Approximate variational theory of bound excitons in strongly correlated systems

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Paradigms for the Mott transition

Hubbard Hamiltonian:

$$H = -t\sum_{\langle i,j\rangle\sigma} c^\dagger_{i\sigma}c_{j\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow}$$

Metal-insulator transition between paramagnetic metal and paramagnetic insulator

- Brinkman-Rice transition
- Single-site DMFT

Exciton binding transition (Capello *et al.*, 2005)

Variational approaches

Gutzwiller wavefunction (GWF):

$$|\Psi_G(\gamma)\rangle = \exp(-\gamma\sum_i n_{i\uparrow}n_{i\downarrow})|FS\rangle$$

Baeriswyl wavefunction (BWF):

$$|\Psi_B(\alpha)\rangle = \exp(-\alpha\sum_{\langle i,j\rangle\sigma} c^\dagger_{i\sigma}c_{j\sigma})|\Psi(\gamma\to\infty)\rangle$$

Combined projection (Baeriswyl-Gutzwiller, BGWF):

$$|\Psi_{BG}(\alpha,\gamma)\rangle = \exp(-\alpha\sum_{\langle i,j\rangle\sigma} c^\dagger_{i\sigma}c_{j\sigma})|\Psi(\gamma)\rangle$$

Gutzwiller wavefunction (GWF)

Exact solution in 1D (Metzner and Vollhardt, 1987): metallic, finite discontinuity in the momentum distribution

QMC in two and three dimensions

Gutzwiller approximation is the exact solution in ∞-dimensions: Brinkman-Rice transition

For finite dimensions GWF is metallic:

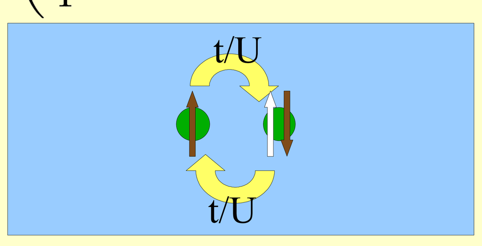
$$D_c = \left\langle \Psi_G \left| \frac{\partial^2 H_t(\Phi)}{\partial\Phi^2}\right| \Psi_G\right\rangle$$

Insulation implemented via non-centro-symmetric correlations between holes and double occupations (Capello, *et al.*, 2005)

Baeriswyl wavefunction (BWF)

- Finite dimensions, finite U: BWF is insulating (Dzierzawa *et al.*, 1997)
- Insulating state is characterized by bound excitons (Baeriswyl, 2000)

$$\langle X^2\rangle = \langle D\rangle = 2\sum_{\langle i,j\rangle}\frac{t^2}{U^2}\left(\frac{1}{4} - \langle\Psi_G(\infty)|\mathbf{S}_i\cdot\mathbf{S}_j|\Psi_G(\infty)\rangle\right)$$



Gutzwiller approximation →GWF

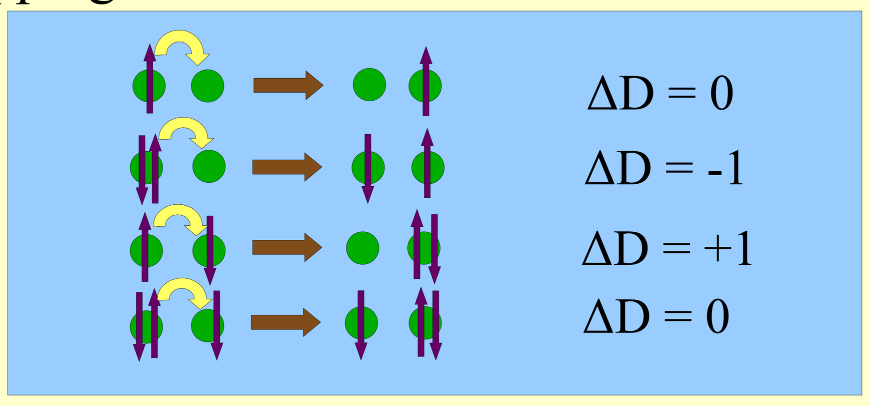
Combinatorial approach:

- Sampled configurations have one electron of a particular spin at each site
- Statistical weight of a particular configuration: $P(\Gamma) = \exp[-2\gamma D(\Gamma)]$
- Expectation value of an operator diagonal in coordinate space:

$$\langle A\rangle_B = \frac{\sum_\Gamma P(\Gamma)A(\Gamma)}{\sum_\Gamma P(\Gamma)}$$

Gutzwiller approximation →GWF

Hopping classification: $H_t = H_t^0 + H_t^+ + H_t^-$



$$\langle c^\dagger_{i\uparrow}c_{j\uparrow}\rangle_G = A\frac{\sum_\Gamma^{\text{hop}\uparrow} P(\Gamma)\exp(-\gamma\Delta D)}{\sum_\Gamma P(\Gamma)}$$

Gutzwiller approximation→BWF

Sample confiugrations in reciprocal space

For the completely projected GWF n_k is uniform

Statistical weight of configurations

$$P(\Gamma) = \exp\left(\sum_{k\sigma}\epsilon_k n_{k\sigma}(\Gamma)\right)$$

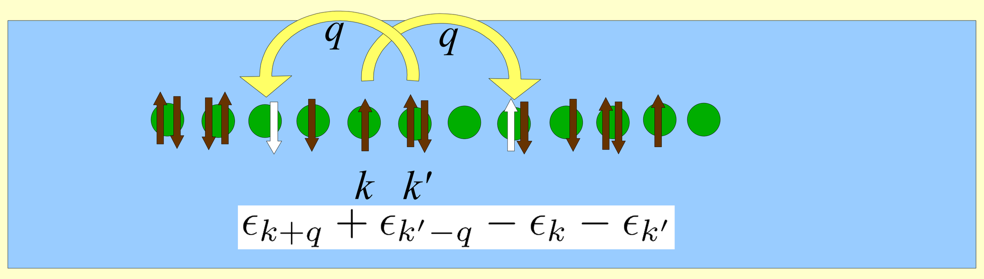
Expectation value of an operator diagonal in reciprocal space

$$\langle A\rangle_B = \frac{\sum_\Gamma A(\Gamma)P(\Gamma)}{\sum_\Gamma P(\Gamma)}$$

Gutzwiller approximation→BWF

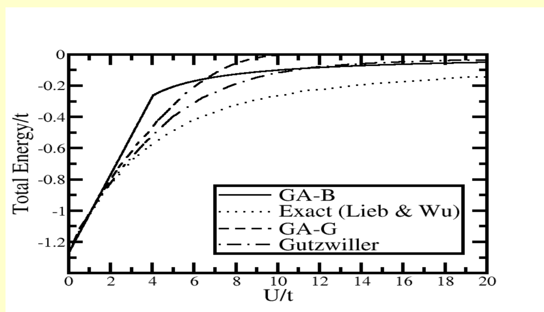
Interaction:

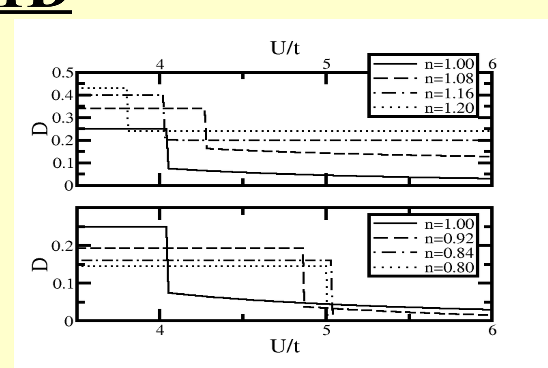
$$\sum_i n_{i\uparrow}n_{i\downarrow} = \sum_{k,k'} n_{k\uparrow}n_{k'\downarrow} - \sum_{kk'q} c^\dagger_{k+q,\uparrow}c^\dagger_{k'-q,\downarrow}c_{k\uparrow}c_{k'\downarrow}$$

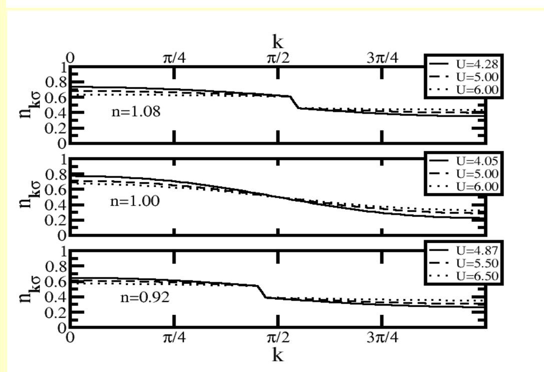


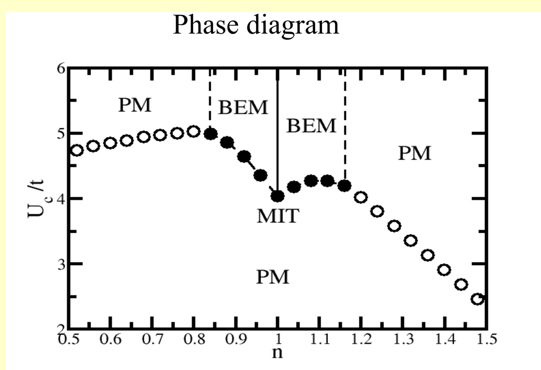
$$\langle c^\dagger_{k+q\uparrow}c^\dagger_{k'-q\downarrow}c_{k\uparrow}c_{k'\downarrow}\rangle = B\frac{\sum_\Gamma^{k-\text{hop}} P(\Gamma)\exp[-\alpha(\epsilon_{k+q}+\epsilon_{k'-q}-\epsilon_k-\epsilon_{k'})]}{\sum_\Gamma P(\Gamma)}$$

GA→BWF Results, 1D



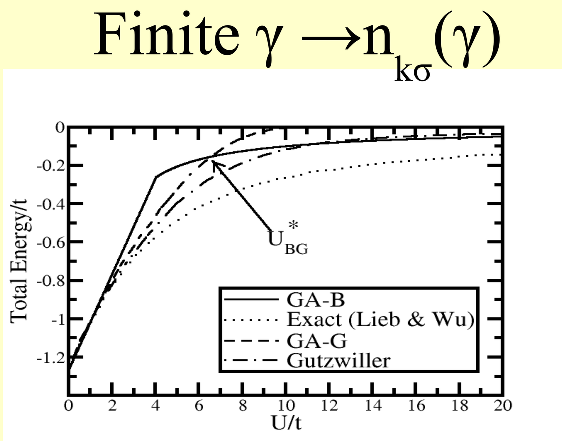


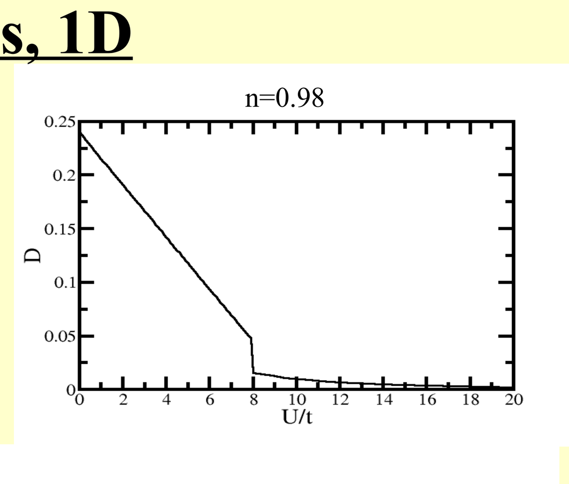


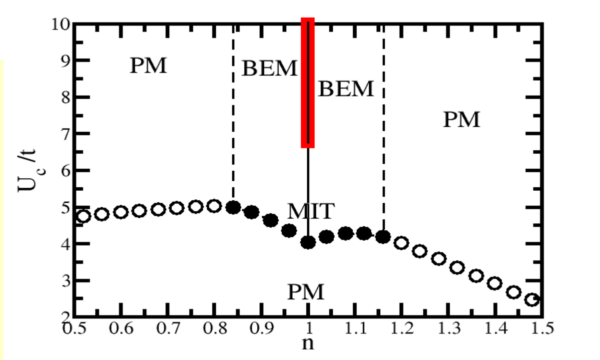


GA→BGWF Results, 1D

Finite γ →$n_{k\sigma}(\gamma)$







Total position operator

Ill-defined for a periodic system

One can construct it using the total momentum shift operator: $\mathfrak{U} = \exp\left(i\frac{2\pi X}{L}\right)$

Two common approaches:

- Resta (1998): $\bar{X}_R = \frac{L}{2\pi}\text{Im}\ \ln\langle\mathfrak{U}\rangle$

  $\bar{\sigma}^2{}_R = \frac{L^2}{2\pi^2}\text{Re}\ \ln\langle\mathfrak{U}\rangle$

  higher powers are not accessible
- Sawtooth operator:

$$\bar{X}_{st} = \sum_{m=1}^{L-1}\left(\frac{1}{2} + \frac{\mathfrak{U}^m}{\exp\left(-i\frac{2\pi m}{L}\right)-1}\right)$$

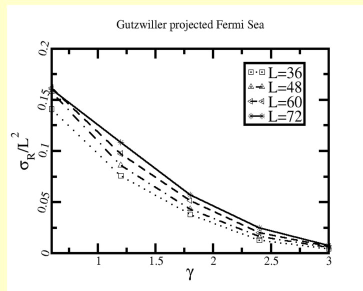
all powers are accessible→cumulants

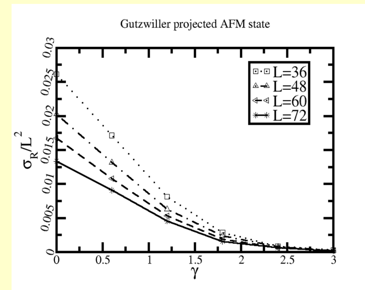
$$U_2 = 1 - \frac{\langle X^2\rangle}{3\langle X\rangle\langle X\rangle} \qquad U_4 = 1 - \frac{\langle X^4\rangle}{3\langle X^2\rangle\langle X^2\rangle}$$

Finite size scaling of localization for MIT

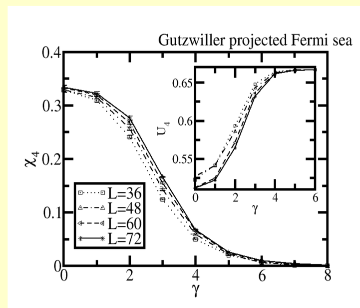
Metallic vs. Insulating GWFs:

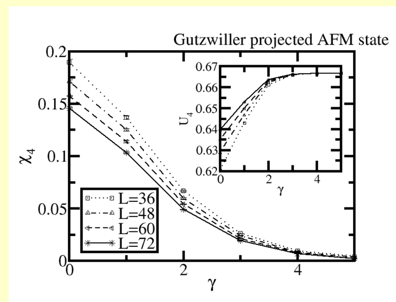
Resta:





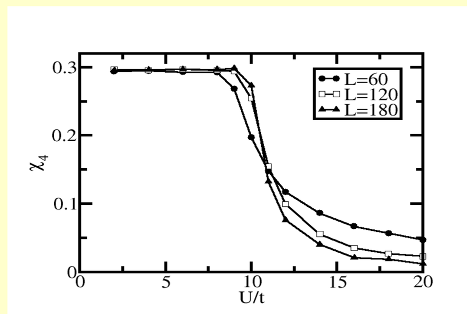
Sawtooth:



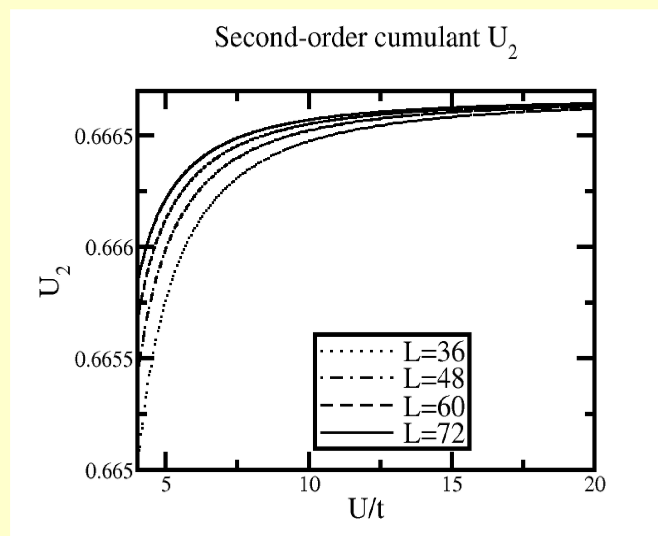


–Brinkman-Rice transition:

$$\chi_4 = \frac{\sqrt{\langle X^4\rangle - \langle X^2\rangle\langle X^2\rangle}}{L^2}$$



Cumulant for BWF at half-filling



BWF state is localized

Conclusion

- Gutzwiller approximation can be applied to the Baeriswyl wavefunction
- Half-filling: metal insulator transition between HF metal and insulator characterized by bound excitons
- Away from half-filling: metal-metal transition between HF metal and metallic state with bound excitons
- Baeriswyl-Gutzwiller wavefunction gives similar results, but HF metal replaced by Gutzwiller correlated metal