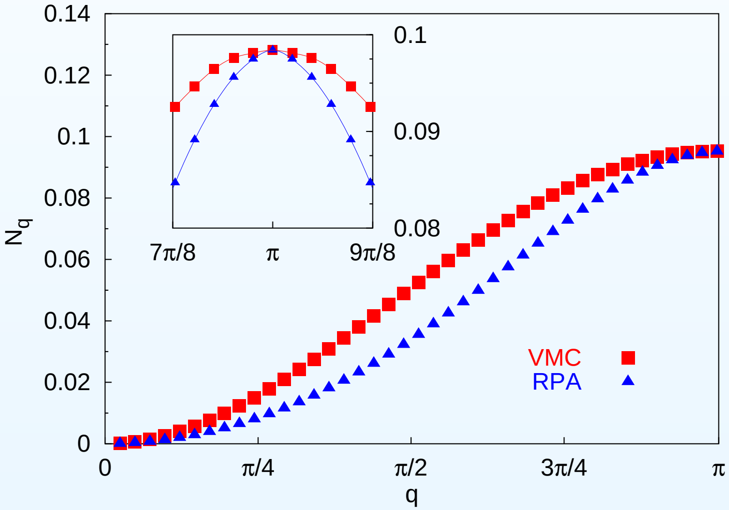
The long-range Jastrow acts as the canonical transformation

Reatto-Chester relation for N(q)

$$N(q) = \frac{\langle\Psi|n_{-q}n_q|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$

$$N(q) = \frac{N^0(q)}{1 + \gamma v(q) N^0(q)}$$



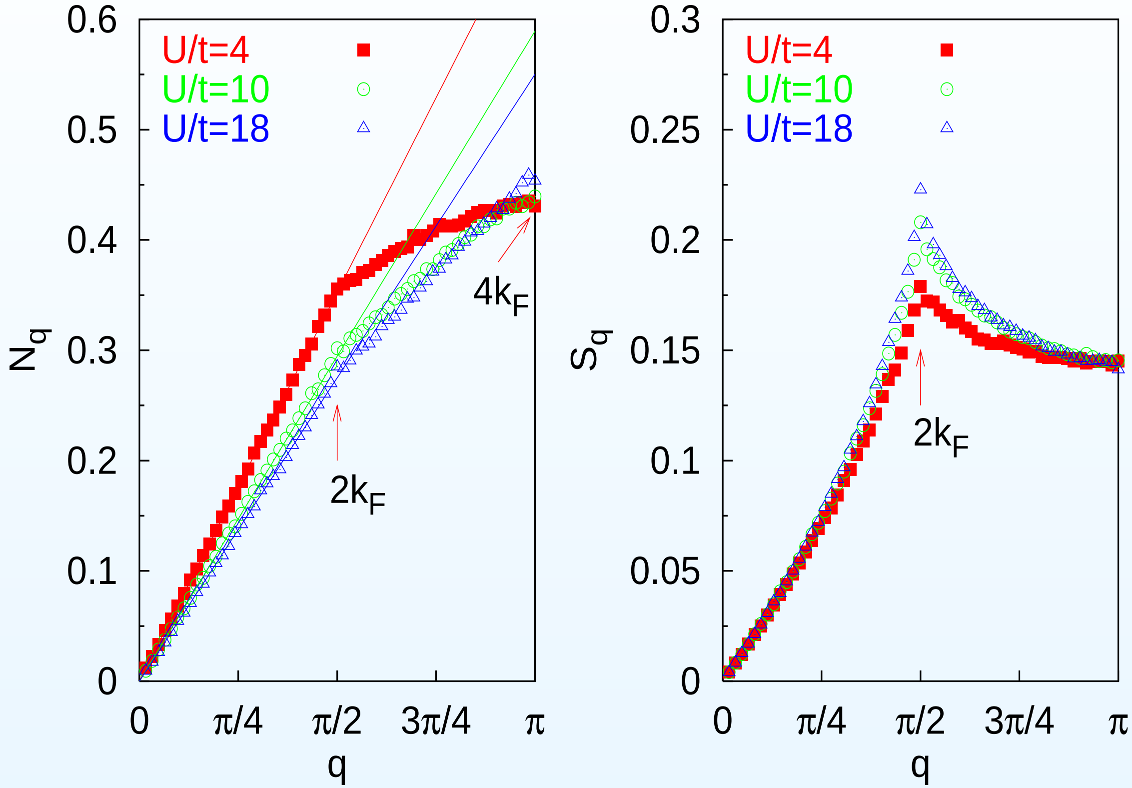


The Reatto-Chester is valid qualitatively for small q

But at half filling:

- the small-q behavior is quantitatively incorrect: $\gamma > 2$
- the Friedel oscillations at $q = 2k_F$ are removed

Luttinger liquid (I): Structure factors



$$N(q) = K_\rho/\pi|q|$$

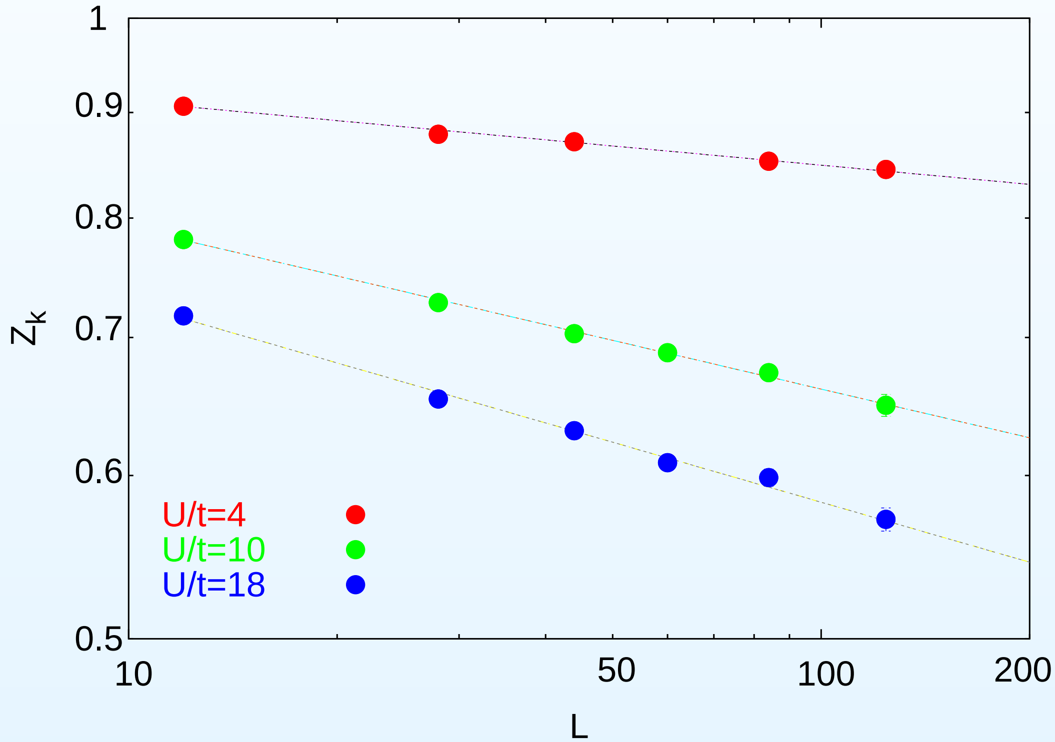
U/t	K_ρ^{exact}	K_ρ
4	0.711	0.705(3)
10	0.594	0.595(3)
18	0.551	0.550(3)

$$\langle n(x)n(0)\rangle \sim \frac{K_\rho}{(\pi x)^2} + A_1\frac{\cos(2k_F x)}{x^{K_\rho+1}} + A_2\frac{\cos(4k_F x)}{x^{4K_\rho}},$$

$$\langle \mathbf{S}(x)\cdot\mathbf{S}(0)\rangle \sim \frac{1}{(\pi x)^2} + B\frac{\cos(2k_F x)}{x^{K_\rho+1}},$$

Luttinger liquid (II): quasiparticle weight

$$Z_q = \frac{|\langle \Psi_{N-1} | c_{q,\sigma} | \Psi_N \rangle|^2}{\langle \Psi_N | \Psi_N \rangle \langle \Psi_{N-1} | \Psi_{N-1} \rangle} \quad with \quad |\Psi_{N-1}\rangle = \mathcal{J}\, c_{q,\sigma}\, |\mathcal{FS}\rangle$$



$$Z_{k_F} \sim 1/L^{\theta}$$

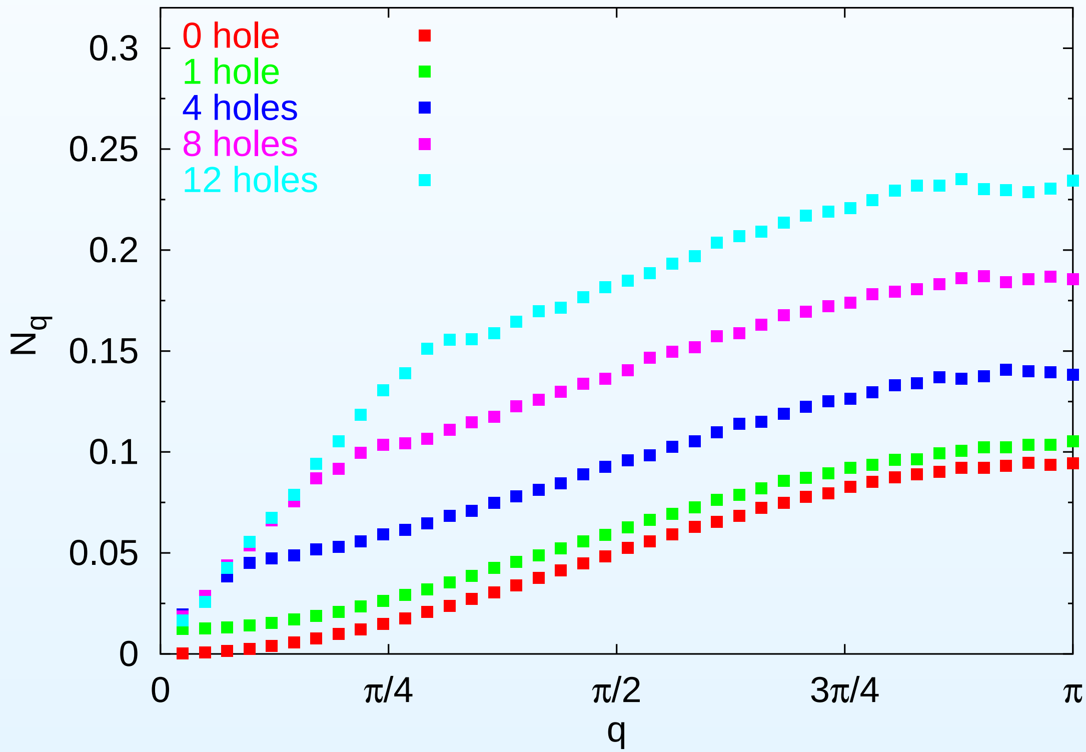
$$\theta_c = (K_\rho + K_\rho^{-1} - 2)/4$$

U/t	θ	θ_c
4	0.031(5)	0.031(3)
10	0.078(5)	0.072(3)
18	0.097(5)	0.092(3)

$Z_{k_F} \longrightarrow 0$: NO quasiparticles defined

From Luttinger liquid to Mott insulator

The linear part of $N(q)$ (from $q = 0$ to $4k_F$) shrinks when decreasing the doping and $N(q) \sim q^2$ at half filling:



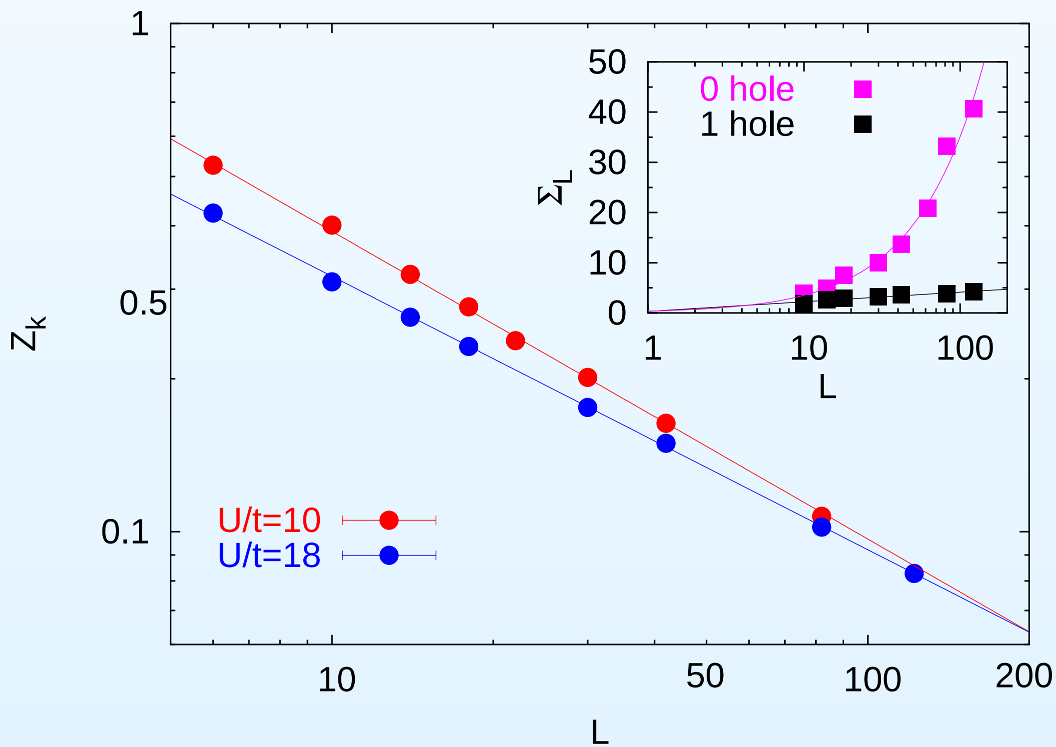
$$N_q \sim \frac{K_\rho |q|}{\pi} \Theta(4k_F - q) + (c + q^2)\Theta(q - 4k_F)$$

Mott insulator: quasiparticle weight

We get very different Jastrow at half filling and for the one hole

$$\Sigma_L = 1/L \sum_{q \neq 0} v(q)$$

diverges *linearly* at 1/2 filling and *logarithmically* at finite doping



Minimizing BOTH Jastrows:

$$Z_{k_F} \sim 1/L^\theta$$

U/t	θ	θ_{exact}
10	0.60(5)	0.5
18	0.55(5)	0.5

Half filling in 2D: coming from $U/t \gg 1$

The unbiased minimization gives a singular v_q

$$\mathcal{J} = \exp\left[-\frac{1}{2}\sum_{i,j} v_{ij}(n_i-1)(n_j-1)\right] \qquad v_q \sim \pi\beta/q^2$$

Holons: charged particles with $q_i = 1$

Doublons: charged particles with $q_i = -1$

Singly occupied sites: neutral background $q_i = 0$

Two-component classical Coulomb gas in 2D

Laughlin wave function for the FQHE maps onto the one-component Coulomb gas

First-order transition between a plasma and a Wigner crystal

What does it mean? Feynman answers

In analogy with the Feynman's construction for Helium

$$|\Psi_q\rangle = n_q|\Psi_0\rangle \qquad E_q - E_0 \sim \frac{\langle -K\rangle q^2}{2N_q}$$

For a gapped system $\Longrightarrow$ $N_q \sim q^2$

Strong consequences on the form of $|\Psi_0\rangle$

For operators that depend upon only on electronic positions

$$\langle\Theta\rangle = \frac{\langle\Psi_0|\Theta|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} = \sum_x \langle x|\Theta|x\rangle |\Psi_0(x)|^2$$

$$|\Psi_0(x)|^2 = e^{-\frac{V(x)}{T^{eff}}}$$

When Feynman met Jastrow

In the limit $U/t \gg 1$ small charge fluctuations

Only the two-body term is relevant

all multi-particle interactions are negligible

$$V(x) = \sum_{q \neq 0} v_q^{eff} n_q(x) n_{-q}(x)$$

$N_q \sim q^2 \Longrightarrow$ fluctuations of the classical variable n_q vanish and v_q^{eff} must diverge for small q's.

$$N_q \sim T^{eff}/v_q^{eff}$$

$$v_q^{eff} \propto 1/q^2$$

2D classical Coulomb gas on the lattice

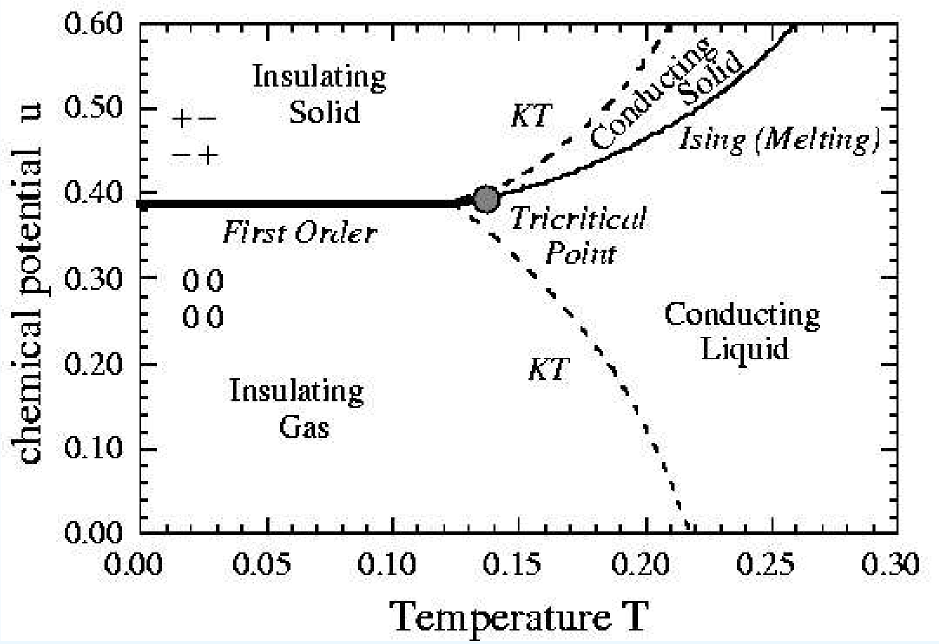
$$\langle n(r)n(0)\rangle \sim \begin{cases} \left(\frac{1}{r}\right)^{1/(T\epsilon)} & T < T_c \\ e^{-r/\lambda} & T > T_c \end{cases}$$

$$\frac{1}{\epsilon} = \lim_{q\to 0}\left[1 - \frac{2\pi}{Tq^2}N_q\right]$$

$1/\epsilon$ has a finite jump at the transition

$1/\epsilon = 0$ for $T > T_c$

$1/\epsilon > 0$ for $T < T_c$



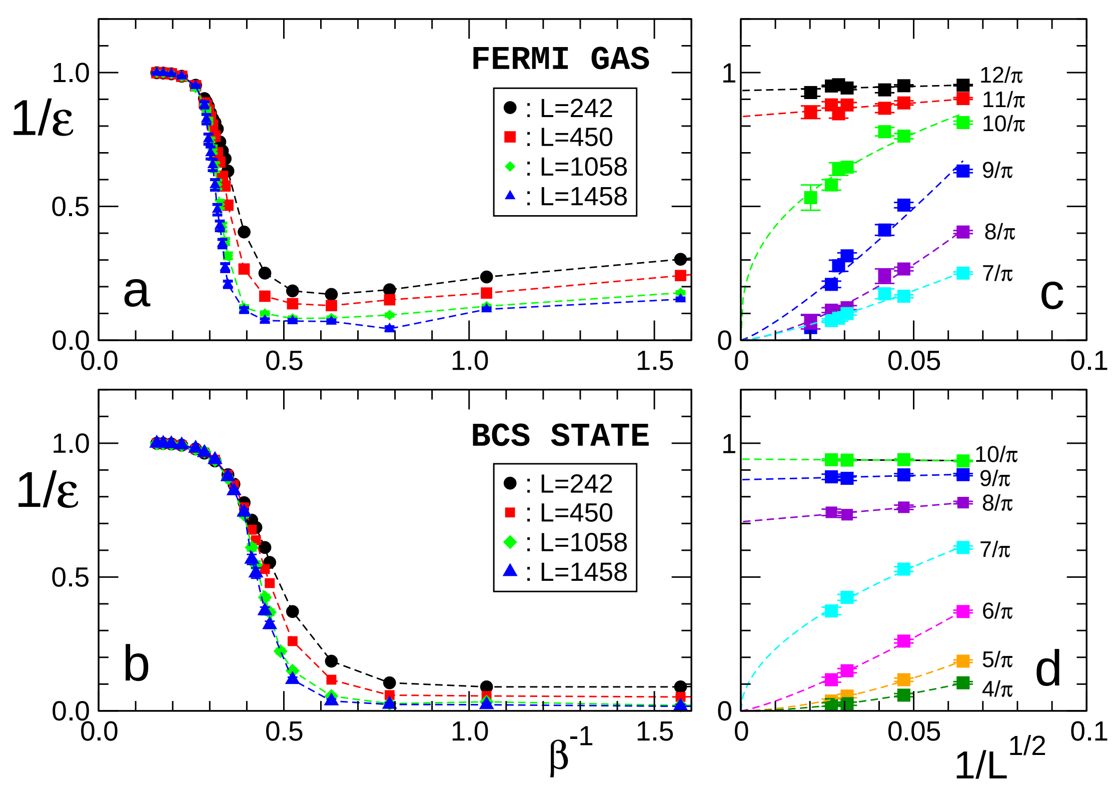
From J. Lee and S. Teitel, Phys. Rev. B **46**, 3247 (1992)

KT transition at small densities

(small fugacities)

The “dielectric function”

Evidence for a transition



Static structure factor: metal and insulator

small β:

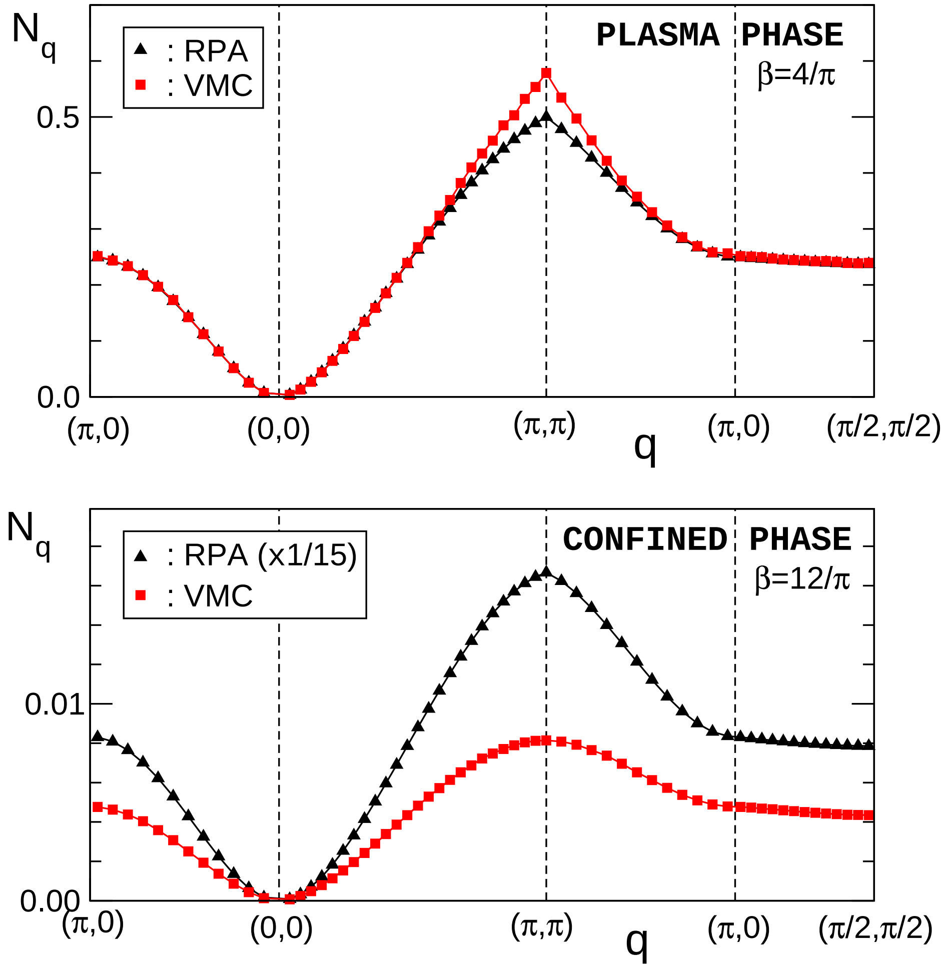
RPA is correct

$2k_F$ singularities

large β:

RPA is NOT correct

NO $2k_F$ singularities



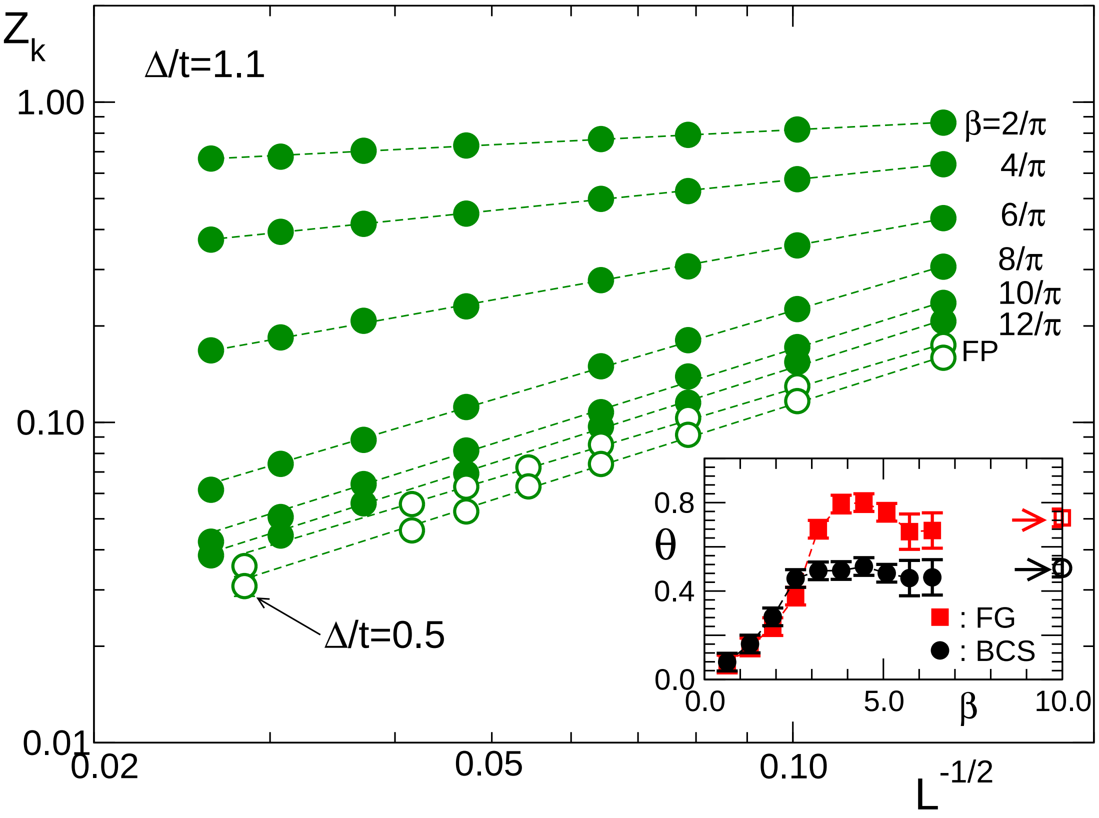
The quasiparticle weight: non-Fermi liquid properties?

$Z_k \sim 1/L^\theta$

θ constant in the confined phase! Universal properties of the FPWF

$\theta \longrightarrow 0$ in the plasma phase

Bares and Wen (1993)
Valenti and Gros (1992)



Conclusions

- The Jastrow wave functions are very flexible
- In 1D: Insulators, conducting LL and dimerized states
  [not shown, see M. Capello *et al.* PRL **94**, 026406 (2005)]
  $v_q \sim \beta/q^2 \Longrightarrow$ Insulator for any β
  $v_q \sim 1/q \Longrightarrow LL$
- In 2D: much more appealing scenario
  $v_q \sim \beta/q^2$ maps onto the 2D classical CG
  For small β's $\Longrightarrow$ metal with $Z_k \to 0$
  For large β's $\Longrightarrow$ insulator with power-law correlations
- What about finite doping? strange “metal”?
- Is it a reliable situation? Call for microscopic 2D models