Local electron correlation in quasi-periodic systems

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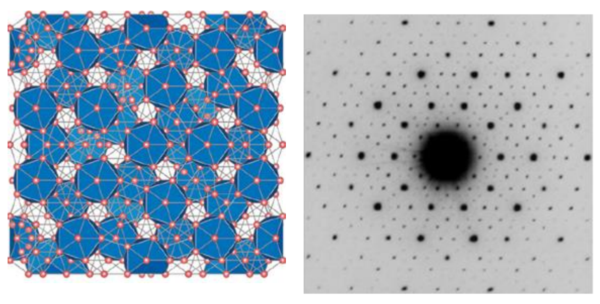
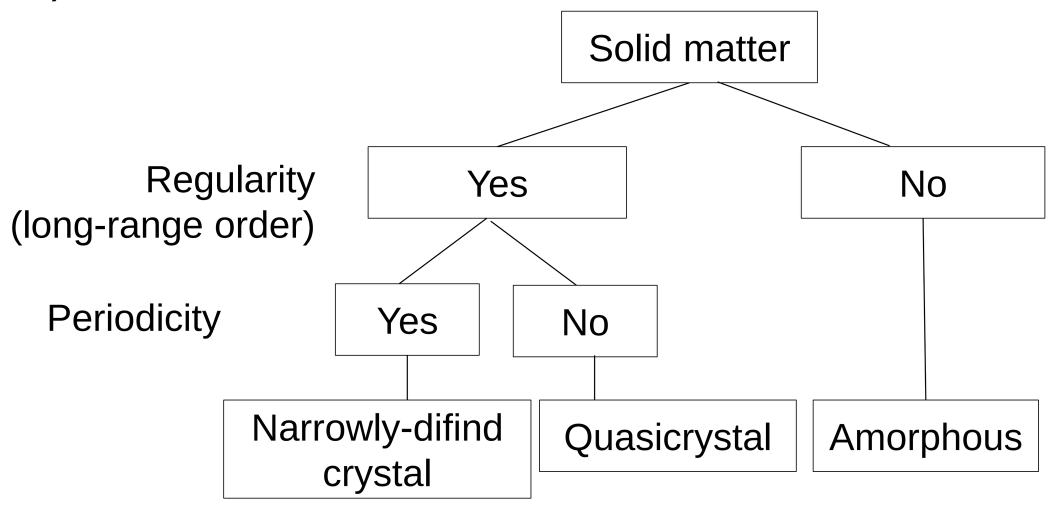
1. Introduction

Quasicrystal in Al-Mn alloys (1984)[1]

- No translational symmetry
- Rotational symmetry
  5-fold, 8-fold, 10-fold…



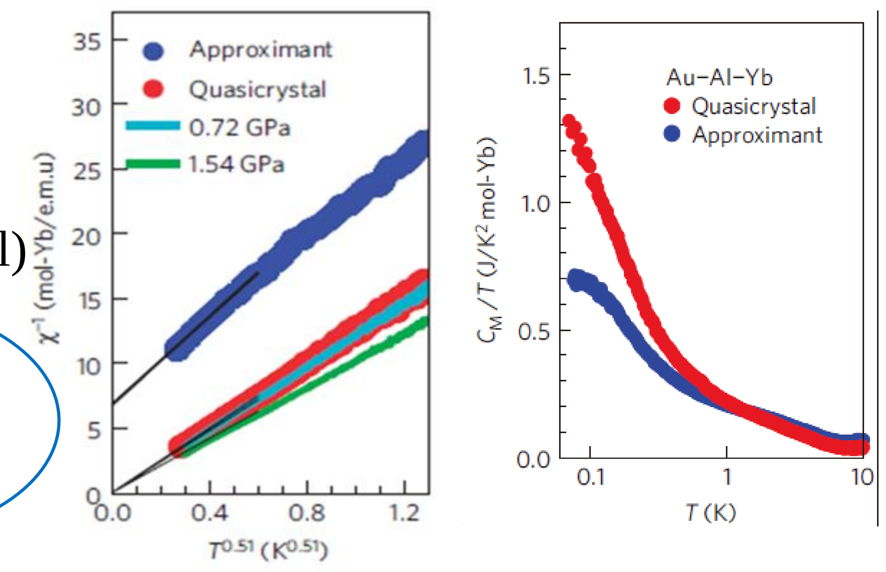


◆Quantum criticality (2012)[4]:

- $Au_{51}Al_{34}Yb_{15}$: Quasicrystal
- $Au_{51}Al_{35}Yb_{14}$: Approximant (crystal)

Metal Itinerancy ⇔ Yb Localization correlation

- Quasiperiodicity
- Local correlation

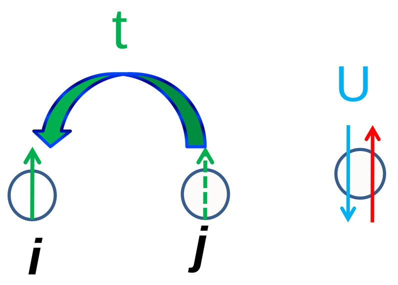


K. Deguchi, *et al*., Nmat. **11**, 1013-1016 (2012)

2.Model

◆ Hubbard model: itinerancy and localization

$$H = \boxed{-\sum_{\langle i,j\rangle} t(c_{i\sigma}^\dagger c_{j\sigma} + h.c.)} + \boxed{U\sum_i n_{i\uparrow}n_{i\downarrow}}$$



Local correlation effect

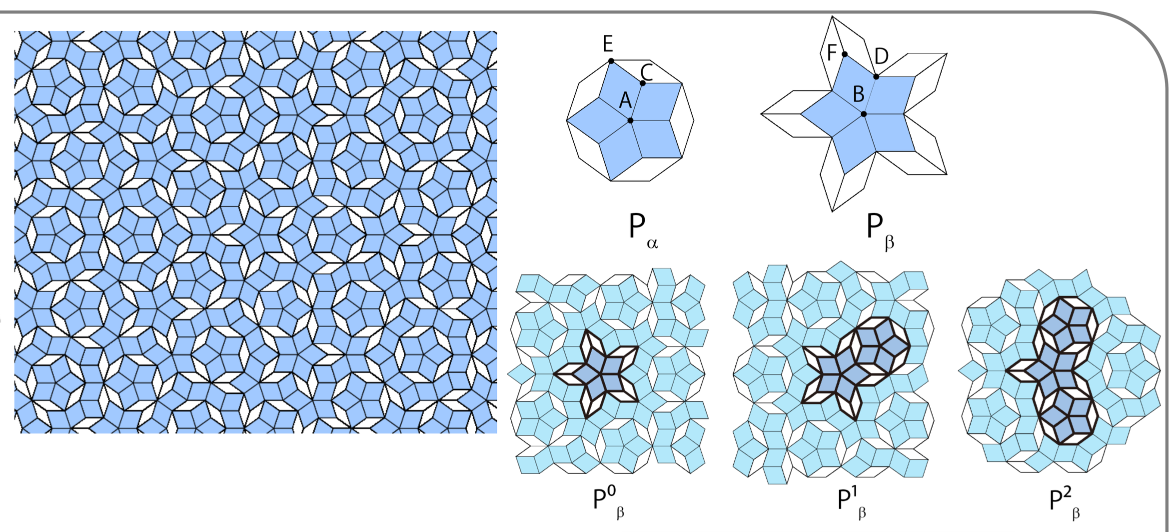
$\Sigma(\omega)$: Self-energy

ω dependency

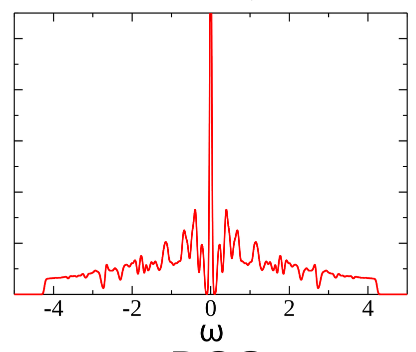
◆ Quasiperiodic lattice

Penrose lattice(2D)[5,6,7](C-model, V-model)

- Number of bonds different for each site
- Delta function like DOS(ω=0)
- Exact wave functions with no-correlation
  confined states



➡ How it would be in strongly correlated region?

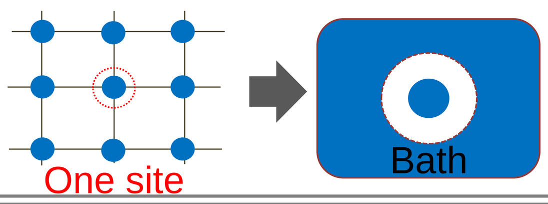


3.Methods

- Real-space Dynamical Mean Field Theory[8](RDMFT) + Continuous-time QMC[9]

Quantum fluctuation effect

Non perturbative approach



$\mathcal{G}_0^i(i\omega_n) \rightarrow$ Impurity Solver $\rightarrow G_{\rm loc}^i(i\omega_n) = G_{\rm imp}^i(i\omega_n)$

$\Sigma_i(i\omega_n) = \mathcal{G}_{0i}^{-1} - {G_{\rm loc}^i}^{-1}$

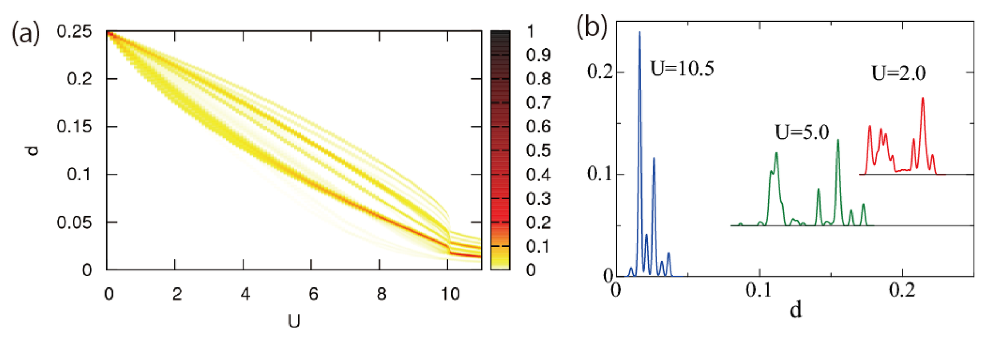
$G_{\rm loc}^i(i\omega_n) = G_{\rm latt}^{ii}(i\omega_n)$

${\mathcal{G}_0^i}^{-1}(i\omega_n) = {G_{\rm loc}^i}^{-1}(i\omega_n) + \Sigma_i(i\omega_n)$

4.Results

At Half-filling, 4181 sites

- Double occupancy (QMC)



Double occupancy

$d = \langle n_{f\uparrow} n_{f\downarrow}\rangle$

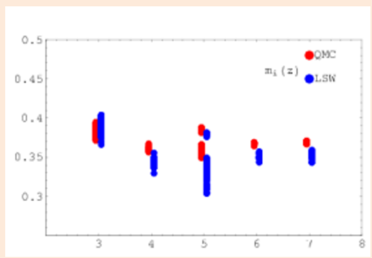
Renormalization factor

$z = \left[1 - \frac{\partial \mathrm{Re}\Sigma(\omega)}{\partial\omega}\Big|_{\omega=0}\right]^{-1}$

$\Sigma(\omega)$: Self-energy

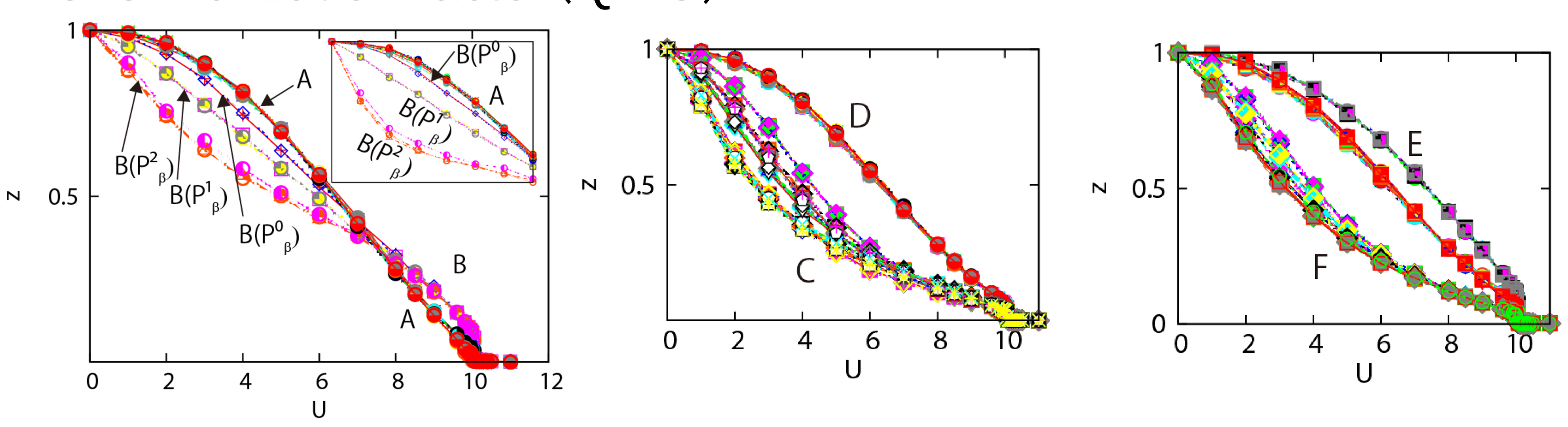
◆ Mott transition and quasiperiodicity

- Site-dependent renormalization
- Site-independent Mott transition
  Irrelevant to confined states, #bond
- 5 classes($U>U_c$):
  Coordination number 3 to 7



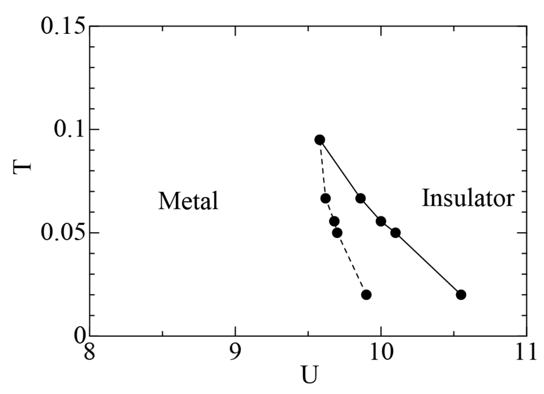
Heisenberg model
A. Jagannathan, et al.,
PRB **75**(21):212407 (2007)

- Renormalization factor (QMC)



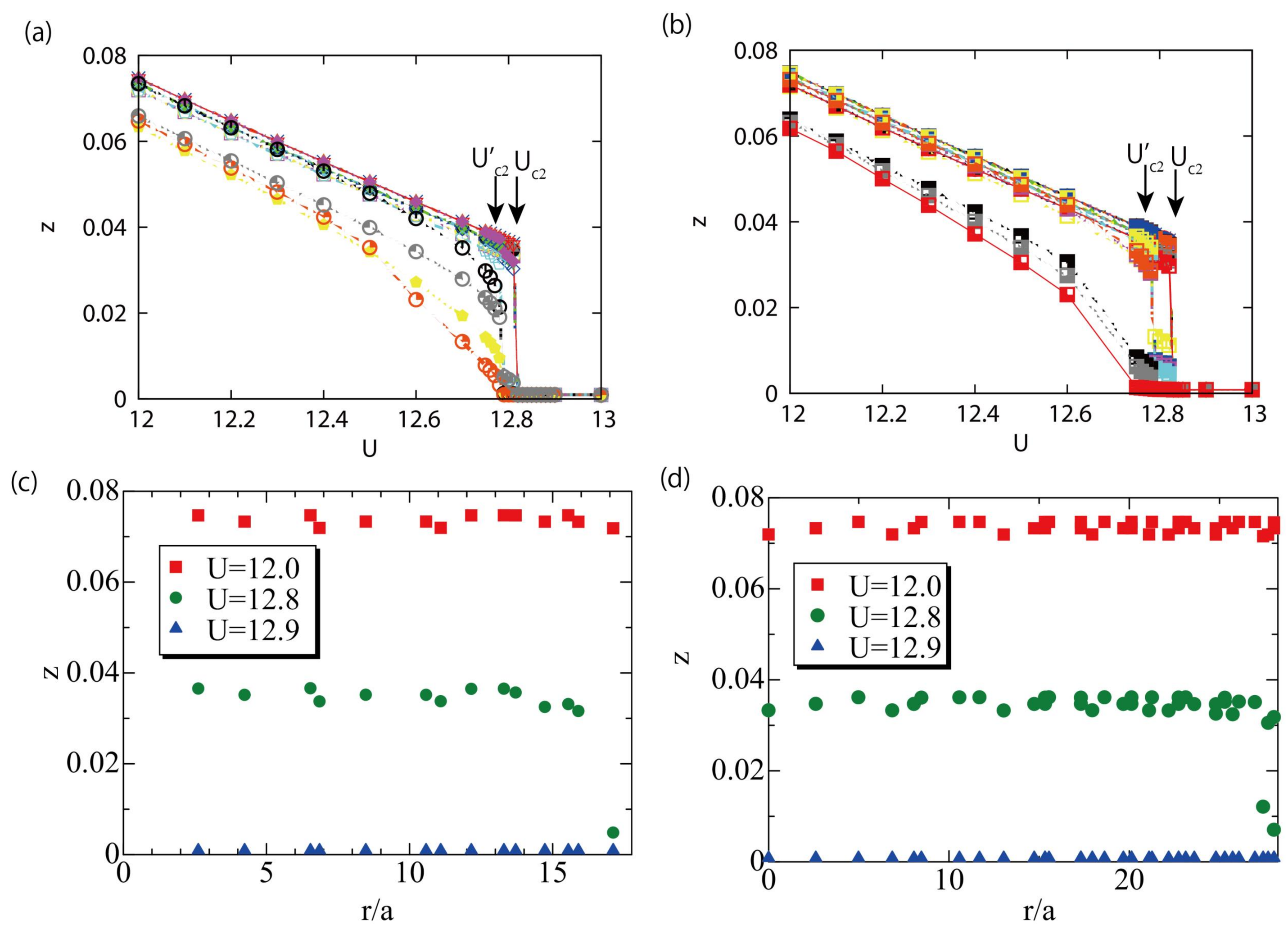
- The overlap structure effectively decreases hopping integrals between B and D sites in weak coupling

- Phase diagram



Critical end point: (U/D, T/D)~(9.5, 0.094)

- Effect of open boundary



Sites in edge experience transitions 2 times

With increasing system size

- Thickness of the edge: same
- Characteristic in quasicrystal system
  × square lattice

5.Conclusion

- Correlation effects in quasiperiodic system (RDMFT)
- Mott transition point: characteristic behavior
  Geometrical structure around the site

6.References

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