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The Hubbard model on small clusters from symmetry-projected wave-functions

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Computational Challenges in Nuclear and Many-Body Physics
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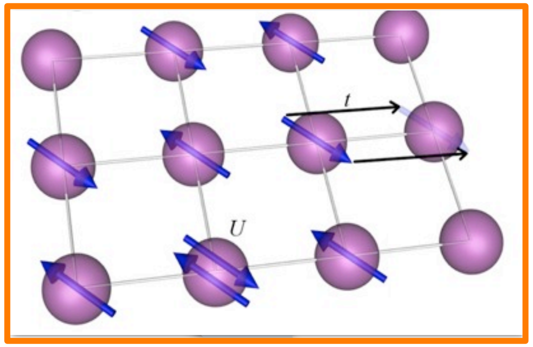
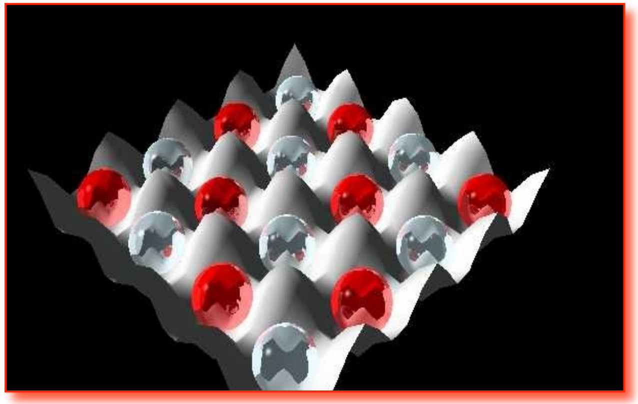
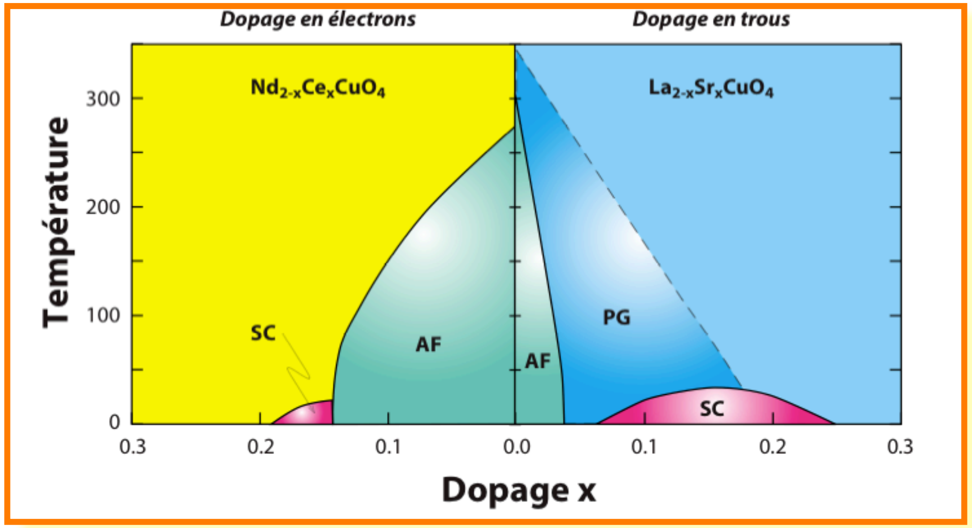
The Hubbard model

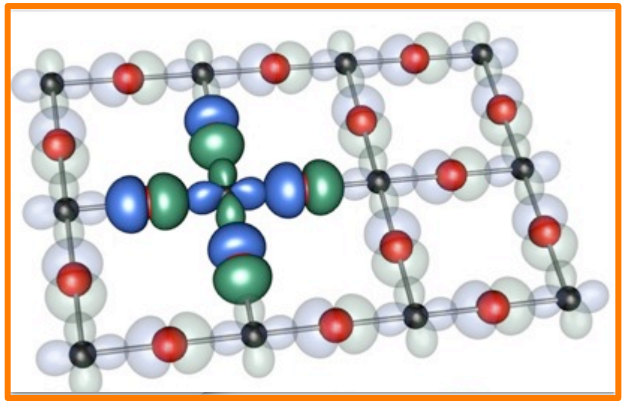
$$\hat{H} = -t \sum_{\substack{\langle \vec{r},\vec{r}' \rangle \\ \sigma=\uparrow,\downarrow}} \hat{c}^{+}_{\vec{r}\sigma}\hat{c}_{\vec{r}'\sigma} + U\sum_{\vec{r}} \hat{n}_{\vec{r}\uparrow}\hat{n}_{\vec{r}\downarrow}$$





Ultracold fermions loaded in optical lattice





Cuprates

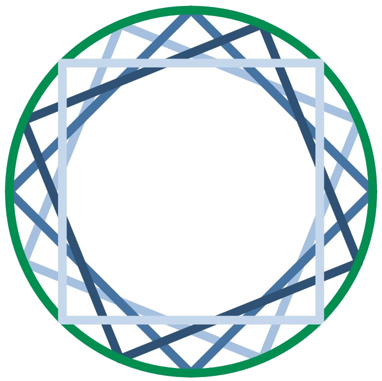
Beyond mean-field : Symmetry-projected wave-functions

Hamiltonian invariant under :
- Spin rotational symmetry
- Translational symmetry
- Lattice C_{4v} transformations

Projection on quantum numbers related to the symmetries of the Hamiltonian (spin,momentum,lattice)

$$\hat{P}^{(\Gamma)} \propto \sum_{g} \left(\chi_{g}^{(\Gamma)}\right)^{*} \hat{U}_{g} \longrightarrow$$ Linear combination of symmetry transformations

Illustration :



$$\hat{P}^{S=0}\left|\downarrow\uparrow\downarrow\uparrow\ldots\right\rangle = \left|\uparrow\downarrow\uparrow\downarrow\ldots\right\rangle + \left|\nearrow\swarrow\nearrow\swarrow\ldots\right\rangle + \left|\leftarrow\rightarrow\leftarrow\rightarrow\ldots\right\rangle + \left|\searrow\nwarrow\searrow\nwarrow\ldots\right\rangle + \ldots$$

Interferences between transformed states induce correlations

Beyond mean-field : Symmetry-projected wave-functions

Here we consider :

Projection onto spin-singlet subspace

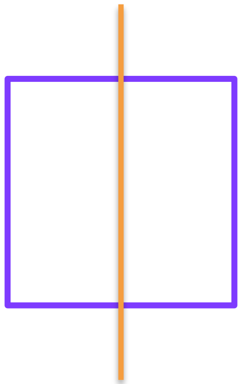
$$\hat{P}^{(S=0)} = \frac{1}{8\pi^2}\int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \sin(\beta) \int_0^{2\pi} d\gamma \; \hat{R}_z(\alpha)\hat{R}_y(\beta)\hat{R}_z(\gamma)$$

Projection onto zero total momentum subspace

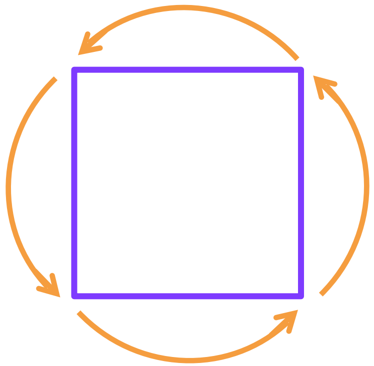
$$\hat{P}^{(\vec{K}=\vec{0})} = \frac{1}{L}\sum_{\vec{a}} \hat{T}_{\vec{a}}$$

$\hat{T}$: translation operator of a lattice vector $\vec{a}$

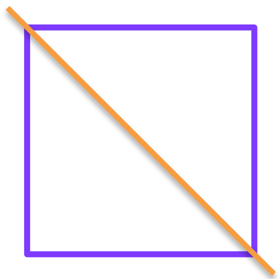
Lattice symmetries C_{4v}



Vertical mirror



$+\frac{\pi}{2}$ rotation



Diagonal mirror

Beyond mean-field : Symmetry-projected wave-functions

Ground state approximation : $|\Psi_0\rangle \rightarrow \hat{P}^{(\Gamma)}|\Phi_{ref}\rangle \propto \sum_g \left(\chi_g^{(\Gamma)}\right)^* \hat{U}_g |\Phi_{ref}\rangle$

$$\langle \hat{H} \rangle_{\Psi_0} = \frac{\langle \Phi_{ref} | \hat{H}\hat{P}^{(\Gamma)} | \Phi_{ref} \rangle}{\langle \Phi_{ref} | \hat{P}^{(\Gamma)} | \Phi_{ref} \rangle} = f[\rho]$$

Wick's theorem

$$h_{ij}^{(\Gamma)} = \frac{\partial \langle \hat{H} \rangle_{\Psi_0}}{\partial \rho_{ji}} \rightarrow h^{(\Gamma)} = \frac{1}{\sum_g \left(\chi_g^{(\Gamma)}\right)^* \det A_g} \sum_g \left(\chi_g^{(\Gamma)}\right)^* A_g^{-1} \left\{ h\left[R_g\right] U_g B_g^{-1} + \left(U_g - 1\right)\left(\mathcal{E}\left[R_g\right] - \langle \hat{H} \rangle_{\Psi_0}\right) \right\}$$

Effective one-body Hamiltonian

with $A_g = 1 + \left(U_g - 1\right)\rho$

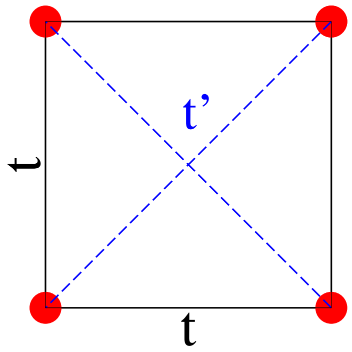
$B_g = 1 + \rho\left(U_g - 1\right)$

$R_g = \rho U_g A_g^{-1}$ $\longrightarrow$ One-body transition density matrix

The approach is variational : $\left[h^{(\Gamma)}, \rho\right] = 0$

Beyond mean-field : Symmetry-projected wave-functions

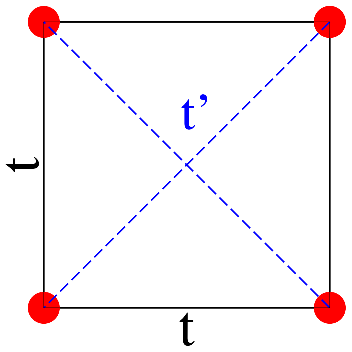
Ground state energy of the Hubbard model (C_{4v} symmetry)



Doping 1/8

		Energy/t	$S_S(\pi,\pi)$	$S_C(\pi,\pi)$
4×4 $U=4t$ $t'=0$	Ex. Diag.	-15.744	2.14	0.424
$S=0, S_z=0, \mathbf{K}=(0,0)$	SPWF	-15.718	2.198	0.428
4×4 $U=4t$ $t'=0$	Ex. Diag.	-15.744	2.18	0.424
$S=0, S_z=0, \mathbf{K}=(\pi,\pi)$	SPWF	-15.71	2.234	0.434
4×4 $U=8t$ $t'=-0.3t$	Ex. Diag.	-12.502	0.965	0.279
$S=0, S_z=0, \mathbf{K}=(0,0)$	SPWF	-12.356	0.944	0.285

Ground state energy of the Hubbard model (C_{4v} symmetry)

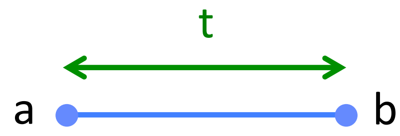


Half-filling

		Energy/t	$S_S(\pi,\pi)$	$S_C(\pi,\pi)$
4×4 $U=4t$ $t'=0$	Ex. Diag.	-13.622	3.64	0.385
$S=0, S_z=0, \mathbf{K}=(0,0)$	SPWF	-13.616	3.656	0.386
4×4 $U=8t$ $t'=-0.3t$	Ex. Diag.	-8.488	4.985	0.192
$S=0, S_z=0, \mathbf{K}=(0,0)$	SPWF	-8.485	4.996	0.192
6×6 $U=4t$ $t'=0$	QMC	-30.87(2)	5.82(3)	0.418(2)
$S=0, S_z=0, \mathbf{K}=(0,0)$	SPWF	-30.733	6.028	0.409
8×8 $U=4t$ $t'=0$	QMC	-55.09(6)	8.2(2)	0.412(2)
$S=0, S_z=0, \mathbf{K}=(0,0)$	SPWF	-54.278	9.616	0.429

The two site Hubbard model at half-filling
Symmetry-projected wave-functions

- Exact diagonalization : $E_0 = \dfrac{U - \sqrt{U^2 + 16t^2}}{2}$

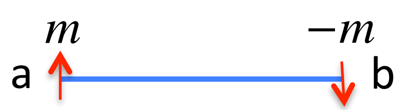


- Spin singlet projection on a Slater determinant with AF order

Single-particle states parametrisation

$$|\phi_1\rangle = \cos\theta |a\uparrow\rangle + \sin\theta |b\uparrow\rangle$$

$$|\phi_2\rangle = \sin\theta |a\downarrow\rangle + \cos\theta |b\downarrow\rangle$$



$$m = \frac{\cos(2\theta)}{2}$$

$$|\Psi\rangle = \hat{P}^{(S=0)} |\Phi_{ref}\rangle$$

Expectation value : $\langle \hat{H} \rangle_\Psi = \dfrac{U\sin^2(2\theta) - 4t\sin(2\theta)}{\sin^2(2\theta) + 1}$ $\Rightarrow$ $\min\left(\langle \hat{H} \rangle_\Psi\right) = E_0$

The two site Hubbard model at half-filling

- Gutzwiller approach : $\left|\Psi\right\rangle = \hat{P}_G \left|\Phi_{ref}\right\rangle$

$$\hat{P}_G = \prod_i \left(1 + (g-1)\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}\right)$$

$$\hat{P}_G \left|a\uparrow a\downarrow\right\rangle_- = g\left|a\uparrow a\downarrow\right\rangle_-$$

$$\hat{P}_G \left|a\uparrow b\downarrow\right\rangle_- = \left|a\uparrow b\downarrow\right\rangle_-$$

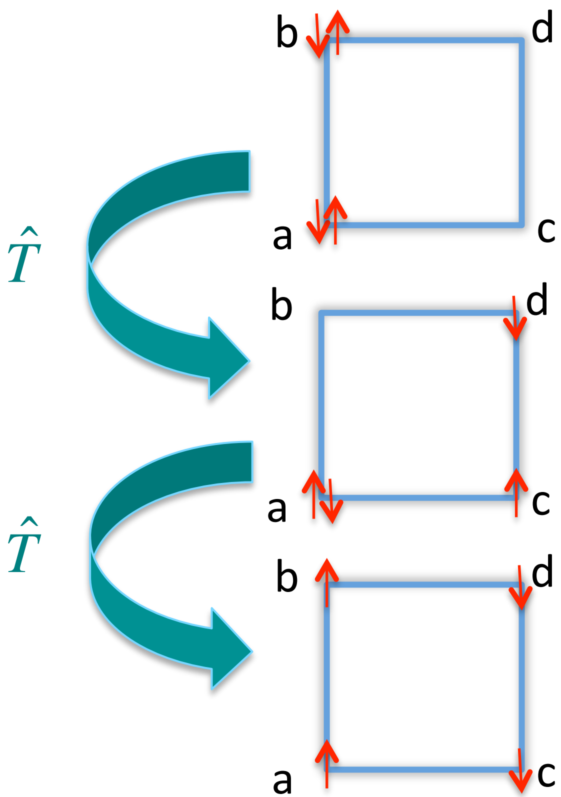
$$\left|\Phi_{ref}\right\rangle = \hat{c}^{+}_{\vec{k}=\vec{0},\uparrow}\hat{c}^{+}_{\vec{k}=\vec{0},\downarrow}\left|\ \right\rangle$$ Free electron state

Expectation value : $\left\langle \hat{H} \right\rangle_\Psi = \dfrac{-4gt + g^2 U}{g^2 + 1}$ ⇒ $\min\left(\left\langle \hat{H} \right\rangle_\Psi\right) = E_0$

Gutzwiller and symmetry-projected wave-functions approaches are analytically exact for the two site Hubbard model at any coupling

The four site Hubbard model at half-filling
Exact diagonalisation

Ground-state features :
- Zero total spin
- Zero total momentum
- d-wave symmetry



$$|1\rangle = \frac{1}{2}\left(\Delta_a^+ - \Delta_d^+\right)\left(\Delta_b^+ - \Delta_c^+\right)|0\rangle \quad \textit{with} \quad \Delta_i^+ = c_{i\uparrow}^+ c_{i\downarrow}^+$$

$$|2\rangle = \frac{1}{4}\left[\begin{array}{l}\left(\Delta_a^+ + \Delta_b^+\right)\left(c_{c\uparrow}^+ c_{d\downarrow}^+ - c_{c\downarrow}^+ c_{d\uparrow}^+\right) - \left(\Delta_a^+ + \Delta_c^+\right)\left(c_{b\uparrow}^+ c_{d\downarrow}^+ - c_{b\downarrow}^+ c_{d\uparrow}^+\right) \\ -\left(\Delta_b^+ + \Delta_d^+\right)\left(c_{a\uparrow}^+ c_{c\downarrow}^+ - c_{a\downarrow}^+ c_{c\uparrow}^+\right) + \left(\Delta_c^+ + \Delta_d^+\right)\left(c_{a\uparrow}^+ c_{b\downarrow}^+ - c_{a\downarrow}^+ c_{b\uparrow}^+\right)\end{array}\right]|0\rangle$$

$$|3\rangle = \frac{1}{2\sqrt{3}}\left[\begin{array}{l} c_{a\uparrow}^+ c_{b\uparrow}^+ c_{c\downarrow}^+ c_{d\downarrow}^+ + c_{a\downarrow}^+ c_{b\uparrow}^+ c_{c\downarrow}^+ c_{d\uparrow}^+ + c_{a\downarrow}^+ c_{b\downarrow}^+ c_{c\uparrow}^+ c_{d\uparrow}^+ \\ + c_{a\uparrow}^+ c_{b\downarrow}^+ c_{c\uparrow}^+ c_{d\downarrow}^+ - 2\left(c_{a\uparrow}^+ c_{b\downarrow}^+ c_{c\downarrow}^+ c_{d\uparrow}^+ + c_{a\downarrow}^+ c_{b\uparrow}^+ c_{c\uparrow}^+ c_{d\downarrow}^+\right)\end{array}\right]|0\rangle$$

In this three dimensional subspace the Hamiltonian reads: $H = \begin{pmatrix} 2U & 2t & 0 \\ 2t & U & -2\sqrt{3}t \\ 0 & -2\sqrt{3}t & 0 \end{pmatrix}$

The four site Hubbard model at half-filling
Exact diagonalisation

Let the eigenvalues E_k of the Hamiltonian correspond to $E \equiv U - 4t\chi$

Then χ satisfies the depressed cubic equation : $16t^2\chi^3 - \chi\left(16t^2 + U^2\right) - 2tU = 0$

Cardano's formula

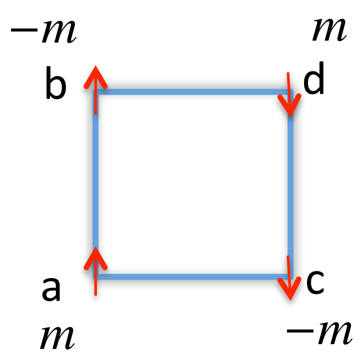
Eigenvalues' final expression : $E_k = U - 2\sqrt{\frac{16t^2 + U^2}{3}}\cos\left(\frac{\beta - 2k\pi}{3}\right)$

with $\cos(\beta) = 4t^2U\left(\frac{3}{16t^2 + U^2}\right)^{\frac{3}{2}}$

$$\begin{cases} k = 0 & \textit{ground-state} \\ k = 1,2 & \textit{excited states} \end{cases}$$

The four site Hubbard model at half-filling
Symmetry-projected wave-function : analytical approach

Reference state : antiferromagnetic Slater determinant $\left|\Phi_{ref}\right\rangle = \hat{c}^{+}_{\phi_1\uparrow}\hat{c}^{+}_{\phi_2\uparrow}\hat{c}^{+}_{\phi_3\uparrow}\hat{c}^{+}_{\phi_4\uparrow}\left|\ \right\rangle$



Single-particle states parametrisation

$$\left|\phi_1\right\rangle = \frac{1}{\sqrt{2}}\left(\left|a\right\rangle - \left|d\right\rangle\right)$$

$$\left|\phi_2\right\rangle = \frac{1}{\sqrt{2}}\left(\cos\varphi\left|a\right\rangle + \sin\varphi\left|b\right\rangle + \sin\varphi\left|c\right\rangle + \cos\varphi\left|d\right\rangle\right)$$

$$\left|\phi_3\right\rangle = \frac{1}{\sqrt{2}}\left(\left|b\right\rangle - \left|c\right\rangle\right)$$

$$\left|\phi_4\right\rangle = \frac{1}{\sqrt{2}}\left(\sin\varphi\left|a\right\rangle + \cos\varphi\left|b\right\rangle + \cos\varphi\left|c\right\rangle + \sin\varphi\left|d\right\rangle\right)$$

Spin rotational invariance restoration : projection onto spin-singlet subspace

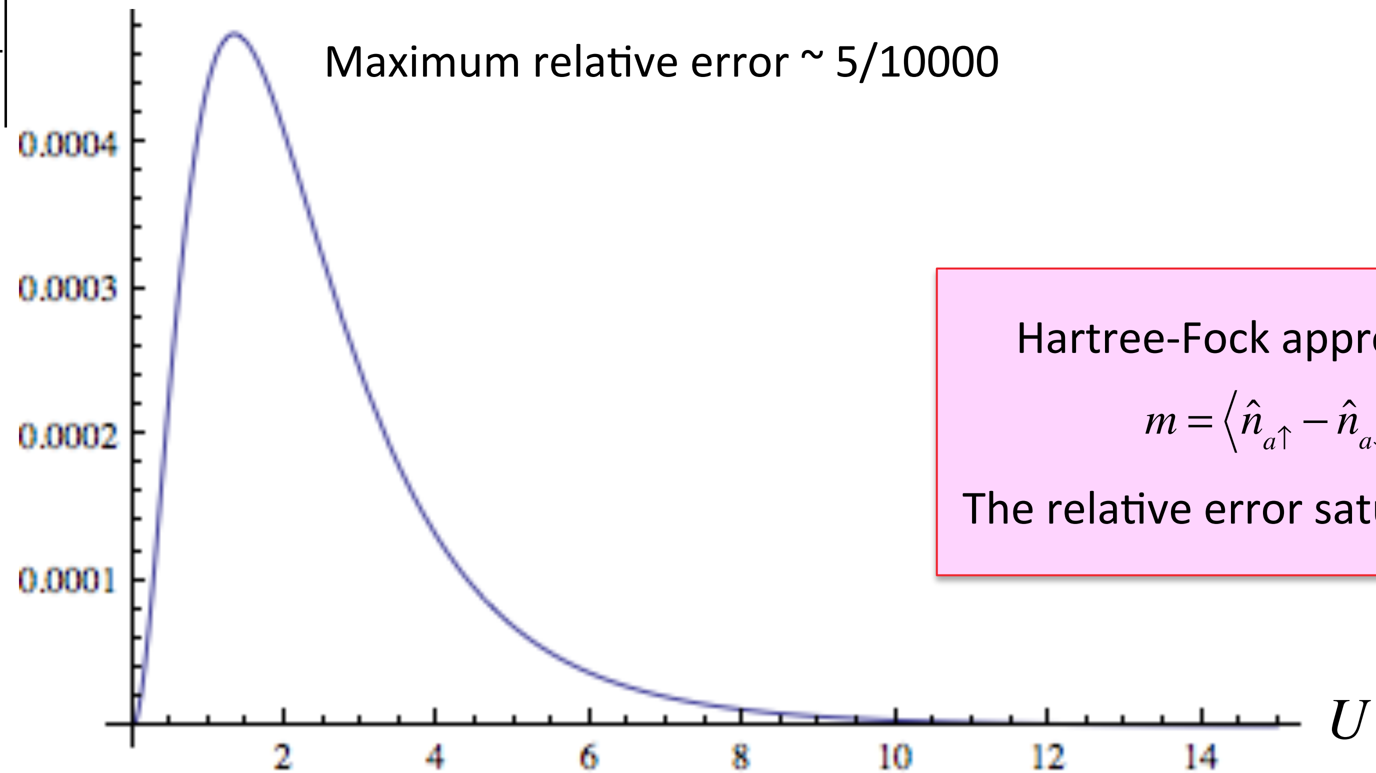
Approximation of the ground-state :

$$\left|\Psi\right\rangle = \hat{P}^{(S=0)}\left|\Phi_{ref}\right\rangle = \sin^2\varphi\left|1\right\rangle - \sin(2\varphi)\left|2\right\rangle - \frac{1+\cos^2\varphi}{\sqrt{3}}\left|3\right\rangle$$

The four site Hubbard model at half-filling
Symmetry-projected wave-function : analytical approach

Expectation value $E^{(S=0)}$ in the state $|\Psi\rangle$: $\left\langle \hat{H} \right\rangle_\Psi = \dfrac{\frac{3}{8}U\left(5-4\cos(2\varphi)-\cos(4\varphi)\right)-12t\sin(2\varphi)}{2+\sin^2(2\varphi)}$

$\left|\dfrac{\left\langle \hat{H} \right\rangle - E_0}{E_0}\right|$



Maximum relative error ~ 5/10000

Hartree-Fock approximation :

$m = \left\langle \hat{n}_{a\uparrow} - \hat{n}_{a\downarrow} \right\rangle_{\Phi_{ref}}$

The relative error saturates to 33%

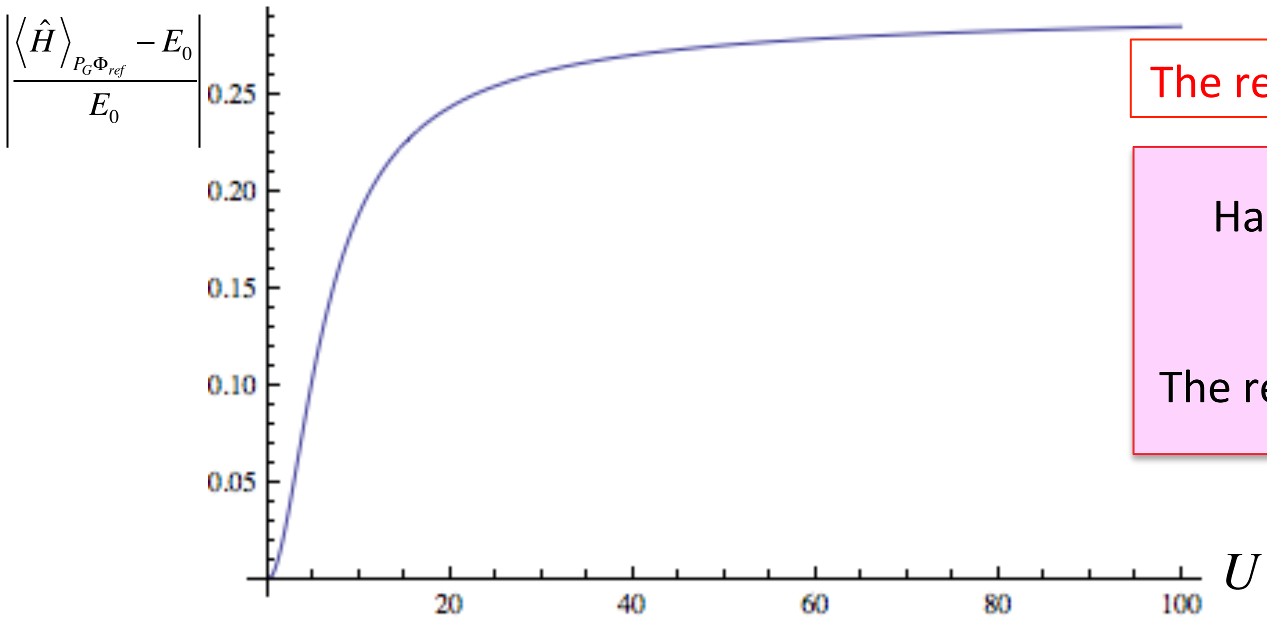
The four site Hubbard model at half-filling

The Gutzwiller wave-function

Gutzwiller projector : $\hat{P}_G = \prod_i \left(1 + (g-1)\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}\right)$

Expectation value: $\left\langle \hat{H} \right\rangle_{P_G\Phi_{ref}} = \dfrac{\left\langle \Phi_{ref} \middle| \hat{P}_G \hat{H} \hat{P}_G \middle| \Phi_{ref} \right\rangle}{\left\langle \Phi_{ref} \middle| \hat{P}_G \hat{P}_G \middle| \Phi_{ref} \right\rangle} = \left\langle \hat{H} \right\rangle(\varphi, g)$

$$\left\langle \hat{H} \right\rangle_{P_G\Phi_{ref}} = \frac{\left(-8tg\sin\varphi\cos\varphi + 2Ug^2\sin^2\varphi\right)\left[(1+g)^2\sin^2\varphi + 4\cos^2\varphi\right]}{4\cos^4\varphi + 8g^2\cos^2\varphi\sin^2\varphi + \left(1+2g^2+g^4\right)\sin^4\varphi}$$



The relative error saturates to 28%

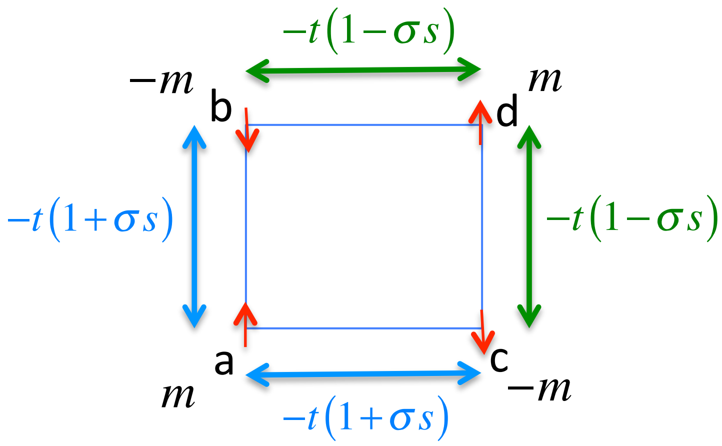
Hartree-Fock approximation :

$$m = \left\langle \hat{n}_{a\uparrow} - \hat{n}_{a\downarrow} \right\rangle_{\Phi_{ref}}$$

The relative error saturates to 33%

The four site Hubbard model at half-filling
Symmetry-projected wave-function : exact results

Symmetry breaking : dress the AF order with bond-spins



$$h_\sigma^{ref}[m,s]=\begin{pmatrix} \frac{U}{2}(1-\sigma m) & -t(1+\sigma s) & -t(1+\sigma s) & 0 \\ -t(1+\sigma s) & \frac{U}{2}(1+\sigma m) & 0 & -t(1-\sigma s) \\ -t(1+\sigma s) & 0 & \frac{U}{2}(1+\sigma m) & -t(1-\sigma s) \\ 0 & -t(1-\sigma s) & -t(1-\sigma s) & \frac{U}{2}(1-\sigma m) \end{pmatrix}$$

Mean-field like Hamiltonian

Lowest energy eigenstates : $\left|\Phi_{ref}\right\rangle$

Translational invariance restoration : projection onto zero momentum subspace

$$\left|\Psi\right\rangle = \hat{P}^{(\vec{K}=\vec{0})}\hat{P}^{(S=0)}\left|\Phi_{ref}\right\rangle$$

The four site Hubbard model at half-filling

Symmetry-projected wave-function : exact results

Expectation value : $E^{(\vec{K}=\vec{0},S=0)} = \dfrac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \dfrac{3\left(-16ab^2t + U\left(2b^2+1\right)\right)}{2\left(4a^2b^2 + 3b^2 - 2ab + 1\right)}$

In terms of the variables : $\begin{cases} a = \dfrac{2\left(2+s^2\right) + \tilde{m}\left(\sqrt{4\left(1+s^2\right)+\tilde{m}^2} + \tilde{m}\right)}{2\left(\sqrt{4\left(1+s^2\right)+\tilde{m}^2} + \tilde{m}\right)} \\ b = \dfrac{2}{\sqrt{4\left(1+s^2\right)+\tilde{m}^2} - \tilde{m}} \end{cases}$ *with* $\tilde{m} = \dfrac{Um}{2t}$

Minimisation with respect to a and b yields :

$$\frac{\partial}{\partial a}\left[E^{(\vec{K}=\vec{0},S=0)}\right] = \frac{\partial}{\partial b}\left[E^{(\vec{K}=\vec{0},S=0)}\right] = 0 \Rightarrow \begin{cases} a^2\left(16b^2t - 4bU\right) - a\left(2b^2U + 16bt - U\right) = bU \\ 32a^2b^3t - 4abU\left(2b^2+1\right) = 8bt\left(3b^2+1\right) - U\left(2b^2+1\right) \end{cases}$$

System of eqs. linear in a and a^2

The four site Hubbard model at half-filling
Symmetry-projected wave-function : exact results

$$\begin{cases} a = f(b) \\ a^2 = g(b) \end{cases} \Rightarrow g(b) - f^2(b) = 0$$

$\Rightarrow$ b solution of a quartic or cubic equation :

- $4b^4(48t^2+U^2) - 16b^3tU + 4b^2(16t^2+U^2) - 8btU + U^2 = 0$ — **No real solution**

- $8b^3t^2 - 6b^2tU + b(U^2 - 8t^2) + tU = 0$

  $\hookrightarrow$ $b - a = b - f(b) = \dfrac{U}{4t}$

$\Rightarrow$

$$16t^2a^3 - a(16t^2+U^2) - 2tU = 0$$

$$E_{\min}^{(\vec{K}=\vec{0},S=0)} = U - 4ta$$

Exact diagonalisation

$$16t^2\chi^3 - \chi(16t^2+U^2) - 2tU = 0$$

$$E = U - 4t\chi$$

The exact ground-state may be obtained by minimizing the energy of a symmetry-projected Slater determinant.

Conclusion

- Conventional Hartree-Fock approximations have been improved to account for electronic correlations

  ↳ Symmetry projections $\hat{P}^{(\Gamma)} \propto \sum_g \left(\chi_g^{(\Gamma)}\right)^* \hat{U}_g$

- Spin-rotational invariance restoration leads to an almost exact description.

- Combining spin-rotational and zero total momentum projections allows to recover the exact energy for any interaction strength.

- The more symmetries we restore, the better the energy of the symmetry-projected wave-function approach is.

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