Single Hole and Two-Hole Doped Mott Antiferromagnets: A DMRG Study

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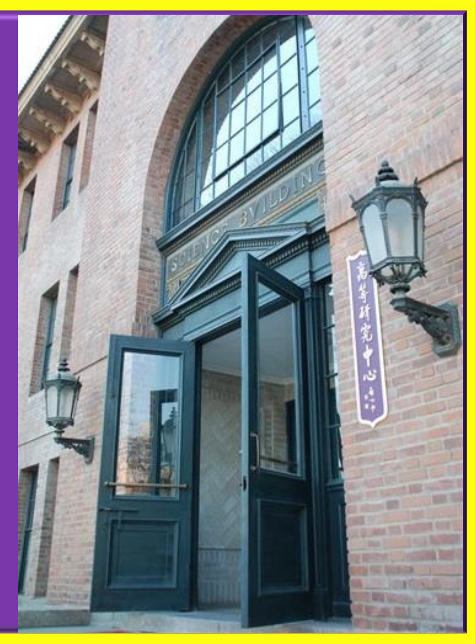
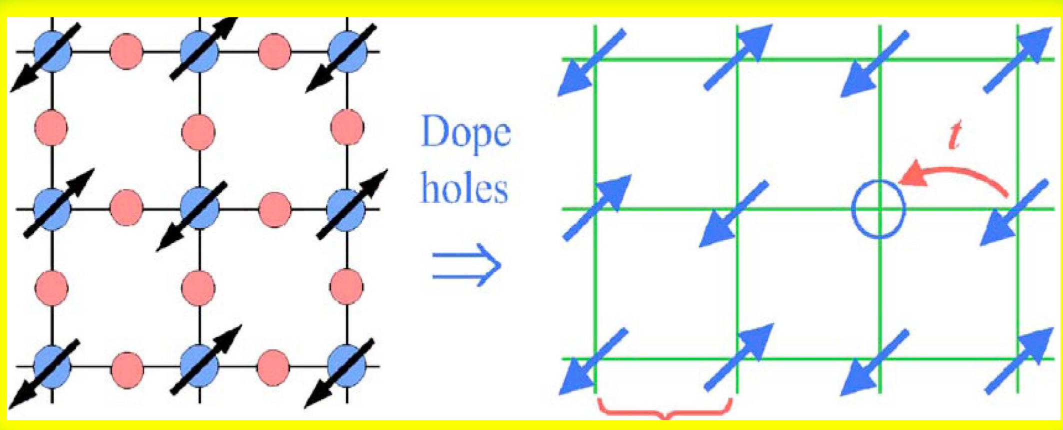


1. Background of Lightly Hole Doped Mott Insulators

The doped Mott insulator is generally believed to be a prototypical picture of many realistic strongly correlated systems notably high-Tc cuprates [1,2]. Important insights into Mott physics can be gained by lightly doped (e.g., single hole and two-hole doped) Mott insulators. It can tell us whether the quasiparticle picture is valid before high-temperature superconductivity sets in and the nature of pairing for doped charge carriers.



➢ **1-hole debate:**
- Spin Polaron Picture/ED (32 sites) → Quasiparticle;
- Phase Strings/Anderson Argument → Non-quasiparticle;
- Experimental Hints[3](ARPES/charge transport/STM) : Broad peak in EDC/nodal Zk=0/low T resistivity- insulator /localized charge state. → Non-quasiparticle;

➢ **2-hole pairing:**
- AFM spin fluctuation pairing "glue" vs. RVB picture

2. Method: Density Matrix Renormalization Group (DMRG) Algorithm

Numerical simulations are performed by standard DMRG method at T=0K. In our DMRG simulations, we keep up to m=5000 states in each block with up to 40 sweeps to get converged results. For the measurement of the ground-state energy and other observables, the total truncation error is of the order or less than 10^{-8} ~10^{-12}.

$$H_{t-J} = -t\sum_{\langle ij\rangle\sigma}\left(c^{\dagger}_{i\sigma}c_{j\sigma}+h.c.\right) + J\sum_{\langle ij\rangle}\left(\mathbf{S}_i\mathbf{S}_j - \frac{1}{4}n_i n_j\right)$$

- Square ladder($N=N_x\times N_y$), N_x=20~ 200, N_y= 1~5;
- J=1 as the unit of energy, t/J=2~10;
- Open boundary condition (OBC) in most cases.

constrained by $\sum_{\sigma} c^{\dagger}_{i\sigma}c_{i\sigma} \le 1$

Advantage:
- No exponential difficulty on the total sites in exact diagonalization (ED);
- No sign problem of quantum Monte Carlo (QMC).

Disadvantage:
- Exponentially difficulty with larger width or with periodical boundary conditions (PBC).

3. One-hole: Self-Localization of the Charge[4] & Destructive Quantum Interference

Evidence:

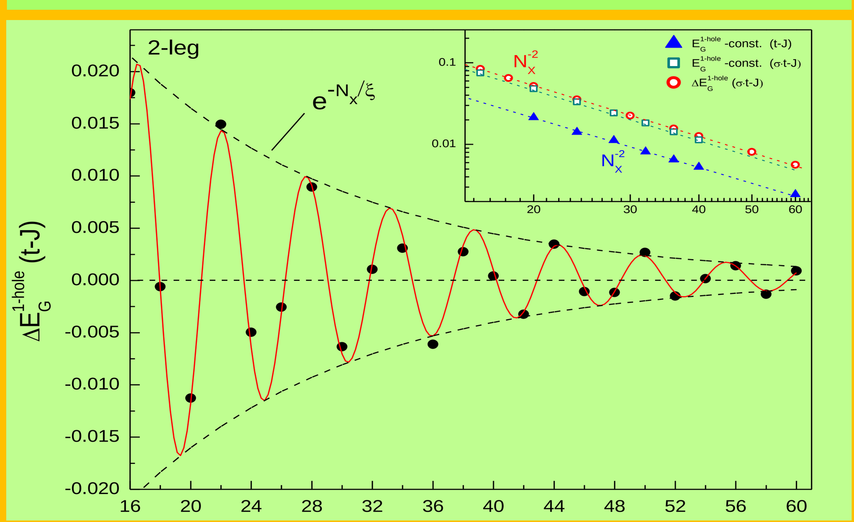
(1). Charge Energy:

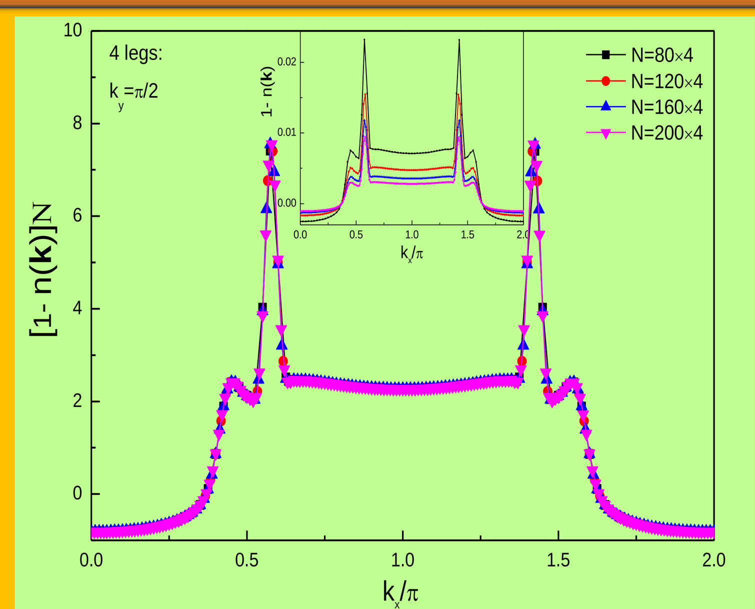
$$\Delta E_G^{1\text{-hole}} \equiv E_G^{1\text{-hole}}(anti-pbc) - E_G^{1\text{-hole}}(pbc)$$

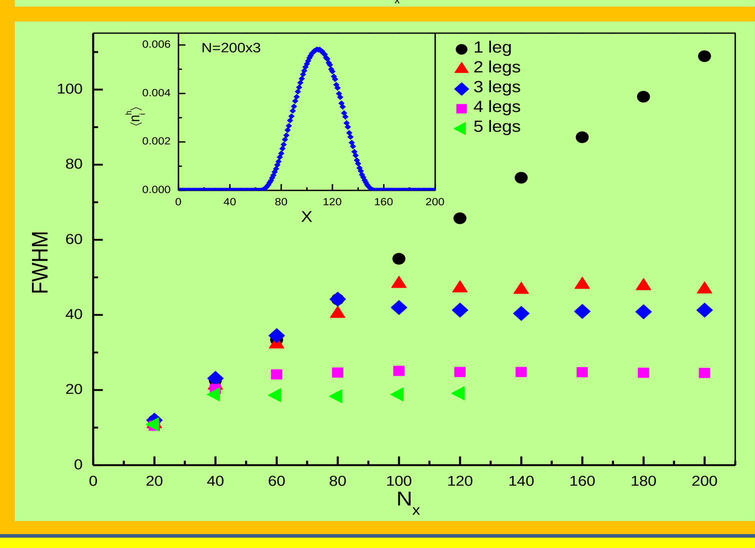
- Oscillates & Exponentially decay with N_x;

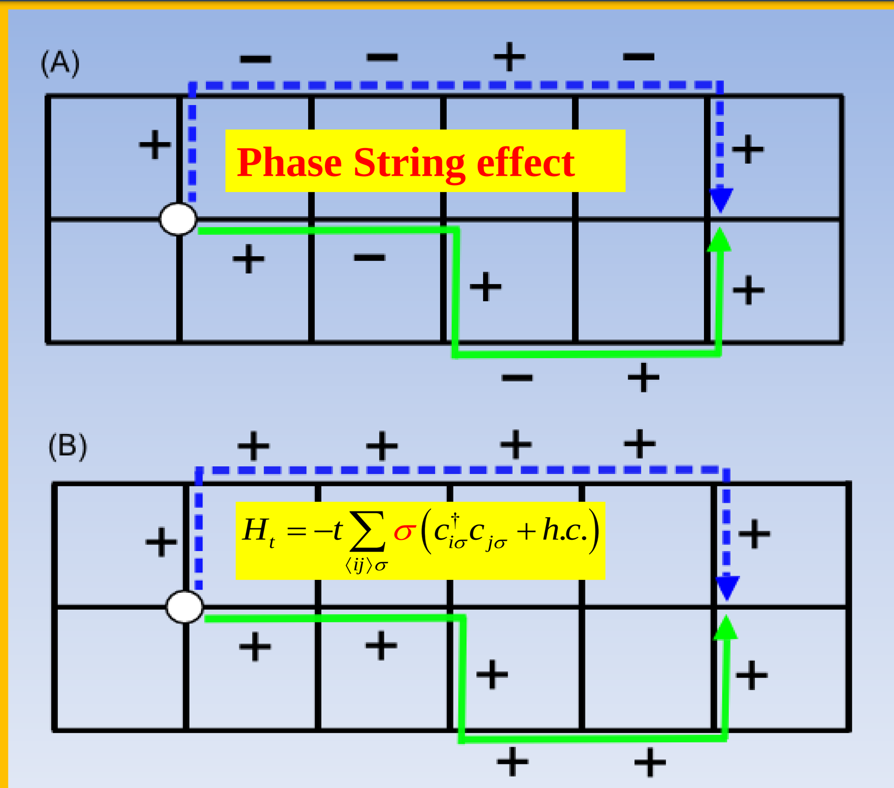
(2). Momentum Space Distribution:
- Vanishing of quasiparticle weight at the Fermi surface in the thermodynamic limit due to the scaling behavior 1-n(k)→[1-n(k)]N;

(3). Real space distribution:
- Saturation of the hole density distribution.





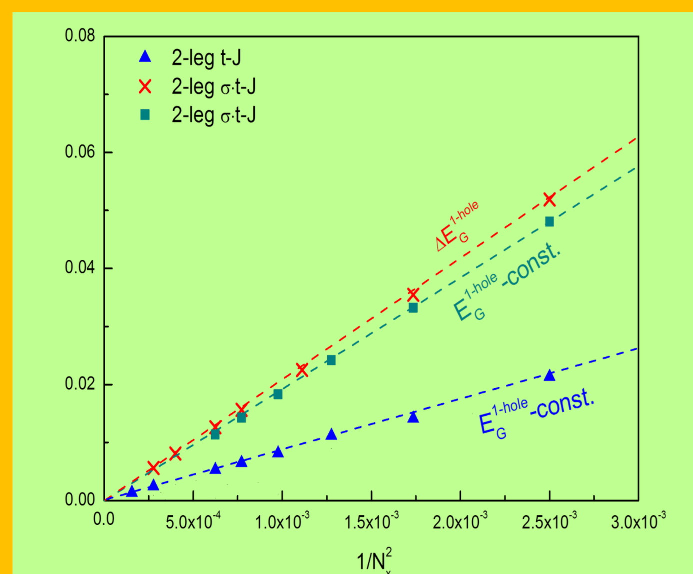


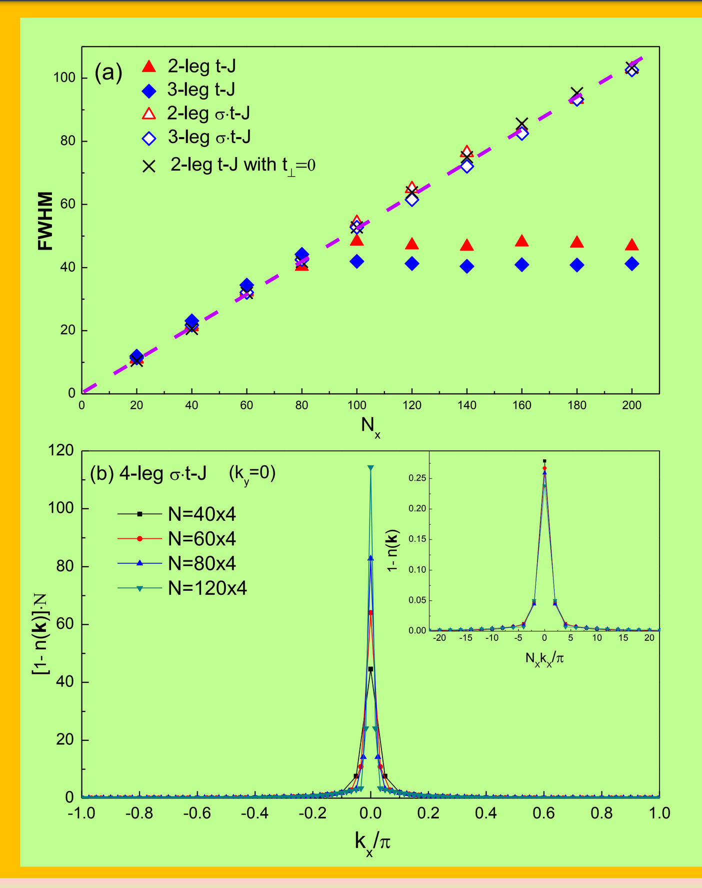


Theorem: For the single hole doped t-J model in a bipartite lattice, the propagation of the hole is superposition of quantum amplitudes of all paths, with each path carrying a sign sequence known as the phase string [5-7]. Then the destructive quantum interference suppress the forward scattering of the hole, leading to self-localization of the charge.

Confirm this explanation:

(1). Turn off the interference;
(2). Turn off phase strings by introducing σ·t-J model .



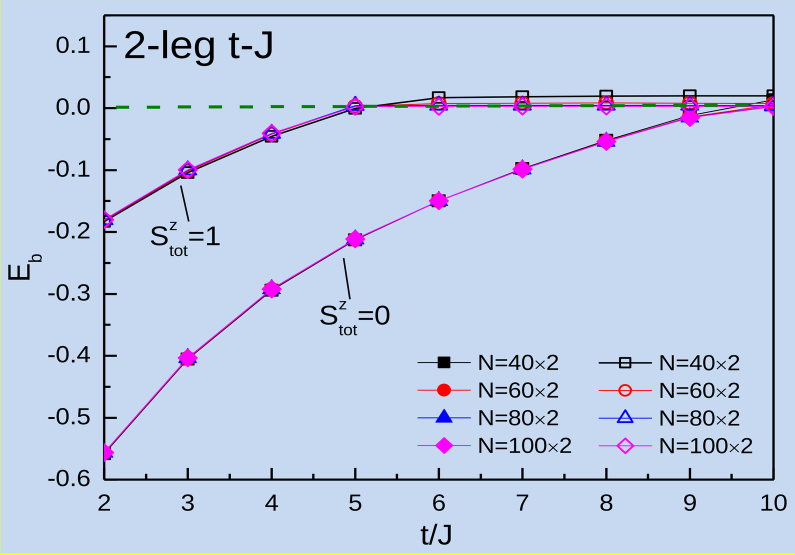


(1). Charge Energy: No oscillation & Power-law decay;
(2). Momentum Space Distribution: Finite quasiparticle weight in the thermodynamic limit due to the scaling behavior $k_x\to k_x\cdot N_x$;
(3). Real space distribution: No saturation of the hole density distribution.

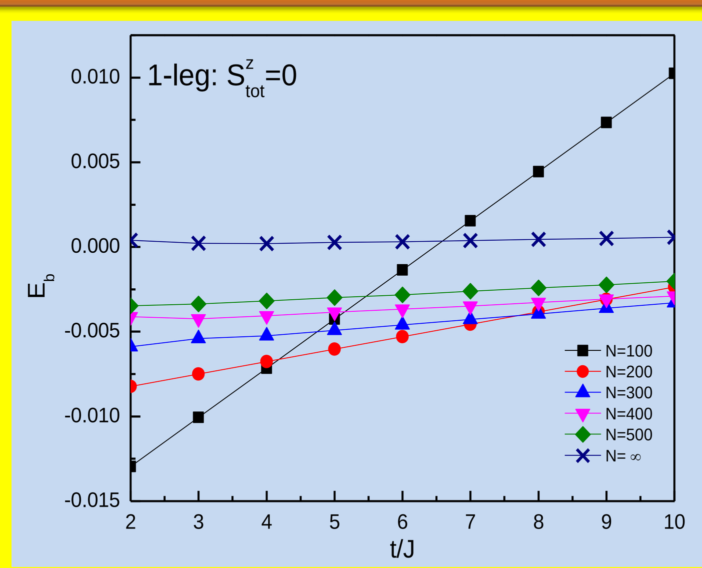
4.Two-hole Binding[8]: Short-ranged Spin-Spin Correlation & Suppressed Coherence of Charge

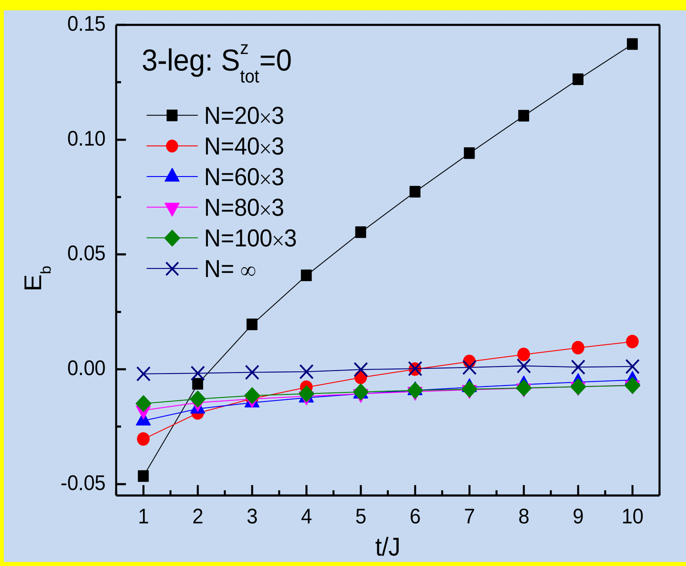
Binding Energy:
$E_b=(E_2-E_0)-2(E_1-E_0)$

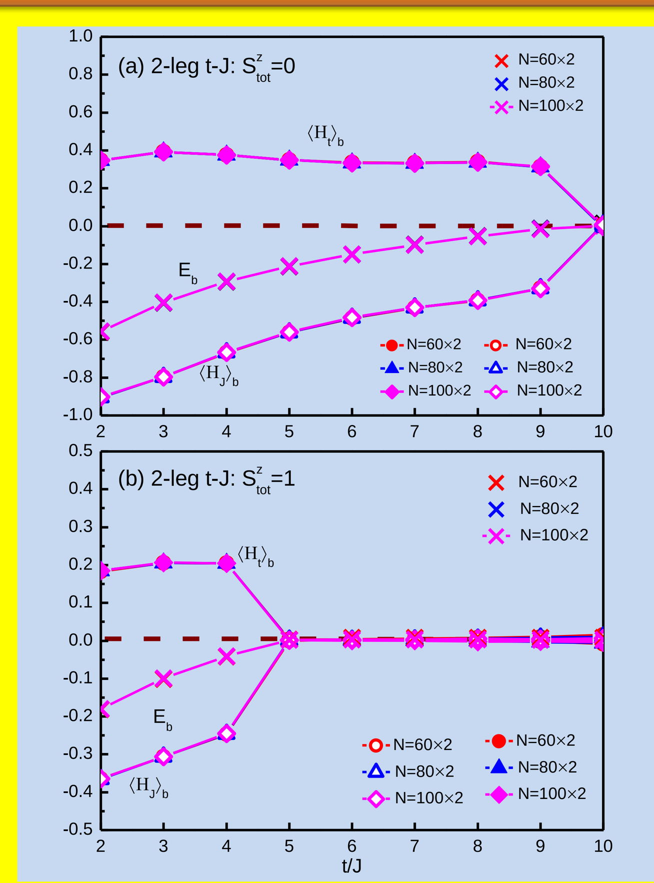
$E_b<0$	Binding of two holes
$E_b\approx 0$	No binding
$E_b>0$	Repulsion of two holes

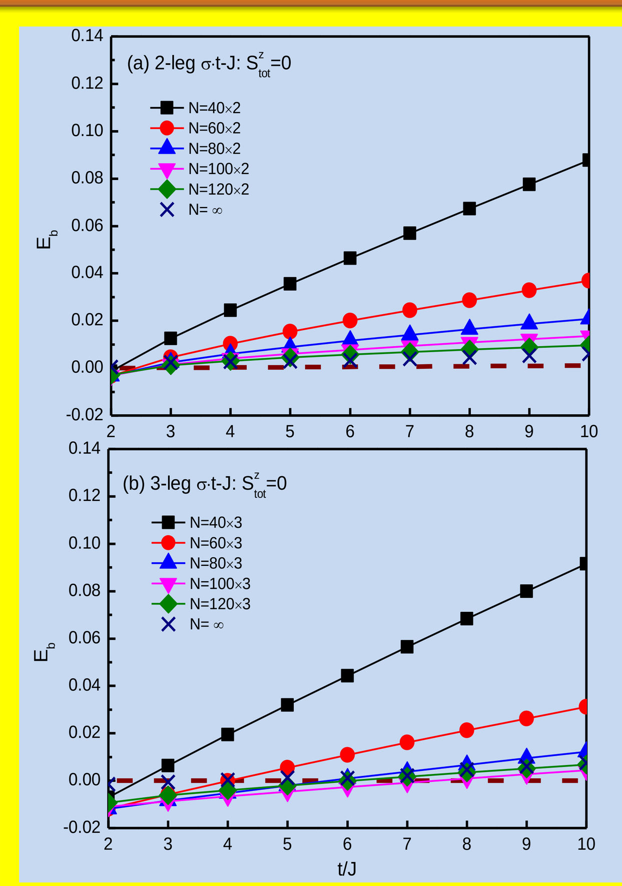


Leg #	Spin Excitation	Binding Energy
Even	Gapped	$E_b<0$
Odd	Gapless	$E_b\approx 0$



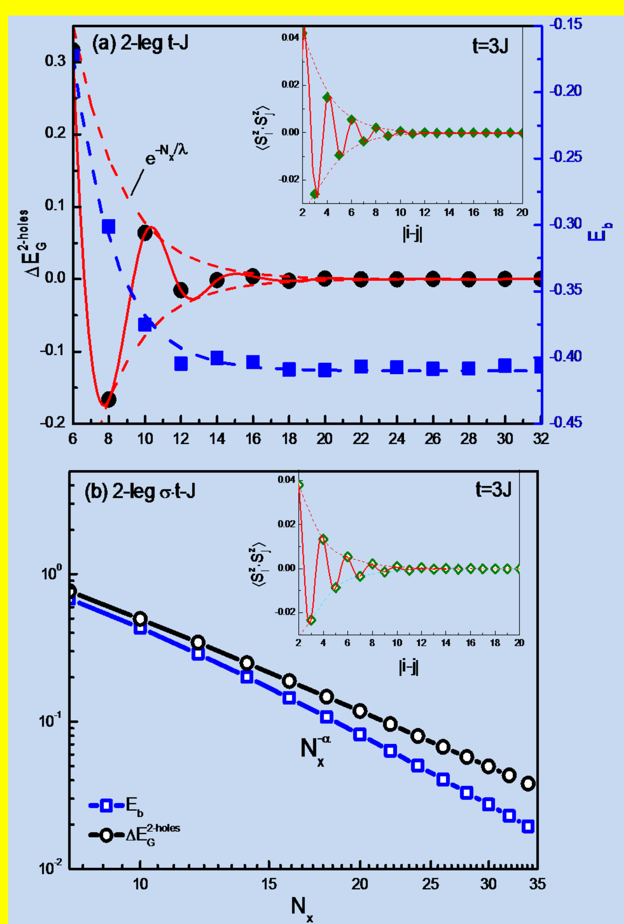




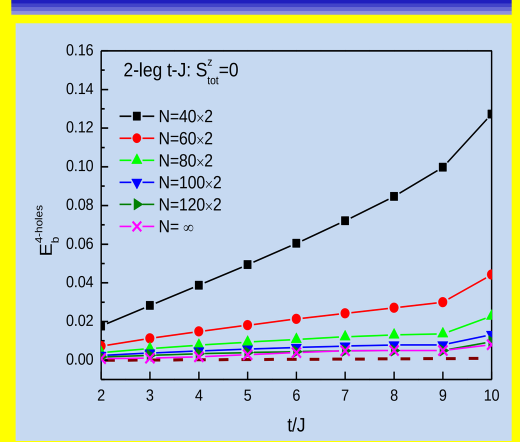


Separated Contribution:
- Driving Force of pairing: Superexchange interaction .
- No strong binding of two holes in σ·t-J model
  → the presence of spin gap is not a sufficient condition.

Pairing Mechanism
- Short-range spin-spin correlation (J-term);
- Suppressed coherence of charge (t-term);



The spin backgrounds of two-hole doped t-J and σ-t-J model are the same. However, the destructive interference of phase strings picked up by the hole from different paths in t-J model suppresses the coherence of the hole, and leads to the strong binding of two holes. But no "droplet" state for four holes.



Summary

Conclusion:

- **Single hole - Self-localizaion of the charge.**
  Localization Mechanism: Destructive quantum interference of different paths.
- **Two holes - Strong binding of two holes.**
  Pairing Mechanism: Short-ranged spin pairing & Suppressed forward charge scattering.

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