Superconductivity in bilayer t-J model: A few variational Monte Carlo results

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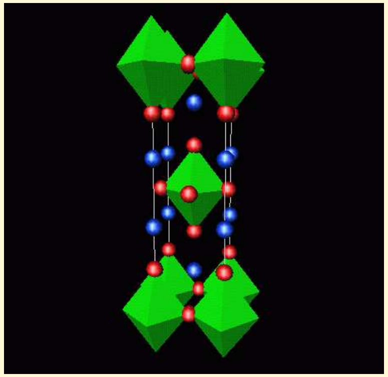
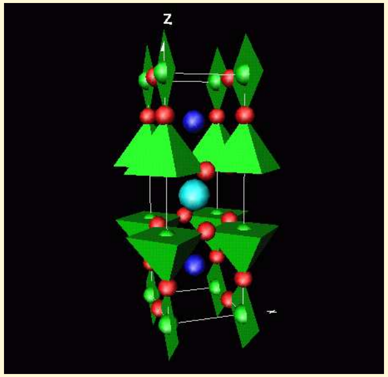
Cuprates



LSCO

YBCO



- Theoretical studies on cuprates - mainly the focus is on a single CuO_2 layer.

- Other important factors to consider - crystal structure details, intrinsic disorder, interlayer couplings etc.

- Bilayer cuprates (e.g. YBa_2CuO_{6+x}) - Interlayer couplings.

Interlayer hopping

Bilayer band splitting (ARPES & ab initio study)	
$t_\perp(\mathbf{k}) = \frac{t_\perp}{4}\left[cos(k_x a) - cos(k_y a)\right]^2$	$t_\perp \sim 0.1 - 0.15$ **eV** **(**$t \sim 0.44$ **eV)**

Interlayer exchange

$J_\perp \sim 0.01$ **eV**
($J \sim 0.13$ **eV)**

- **How the interlayer couplings affect the properties of bilayers?**

Bilayer t-J model

- Variational Monte Carlo
- Pairing symmetry, magnetic and superconducting correlations, coexistence of AF & SC

Interlayer pair-tunneling (ILPT) in bilayer

- Grand canonical VMC
- Energy due to ILPT

Superconductivity in bilayer t-J model

The Model

$$\mathcal{H} = -t \sum_{\langle i,j\rangle\sigma} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + H.c. \right) - t_{\perp} \sum_{\langle i,k\rangle\sigma} \left(c^{\dagger}_{i\sigma} c_{k\sigma} + H.c. \right) + J \sum_{\langle i,j\rangle} \left(\mathbf{S_i}.\mathbf{S_j} - \frac{1}{4} n_i n_j \right) + J_{\perp} \sum_{\langle i,k\rangle} \left(\mathbf{S_i}.\mathbf{S_k} - \frac{1}{4} n_i n_k \right)$$

The operators act in a subspace of no doubly occupied site.

- **Represents bilayer cuprates like, YBa_2CuO_{6+x} (YBCO), $Bi_2Sr_2CaCu_2O_{8+x}$ (Bi2212) etc.**

Parameter values (from exp and theory)

$$\boxed{t_{\perp}/t = 0.05 - 0.20,\ J/t = 0.35,\ J_{\perp}/t = 0.03 - 0.10}$$

Variational Monte Carlo

- ☺ Treats strong correlations exactly, applicable for wide range of parameter values, no sign problem.
- ☹ Biased by the choice of variational wavefunction

Formalism

- Choose the trial wavefunction,

$$|\Psi_{var}\rangle \equiv |\Psi_{var}(\alpha)\rangle, \quad \alpha \text{ is the variational parameter}$$

- Transform $|\Psi_{var}\rangle$ into real space representation

$$|\Psi_{var}\rangle = \sum_R C(R)|R\rangle$$

$|R\rangle = c^\dagger_{i_1\uparrow} \dots c^\dagger_{i_P\uparrow} c^\dagger_{j_1\downarrow} \dots c^\dagger_{j_P\downarrow}|0\rangle$ is an electronic configuration in real space.

- **Expectation value**

$$\langle \hat{A} \rangle = \frac{\langle \Psi_{var} | \hat{A} | \Psi_{var} \rangle}{\langle \Psi_{var} | \Psi_{var} \rangle}$$
$$= \boxed{\sum_R P(R) \frac{\langle \Psi_{var} | \hat{A} | R \rangle}{C^*(R)}} \qquad P(R) = \frac{|C(R)|^2}{\sum_{R'} |C(R')|^2}$$

- **Exact summation is not possible. Use Monte Carlo.**
- **Generate a Markov chain of M ($\ll N$) configurations $|R_1\rangle, |R_2\rangle, \ldots, |R_M\rangle$ according to weights $P(R)$. The sum is approaximated by,**

$$\langle \hat{A} \rangle \approx \langle \hat{A} \rangle_M = \frac{1}{M} \sum_{i=1}^{M} \frac{\langle \Psi_{var} | \hat{A} | R \rangle}{C^*(R)}$$

Wavefunction optimization

- **Calculate energy as a function of α**

$$E_{var}(\alpha) = \frac{\langle \Psi_{var}(\alpha)|\hat{H}|\Psi_{var}(\alpha)\rangle}{\langle \Psi_{var}(\alpha)|\Psi_{var}(\alpha)\rangle}$$

- **Minimize $E_{var}(\alpha)$. Obtain optimized $|\Psi_{var}\rangle$.**

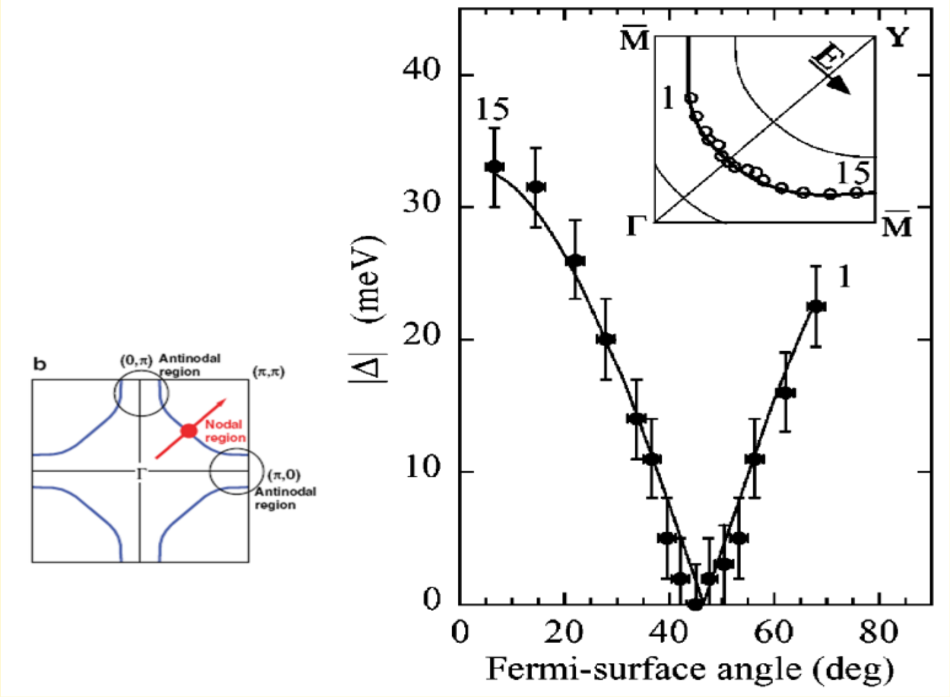
$$E_{min} = E_{var}(\tilde{\alpha}), \quad |\Psi_0\rangle = |\Psi_{var}(\tilde{\alpha})\rangle$$

- **Calculate correlation functions in the optimized wavefunction,**

$$\langle \hat{A}\hat{B}\rangle = \frac{\langle \Psi_0|\hat{A}\hat{B}|\Psi_0\rangle}{\langle \Psi_0|\Psi_0\rangle}$$

Pairing symmetry

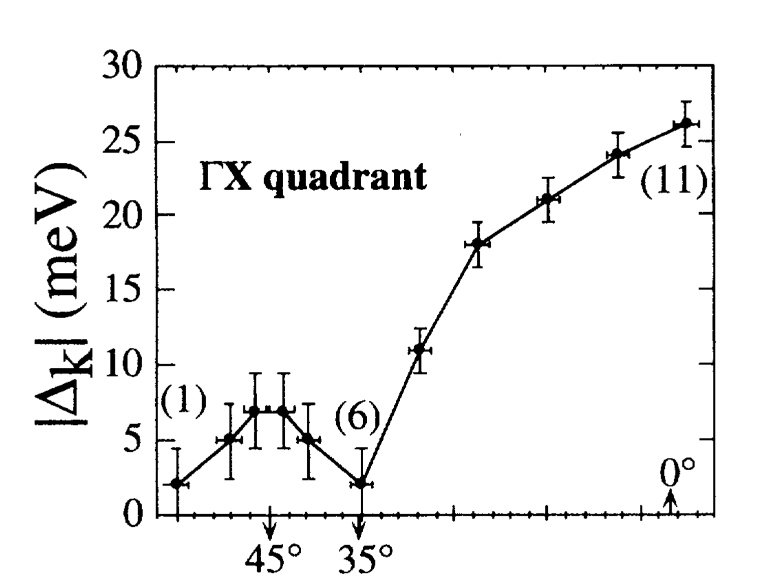
- In cuprates, superconducting pairing symmetry is d-wave ($\Delta_{\mathbf{k}} = \Delta_d(\cos k_x - \cos k_y)$) (ARPES and other exp)



- Supported by numerical and analytical studies of two dimensional (2D) Hubbard and t-J model.

Contradictory reports for bilayered cuprates

- **Could be an extended s-wave with eight line nodes.**
  (Ding et al, PRL 74, 2784 (1995), Vobornik et al, Physica C 317, 589 (1999), Zhao, PRB 75, 140510(R) (2007))



- **Supported by SBMFT study of a bilayer t-J model.**
  (P. A. Lee et al, J. Phys. Chem. Solids 56, 1633 (1995)).

Variational Monte Carlo

- We consider as the variational wavefunction, the Gutzwiller projected BCS state,

$$\boxed{|\Psi_{var}\rangle = \mathcal{P}_G \left(\sum_{\mathbf{k}} \varphi(\mathbf{k}) c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} \right)^{N/2} |0\rangle}$$

with $\varphi(\mathbf{k}) = \frac{\Delta_{\mathbf{k}}}{(\varepsilon_{\mathbf{k}}-\mu)+\sqrt{(\varepsilon_{\mathbf{k}}-\mu)^2+\Delta_{\mathbf{k}}^2}}$

Pairing symmetries considered

(a) $\Delta_{\mathbf{k}} = \Delta_d \left(\cos k_x - \cos k_y\right)$ (d-wave)
(b) $\Delta_{\mathbf{k}} = \Delta_{\parallel} \left(\cos k_x - \cos k_y\right) + \Delta_{\perp} \cos k_z$ ($d + d_z$-wave) (would give eight nodes)
(c) $\Delta_{\mathbf{k}} = \Delta_{\parallel} \left(\cos k_x - \cos k_y\right) + \Delta_{\perp}(1 - \cos k_z)$

Some numerical details

Lattice size=$8 \times 8 \times 2$**.**

Parameter values: $(t_\perp/t, J_\perp/t) = (0.05, 0.10)$**,** $(0.20, 0.10)$**,** $(0.20, 0.03)$**.** $J/t = 0.35$**.**

Monte Carlo sweeps: $10^6 - 10^7$ **for calculation of expectation values.**

Paring symmetry (c): energy always higher - discarded.

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Paring symmetry (b): have lower energy only at $x = 0$ and $(t_\perp, J_\perp) = (0.05t, 0.10t)$.

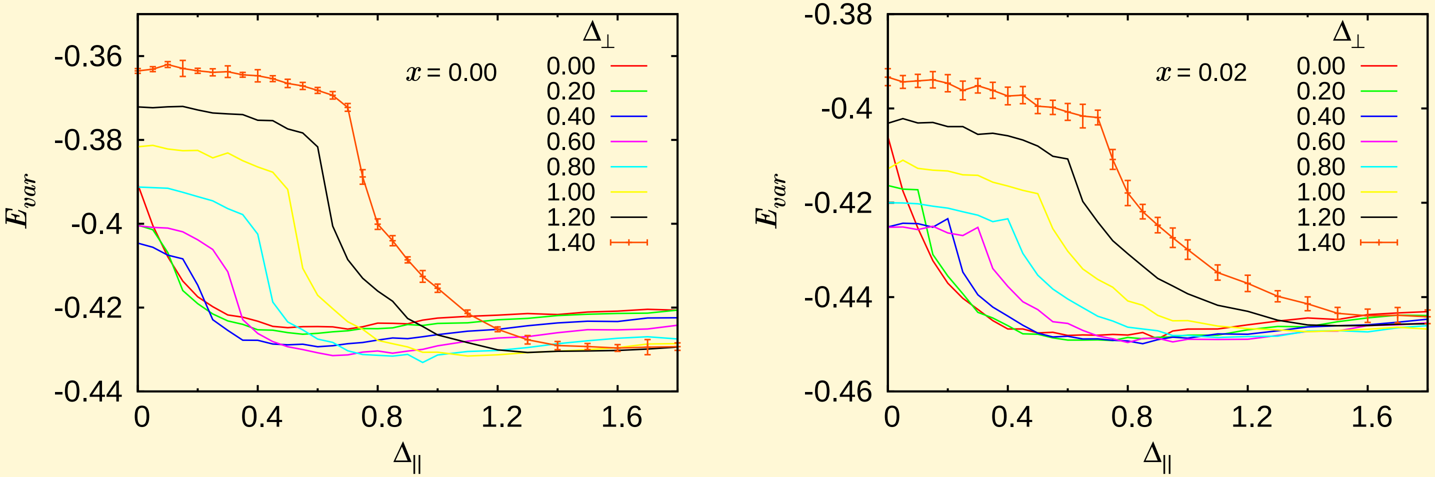

Fig: Energy of the $(d + d_z)$-wave state

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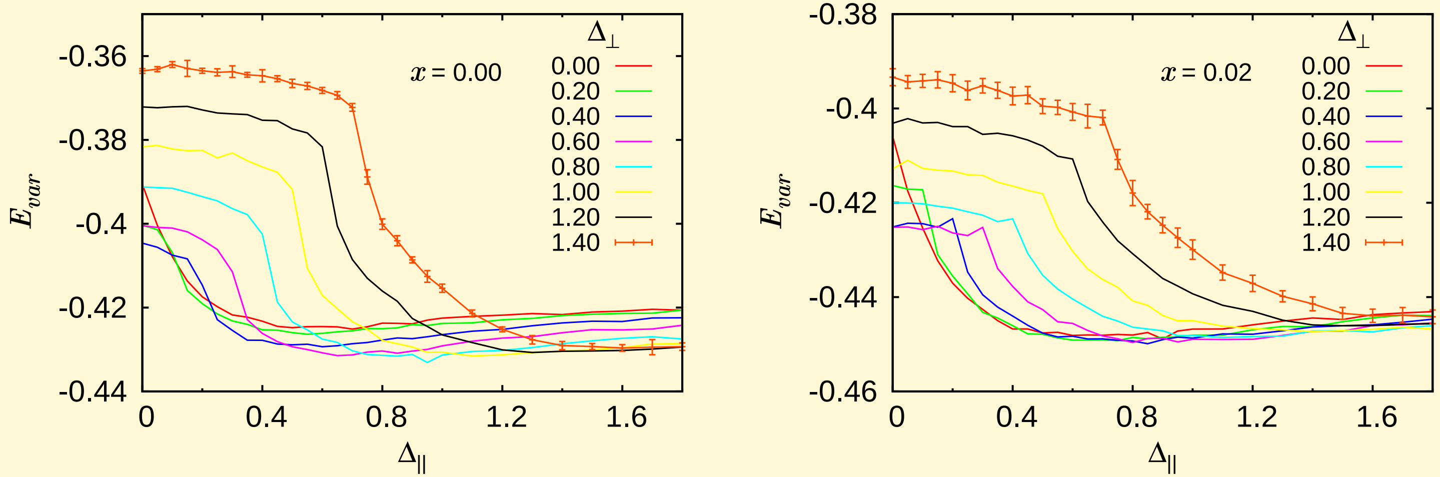
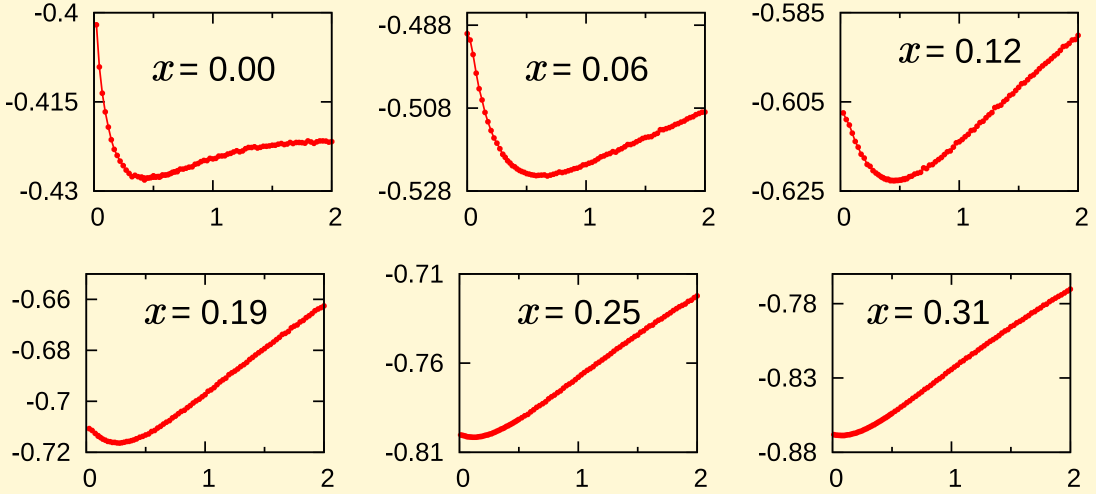


Fig: Energy of the $(d + d_z)$-wave state

Paring symmetry (a): The d-wave state yields lowest energy in all other cases.

Energy of the d-wave state



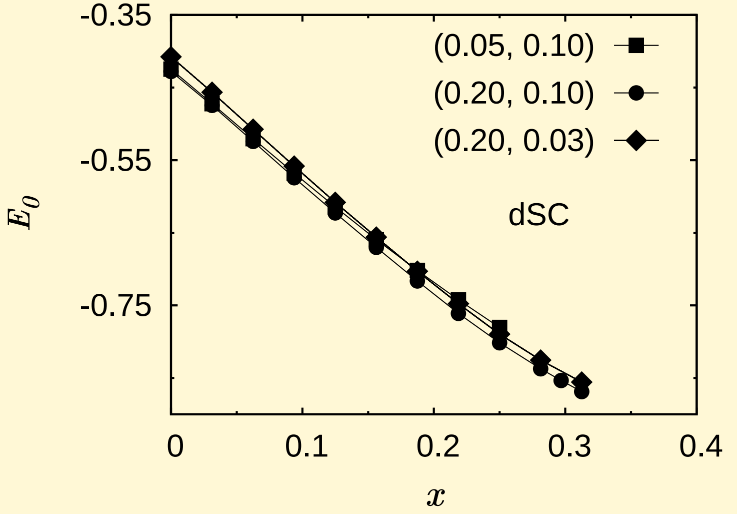
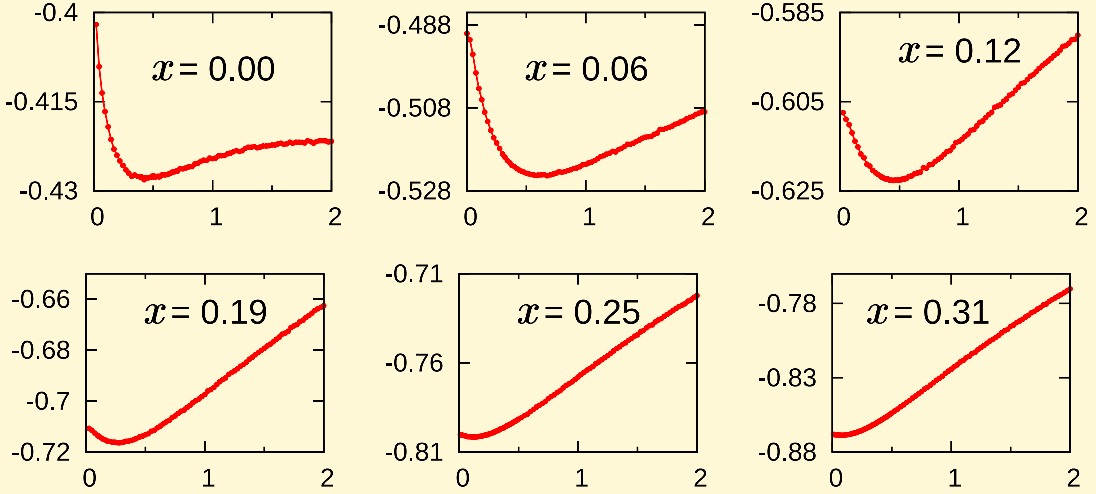


Fig: Variational energy of the d-wave state at various x.

$(t_\perp, J_\perp)$ = (0.20, 0.10).

Fig: Optimal energy, E_0 vs x.



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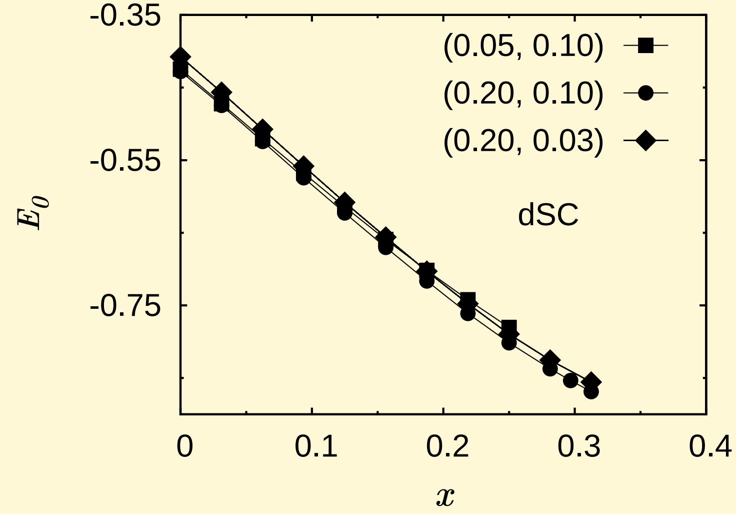
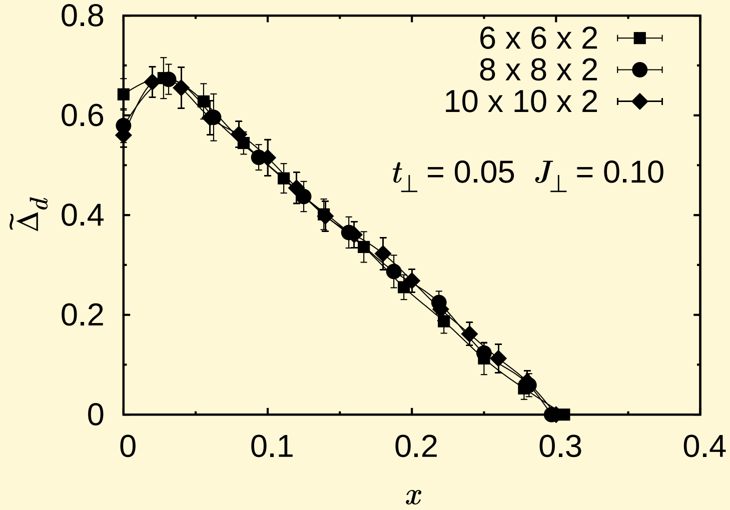
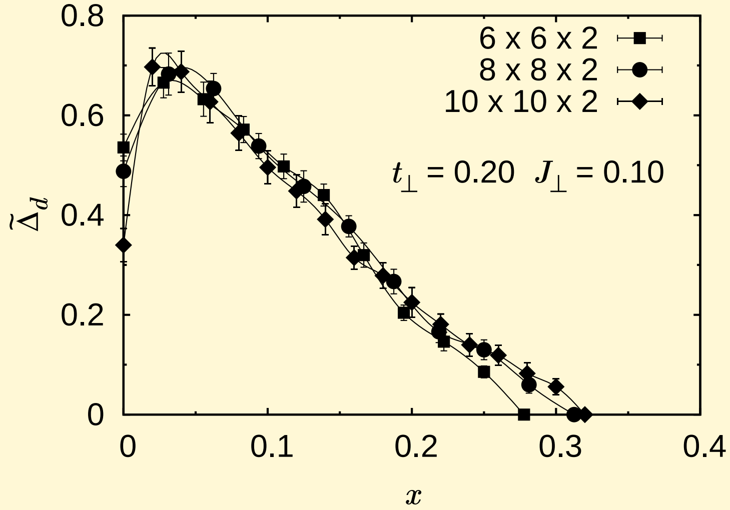


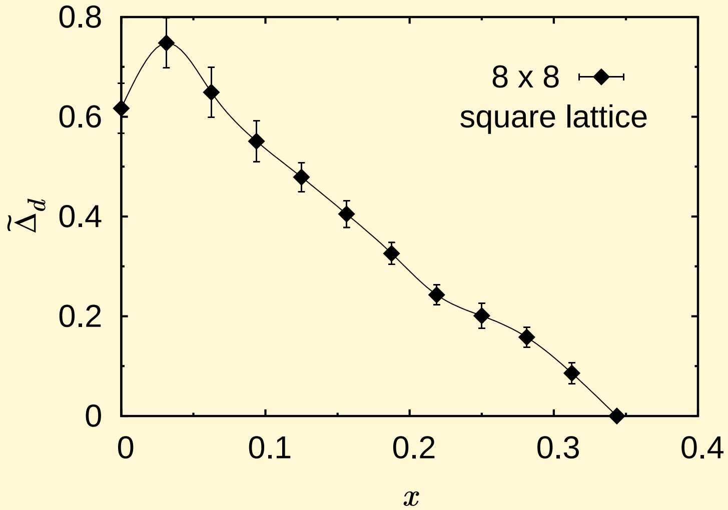
Fig: Optimal energy, E_0 vs x.

Conclusion: Favourable pairing symmetry in bilayer for experimentally relevant parameter values is d-wave.

Doping dependence of the optimal gap parameter







Week magnetic correlations

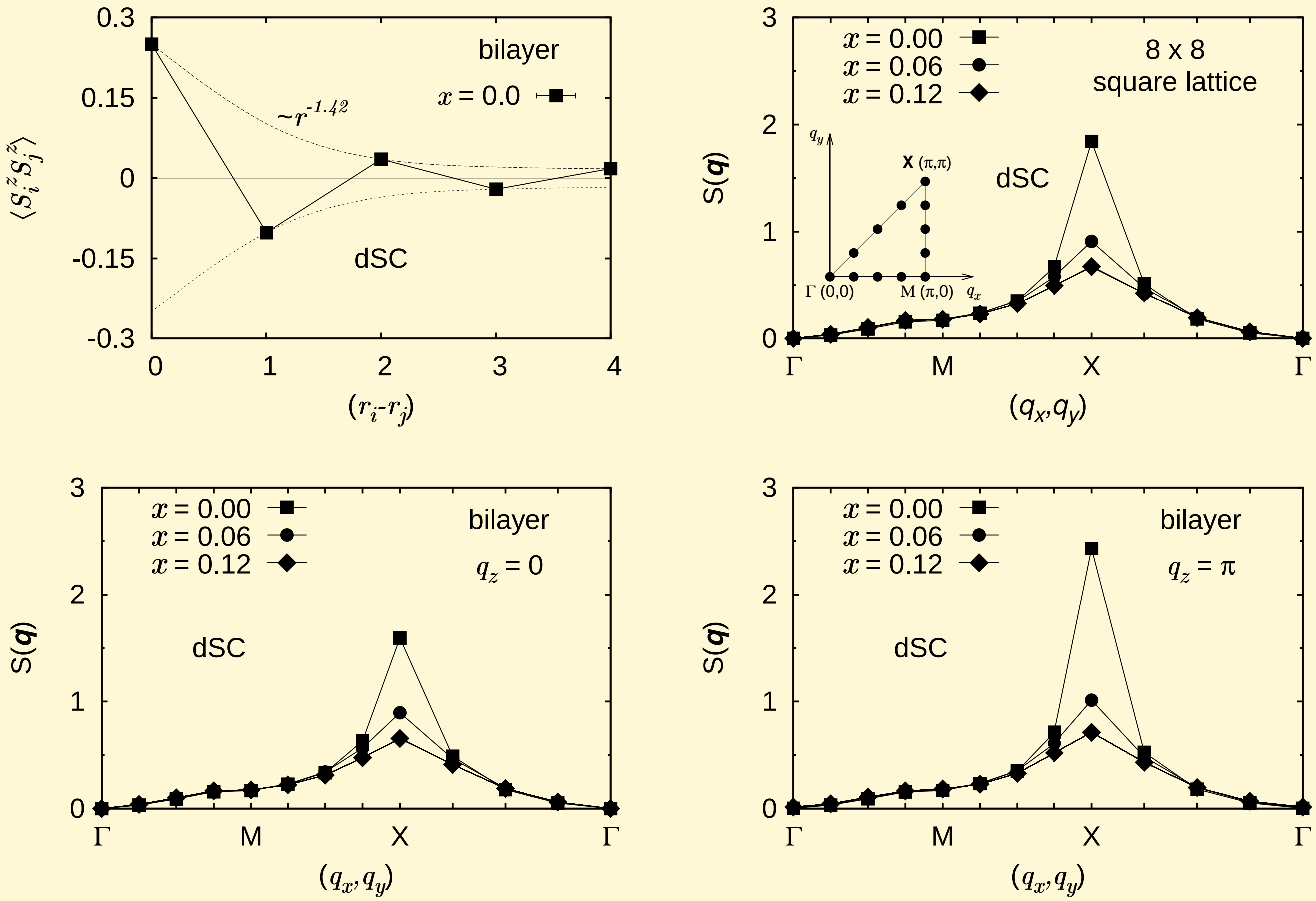


Fig: Spin correlations, $\langle S_i^z S_j^z \rangle$ and spin structure factor, $S(\mathbf{q}) = \sum_{ij} e^{-\mathbf{q}.(\mathbf{r}_i - \mathbf{r}_j)}/N_s$ in the d-wave state.

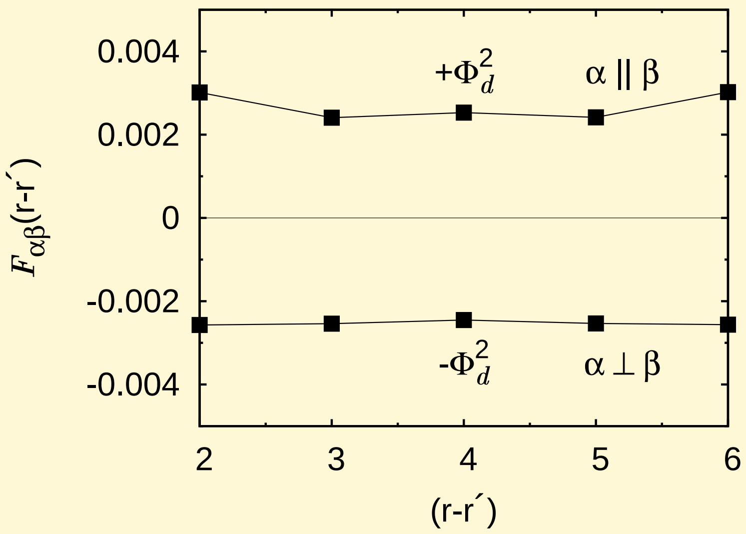
Superconducting correlations

- **SC pair-pair correlation function,**

$$F_{\boldsymbol{\alpha},\boldsymbol{\beta}}(\mathbf{r}-\mathbf{r}') = \left\langle B^{\dagger}_{\mathbf{r}\boldsymbol{\alpha}} B_{\mathbf{r}'\boldsymbol{\beta}} \right\rangle$$

$B^{\dagger}_{\mathbf{r}\boldsymbol{\alpha}} = \frac{1}{2}(c^{\dagger}_{\mathbf{r}\uparrow} c^{\dagger}_{\mathbf{r}+\boldsymbol{\alpha}\downarrow} - c^{\dagger}_{\mathbf{r}\downarrow} c^{\dagger}_{\mathbf{r}+\boldsymbol{\alpha}\uparrow})$ **creates an electron pair at bond** $(\mathbf{r}, \mathbf{r}+\alpha)$**.** α **and** β **are unit vectors** $\hat{x}$**,** $\hat{y}$**, or** $\hat{z}$**.**

- **SC order parameter,** $F_{\boldsymbol{\alpha},\boldsymbol{\beta}}(\mathbf{r}-\mathbf{r}') \rightarrow \pm{\Phi_d}^2$ **for large** $|\mathbf{r}-\mathbf{r}'|$**,** $+$ **(**$-$**) correspond to** $\alpha \parallel$ **(**$\perp$**) to** β **(for planar** α**,** β**).**



Superconducting order parameter

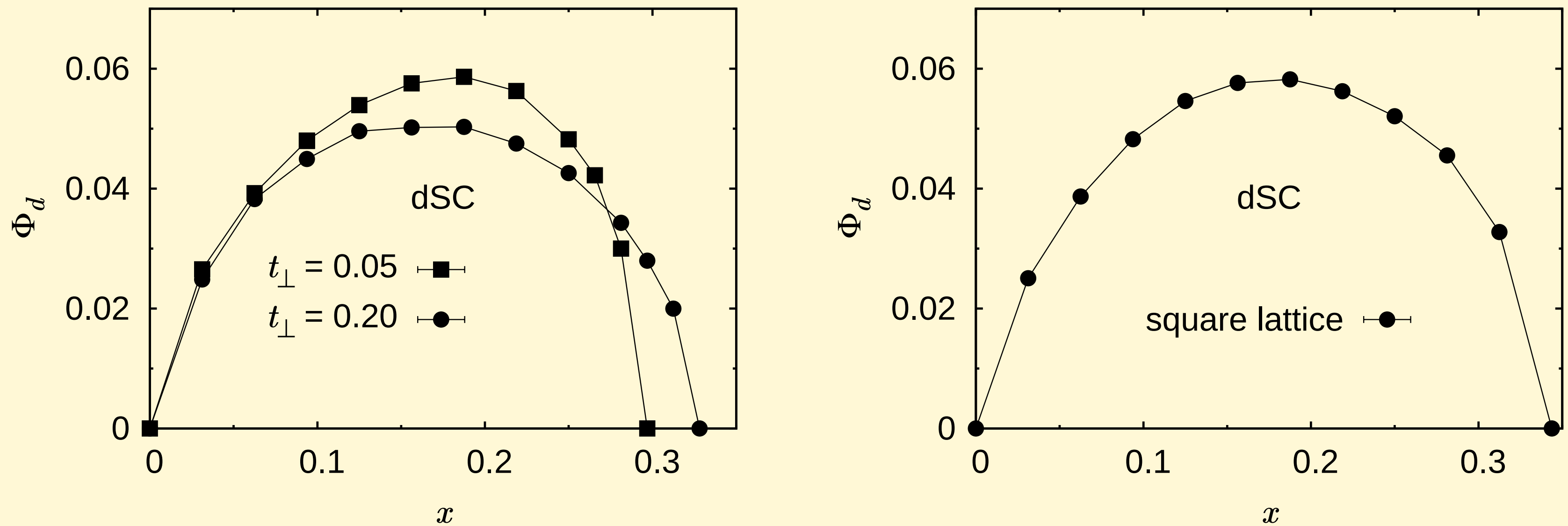


Fig: SC order parameter corresponding to planar correlations ($J_\perp = 0.10t$).

Interplanar correlations are negligibly small

Coexistence of AF & SC

- **Interplay of SC and antiferromagnetism (AF) order has been an important issue in cuprates.**

- **In the t-J model in 2D, there is evidence for coexistence.**

- **What is the scenario in bilayer? How the coexisting AF order affect SC correlations?**

We consider a wavefunction with both SC and AF orders,

$$\boxed{|\Psi_{var}\left(\Delta_{SC}, \Delta_{AF}\right)\rangle = \mathcal{P}_G \mathcal{P}_N \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} d^{\dagger}_{\mathbf{k}\uparrow} d^{\dagger}_{-\mathbf{k}\downarrow} \right) |0\rangle}$$

$$\frac{v_{\mathbf{k}}}{u_{\mathbf{k}}} = \frac{\Delta_{\mathbf{k}}}{(\mp E_{\mathbf{k}} - \mu) + \sqrt{(\mp E_{\mathbf{k}} - \mu)^2 + \Delta_{\mathbf{k}}^2}}, \qquad E_{\mathbf{k}} = \sqrt{\varepsilon_{\mathbf{k}}^2 + \Delta_{AF}^2}$$

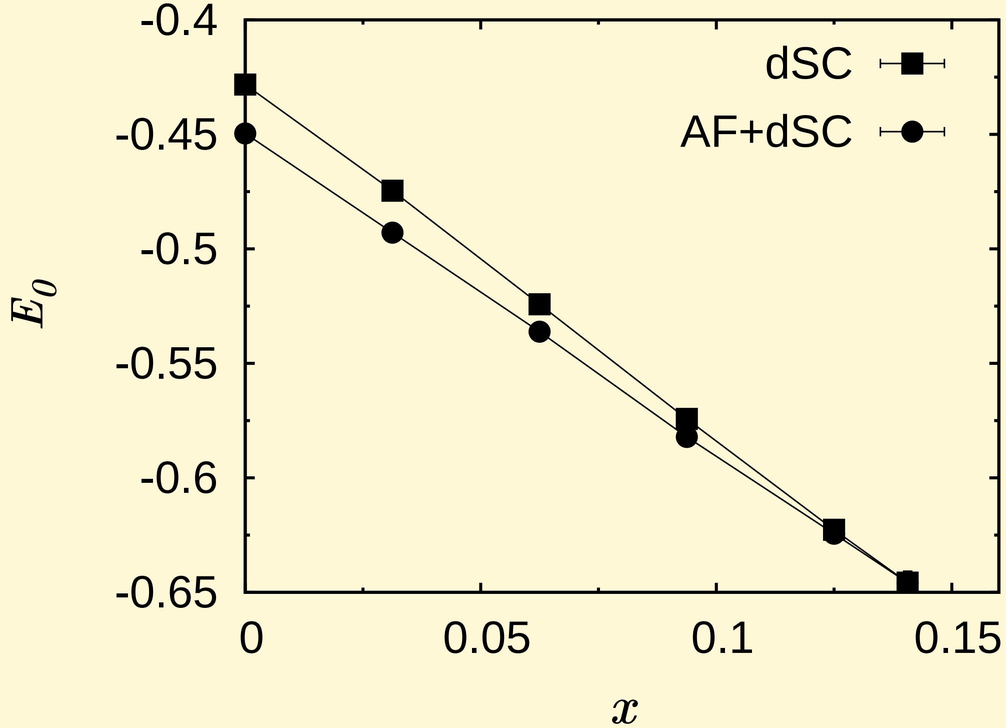
$d^{\dagger}_{\mathbf{k}\sigma} \rightarrow$ **diagonalizes the AF Hartree-Fock Hamiltonian.**

Variational parameters - Δ_{SC} and Δ_{AF}

Phases described by the wavefunction

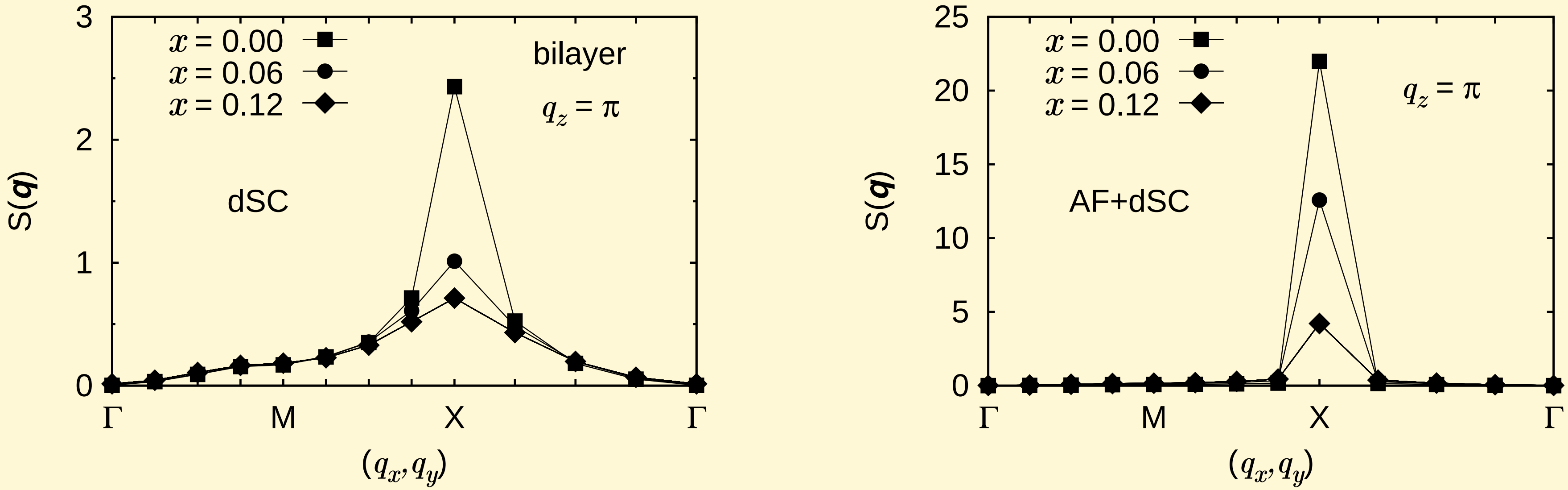
- **AF phase for $\Delta_{AF} \neq 0$ and $\Delta_{SC} \rightarrow 0$.**
- **SC phase for $\Delta_{AF} = 0$ and $\Delta_{SC} \neq 0$**
- **Coexisting AF - SC phase for Δ_{AF}, $\Delta_{SC} \neq 0$**
- **Normal state for Δ_{AF}, $\Delta_{SC} = 0$**

Optimized energy for the pure d-wave state (dSC) and the coexisting state (AF+dSC)



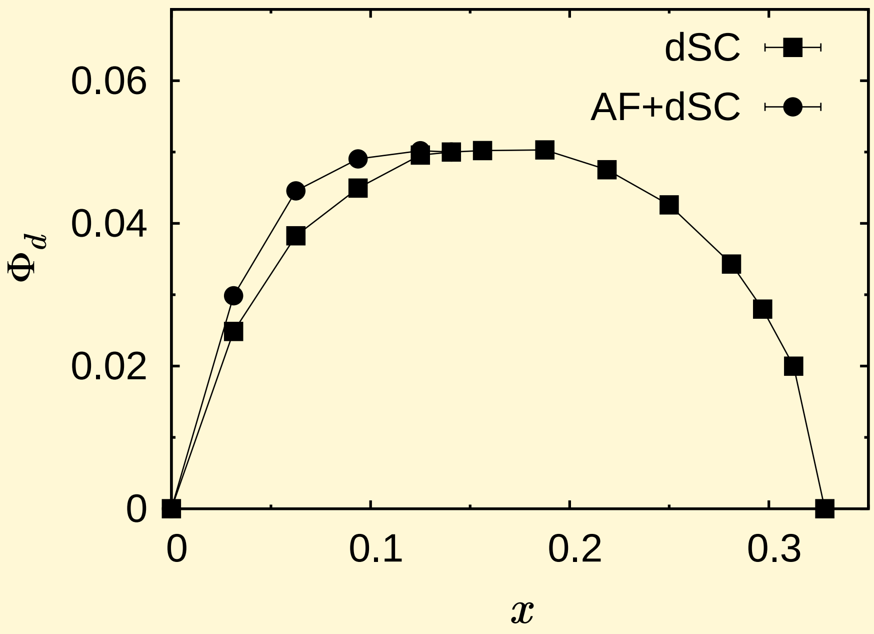
AF coexists with SC in the underdoped region upto hole doping $x \sim 0.14$.

Enhanced magnetic correlations - expected



Spin structure factor in the pure d-wave (dSC) and the coexisting (AF+dSC) states.

Enhanced SC correlations too - interesting



SC order parameter, Φ_d for the pure d-wave (dSC) and the coexisting (AF+dSC) states.

Interlayer pair-tunneling (ILPT)

As a mechanism behind high T_c in cuprates

- Cooper pairs in SC state tunnel across CuO_2 layers by the Josephson tunneling process,

$$\boxed{\mathcal{H}_J = -\sum_{\mathbf{k}} T_J(\mathbf{k}) \left(c^{(1)\dagger}_{\mathbf{k}\uparrow} c^{(1)\dagger}_{-\mathbf{k}\downarrow} c^{(2)}_{-\mathbf{k}\downarrow} c^{(2)}_{\mathbf{k}\uparrow} + h.c. \right)}$$

- It was believed that this lowers kinetic energy in the SC state and provides the large SC condensation energy in cuprates.

- So makes the T_c high.

Experimental contradictions

- c-axis penetration depth, λ_c is related to the condensation energy due to the lowering of kinetic energy.

- Experimentally measured value of λ_c in a number of cuprates differs the predicted value by an order of magnitude.

A relook from a different point of view

- The Gutzwiller projected d-wave BCS wavefunction is used quite often to describe superconductivity in cuprates.
- How well does this state support the ILPT scenario?

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- How well does this state support the ILPT scenario?

We examine this issue using VMC

Model - Consider two 2D t-J layers connected by H_J,

$$\begin{aligned}\mathcal{H} = & - t \sum_{m\langle i,j\rangle\sigma} \left(c_{i\sigma}^{(m)\dagger} c_{j\sigma}^{(m)} + h.c. \right) + J \sum_{m\langle i,j\rangle} \left(\mathbf{S}_i^{(m)} . \mathbf{S}_j^{(m)} - \frac{1}{4} n_i^{(m)} n_j^{(m)} \right) \\ & - \sum_{\mathbf{k}} T_J(\mathbf{k}) \left(c_{\mathbf{k}\uparrow}^{(1)\dagger} c_{-\mathbf{k}\downarrow}^{(1)\dagger} c_{-\mathbf{k}\downarrow}^{(2)} c_{\mathbf{k}\uparrow}^{(2)} + h.c. \right)\end{aligned}$$

m (=1, 2) is the layer index.

Pair tunneling amplitude

$$\boxed{T_J(\mathbf{k}) = \frac{t_\perp^2}{16t}(\cos k_x - \cos k_y)^4}$$

- $t_\perp \sim 0.15$ **eV,** $t \sim 0.4$ **eV.** $t_\perp/t \sim 0.4$**.** $J = 0.35t$**.**

Variational wavefunction

- **Product of two Gutzwiller projected d-wave BCS states with variable particles numbers, one for each layer,**

$$\boxed{|\Psi_{var}\rangle = |\Psi\rangle^{(1)}|\Psi\rangle^{(2)}}$$

$$|\Psi\rangle^{(m)} = \mathcal{P}_G^{(m)}|\Psi_{BCS}\rangle^{(m)} = \mathcal{P}_G^{(m)}\prod_{\mathbf{k}}\left(u_{\mathbf{k}} + v_{\mathbf{k}}c_{\mathbf{k}\uparrow}^{(m)\dagger}c_{-\mathbf{k}\downarrow}^{(m)\dagger}\right)|0\rangle$$

- **Allowing particle number fluctuations is necessary.**

Why GVMC

- Since the particle number is not fixed, it is necessary to perform simulation in grand canonical scheme.

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VMC vs GVMC

- Concentrate on the grandcanonical BCS wavefunction for a single layer

$$|\Psi\rangle = \sum_{N=0,2,\ldots}^{N_s} S_N \left(\sum_{R_N} C(R_N)|R_N\rangle \right)$$

$|R_N\rangle = c^\dagger_{i_1\uparrow} \ldots c^\dagger_{i_{N/2}\uparrow} c^\dagger_{j1\downarrow} \ldots c^\dagger_{j_{N/2}\downarrow}|0\rangle$. $S_N = \pm 1$.

It is a state in a Hilbert space, $\mathbb{H}$ with fluctuating particle number.

Fixed N VMC

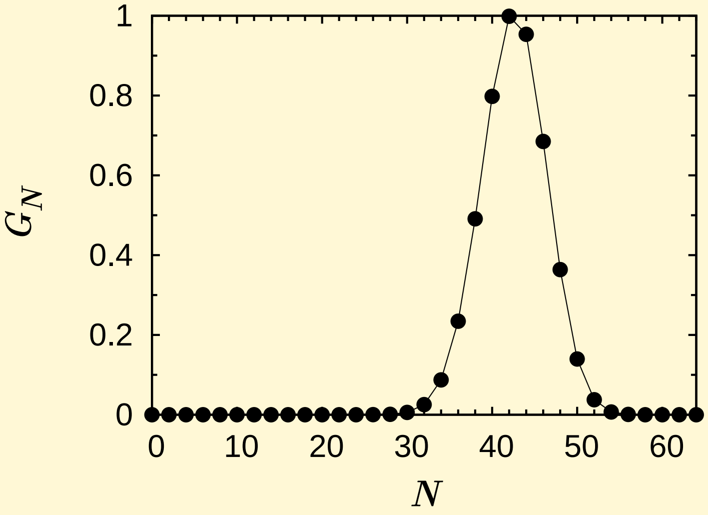
- Generate a Markov chain of states $|R'_N\rangle \rightarrow |R'_N\rangle \rightarrow \ldots$ by doing a random walk in a fixed N subspace, $\mathbb{H}_N$.
- Monte Carlo moves - (i) hopping a spin to a vacant site (ii) exchanging two antiparallel spins.

GVMC

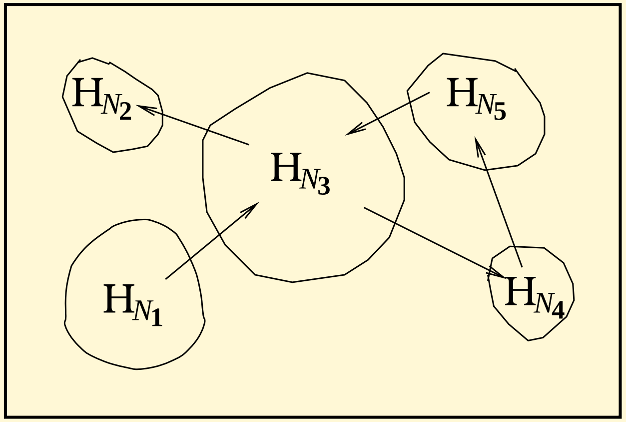
- Generate a Markov chain of states $|R'_{N_1}\rangle \rightarrow |R'_{N_2}\rangle \rightarrow \ldots$ by doing a walk in $\mathbb{H}$.
- Monte Carlo moves - need to create or destroy spins in pairs in addition to (i) and (ii).

A random walk in $\mathbb{H}$

- **Dimension, G_N of a subspace $\mathbb{H}_N$ strongly depend on N.**



G_N vs N for a 8×8 lattice



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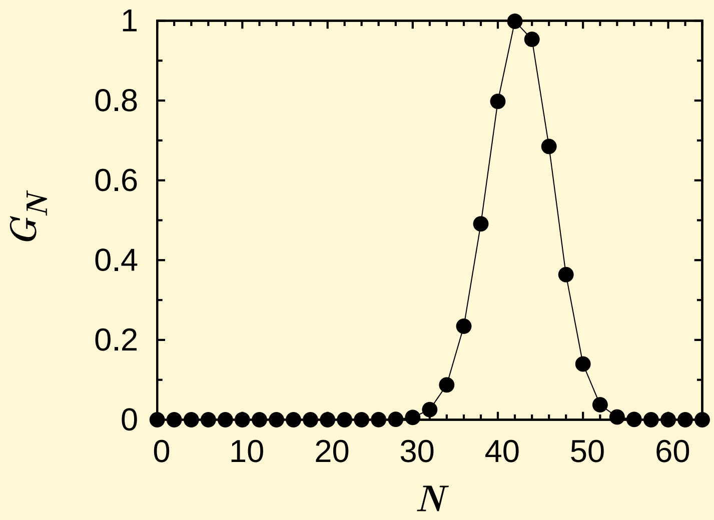

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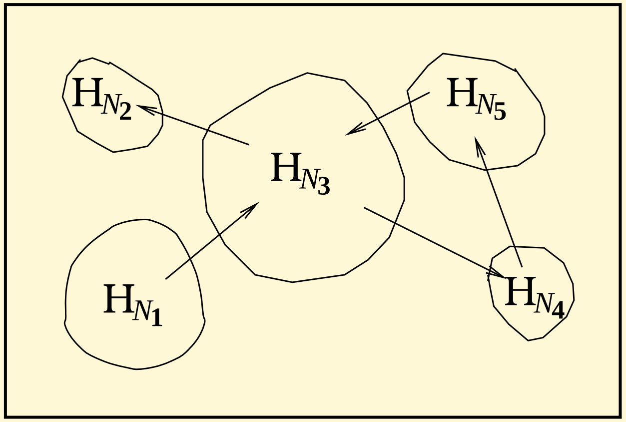

A random walk in $\mathbb{H}$

How often should we attempt jumping to a particular $\mathbb{H}_N$?

- **Should be proportional to G_N. However the actual number may be different. It depends on $C(R_N)$.**

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Consider the hypothetical wavefunction,

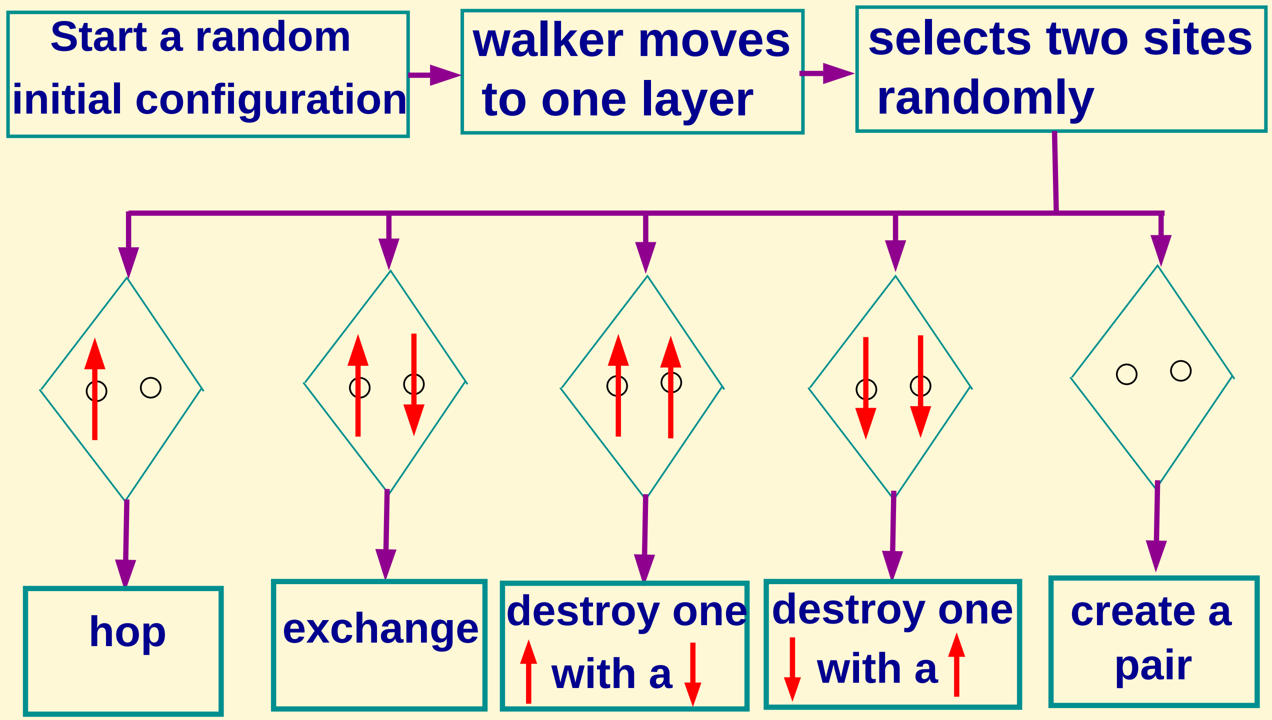
$$|\Psi_{hyp}\rangle = \sum_{N=0,2,...}^{Ns} \sum_{R_N} |R_N\rangle$$

- In simulation of $|\Psi_{hyp}\rangle$, the number of actual jumps, M_N to a $\mathbb{H}_N$ must be proportional to G_N. That is here we require

$$\boxed{M_N \propto G_N}$$

How to satisfy the above condition?

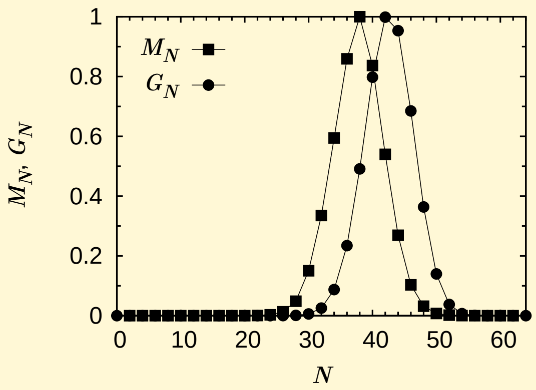
A new algorithm



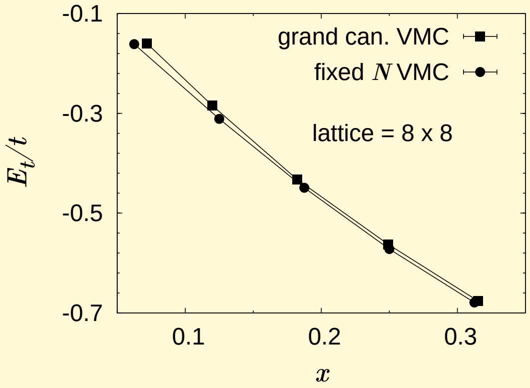
Monte Carlo moves for GVMC simulation

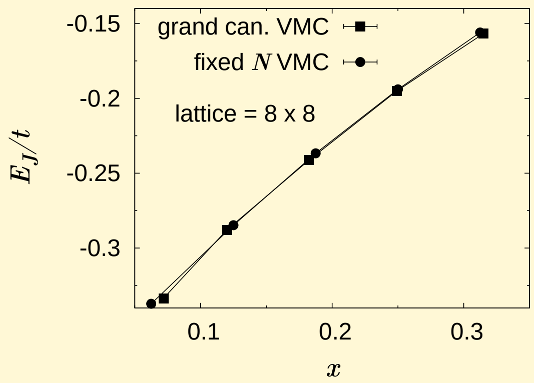
Verifying the algorithm

- Comparison of calculated M_N with G_N



- Energy for the 2D t-J model





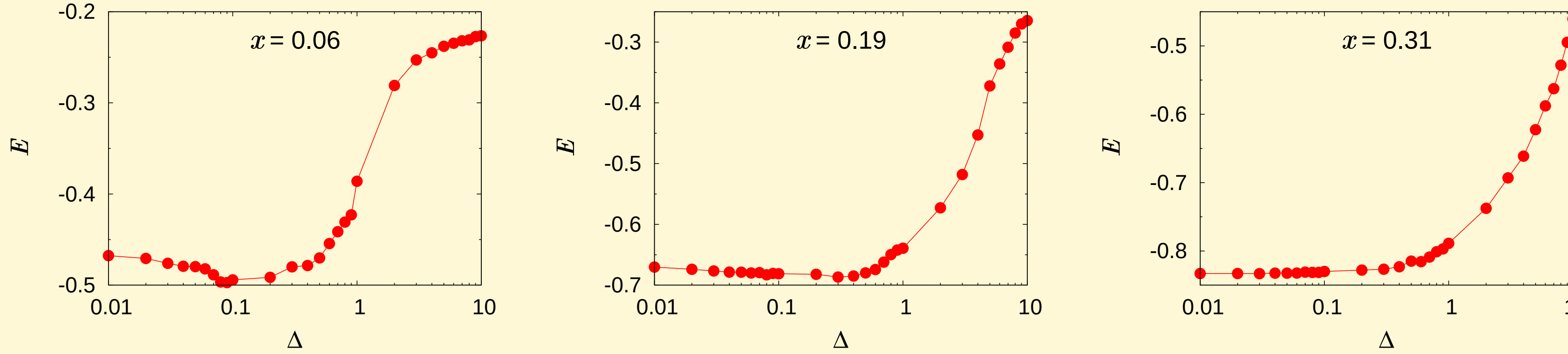
hopping **exchange**

Wavefunction in real space,

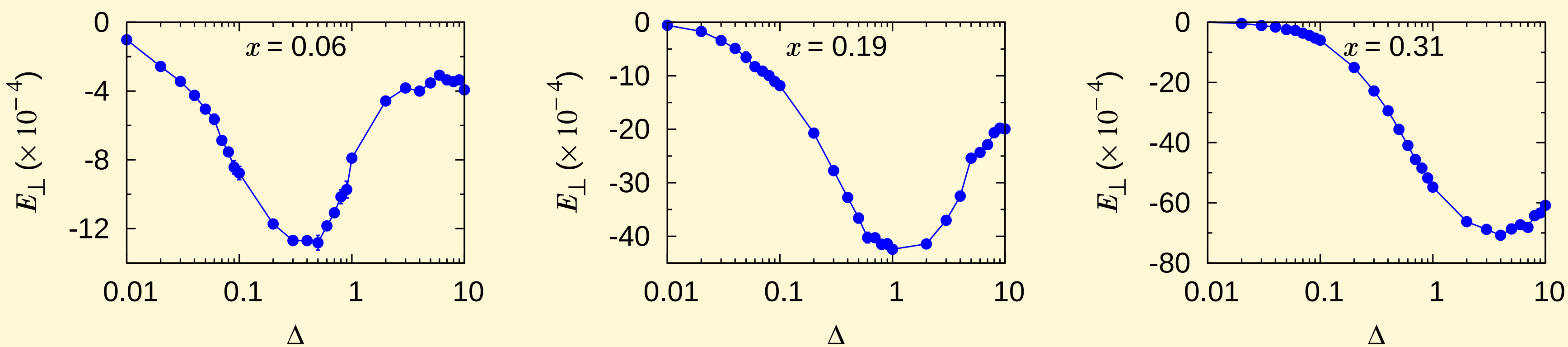
$$|\Psi_{var}\rangle = \sum_{N,N'} S_N S_{N'} \left(\sum_{R_N^{(1)}} \sum_{R_{N'}^{(2)}} C(R_N^{(1)}) C(R_{N'}^{(2)}) |R_N^{(1)}\rangle |R_{N'}^{(2)}\rangle \right)$$

- **Variational parameter is Δ (d-wave SC gap parameter).**
- **Average particle number is fixed by chemical potential, μ.**
- **Lattice parameters: size=$8 \times 8 \times 2$. $J = 0.35t$. $t_\perp/t = 1$.**

Total variational energy, E vs Δ



Pair tunneling energy, $E_\perp$ vs Δ



Interesting variation of $E_\perp$ with Δ.

- $E_\perp$ tends to enhance optimal Δ, thereby SC pairing.
- However the magnitude of Δ is too small to have any appreciable effect eventually.
- Contribution of $E_\perp$ towards the SC condensation energy is only 10% of the total.

Thank You