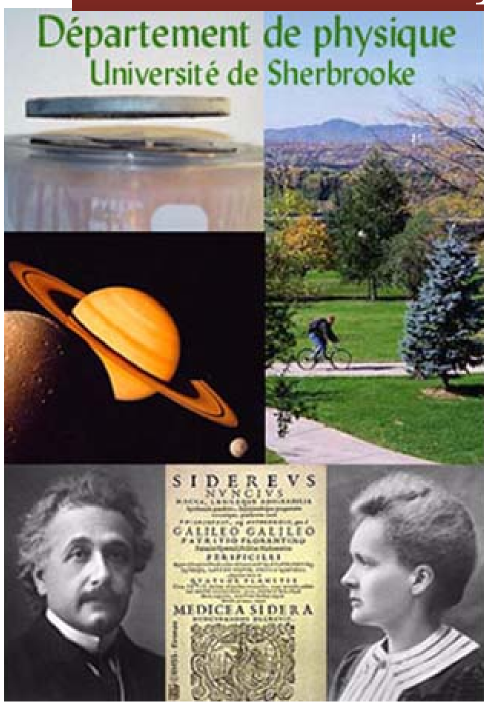
What is the Hamiltonian for parent high-temperature superconductors



André-Marie Tremblay, Alexis Gagné-Lebrun

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CENTRE DE RECHERCHE SUR LES PROPRIÉTÉS ÉLECTRONIQUES
DE MATÉRIAUX AVANCÉS

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Outline

- What is the problem?
- What is the numerical method?
- What are the results?
- Conclusion

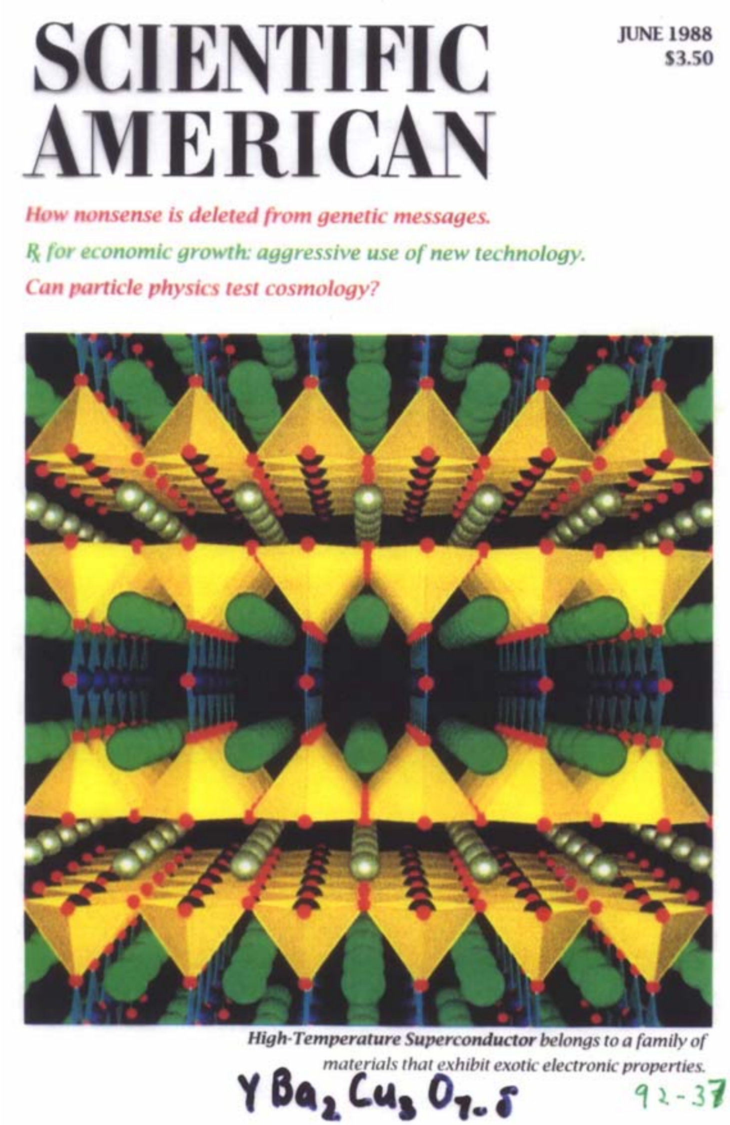
What is the problem ?

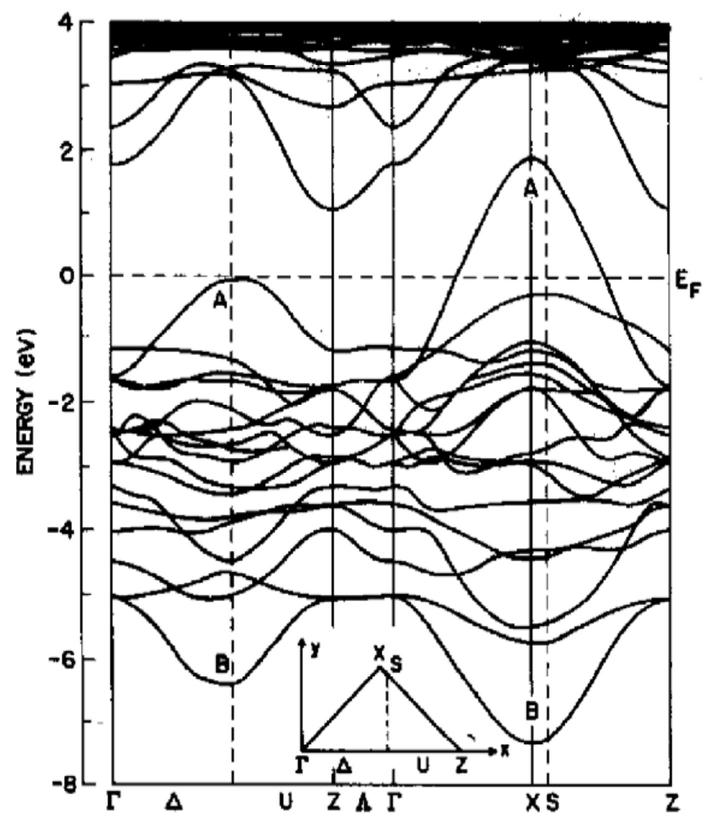
Materials and theoretical considerations

Experiments

Previous theoretical work

What is the problem?





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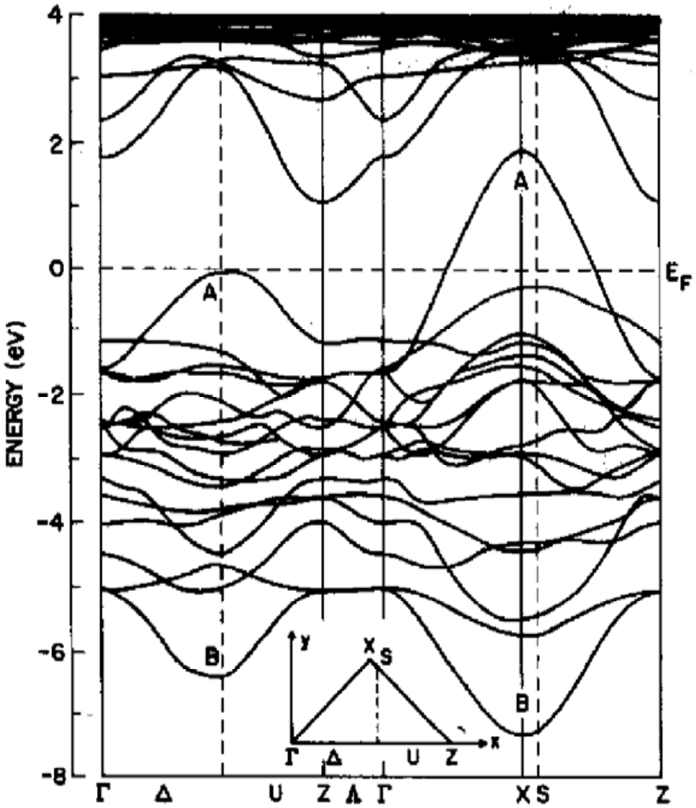
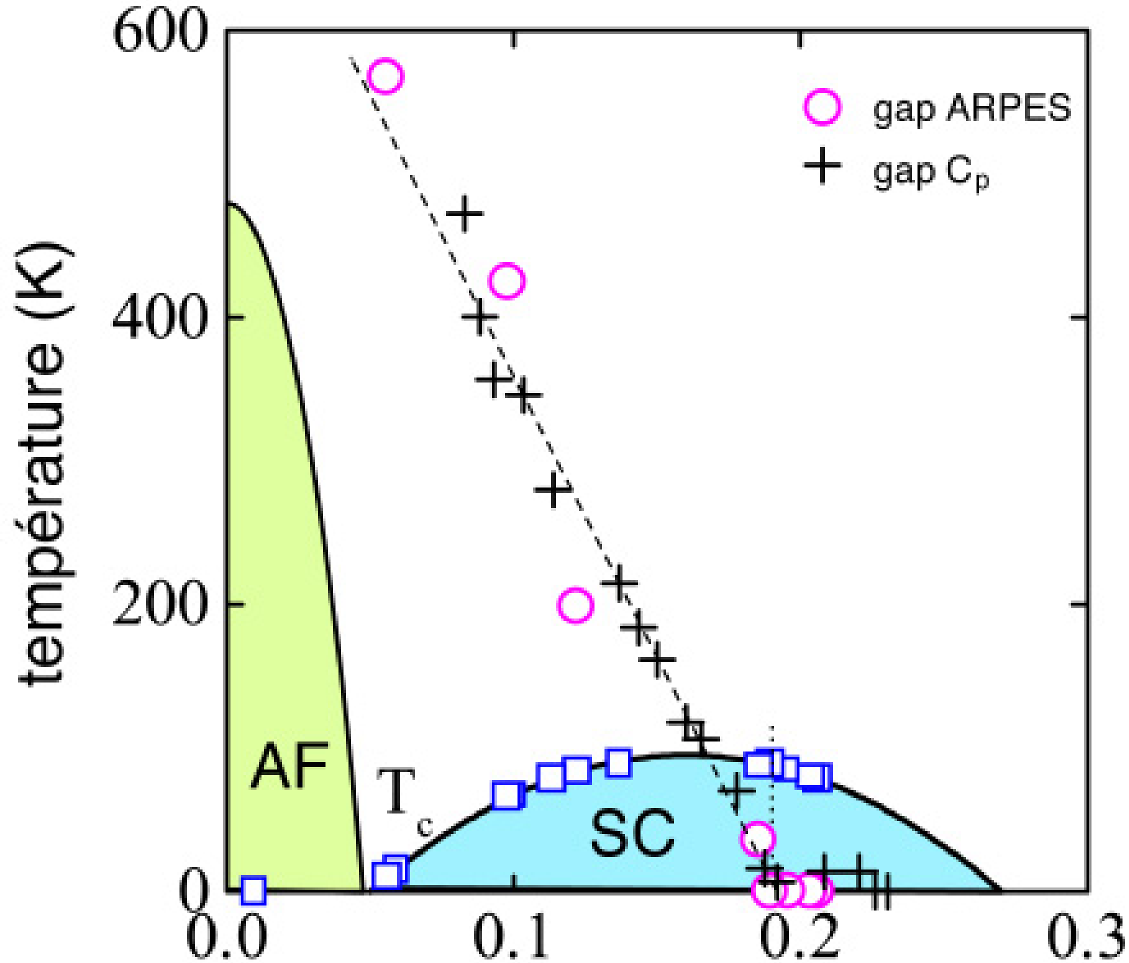
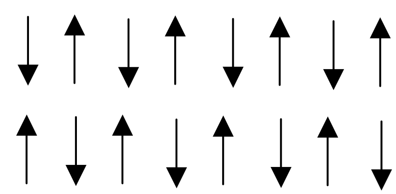




Hole concentration

(doping δ)

Antiferromagnet



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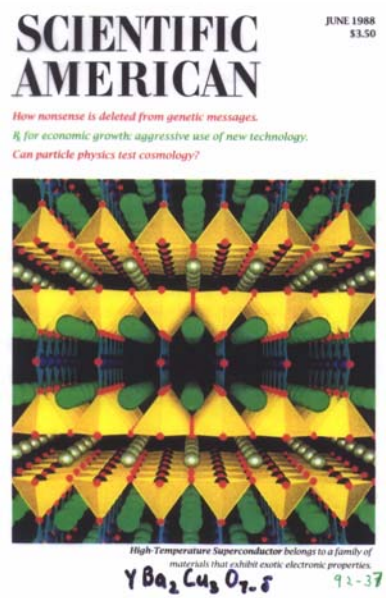
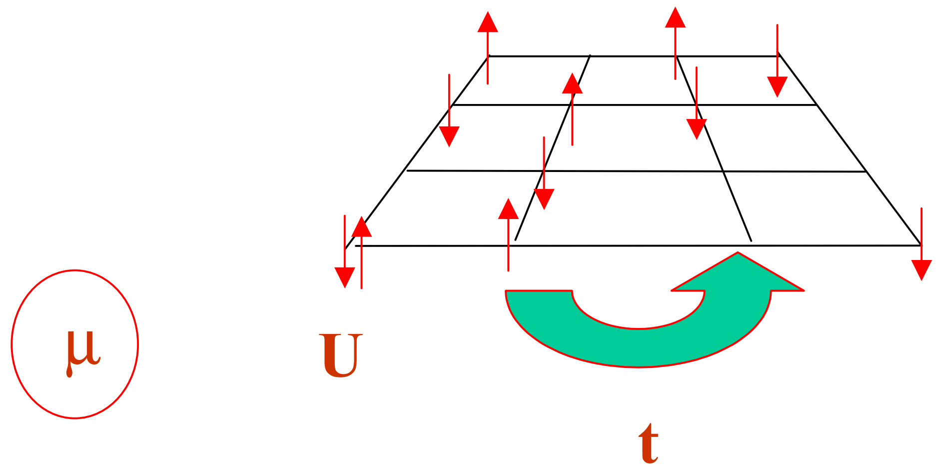
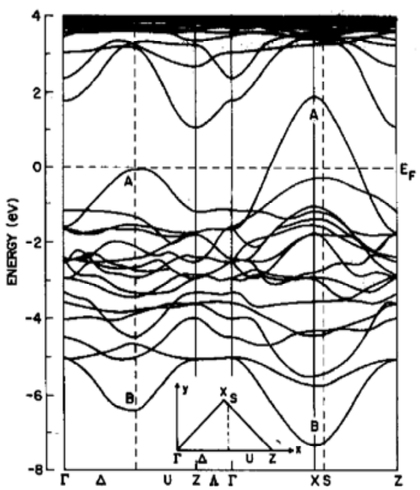
Residual interactions must be added to band structure



The simplest model for $Cu\ O_2$ planes.



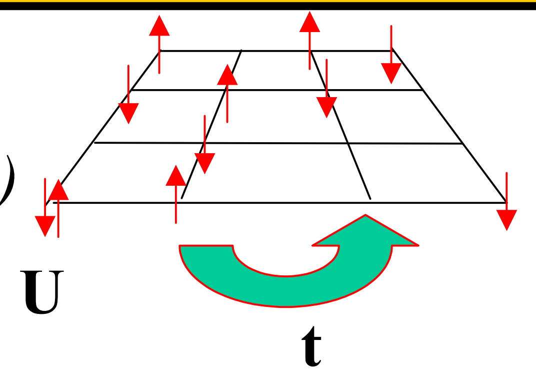


- Size of Hilbert space : 4^N (N = 16)
- With N=16, need 4 GigaBits just for states

Hubbard model (Kanamori, Gutzwiller, 1963) :

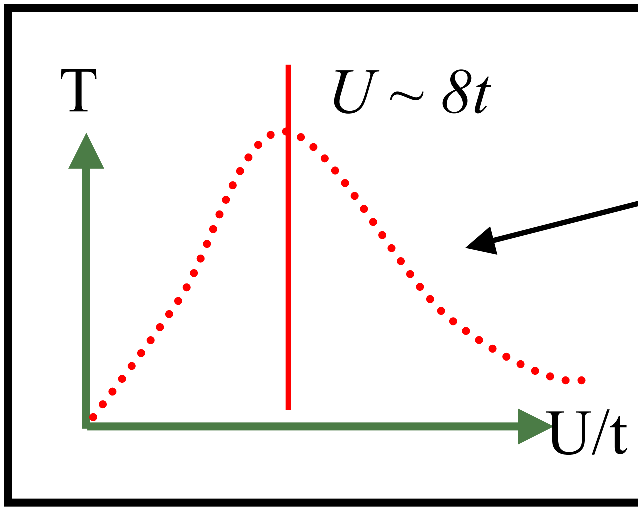
$$H = -\sum_{<ij>\sigma} t_{i,j}\left(c_{i\sigma}^{\dagger}c_{j\sigma} + c_{j\sigma}^{\dagger}c_{i\sigma}\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$

- « Screened » interaction *U*
- *U, T smallest, n = 1 (ou δ=1-n)*
- *a = 1, t = 1,* $\hbar$ *= 1*



Strong *vs* weak coupling

- *t* from band structure,
- *U* harder



Strong coupling

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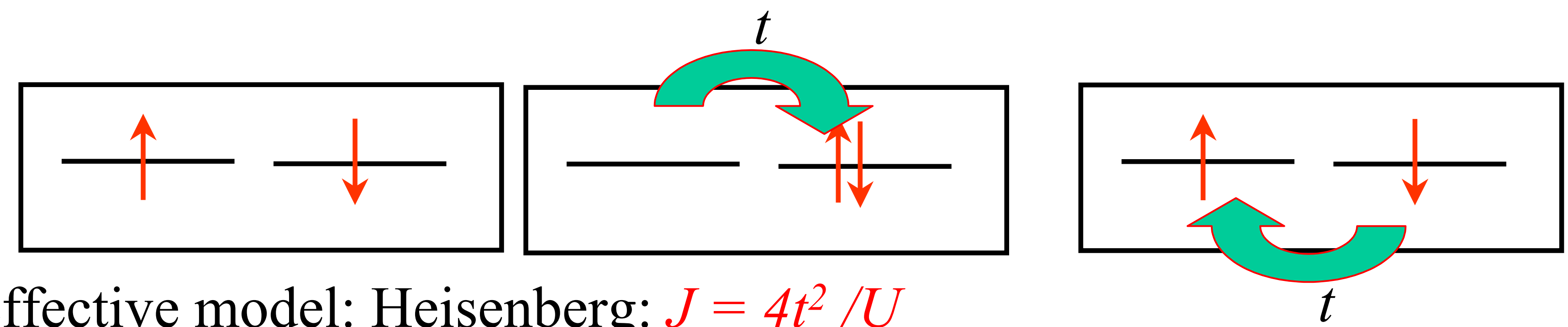
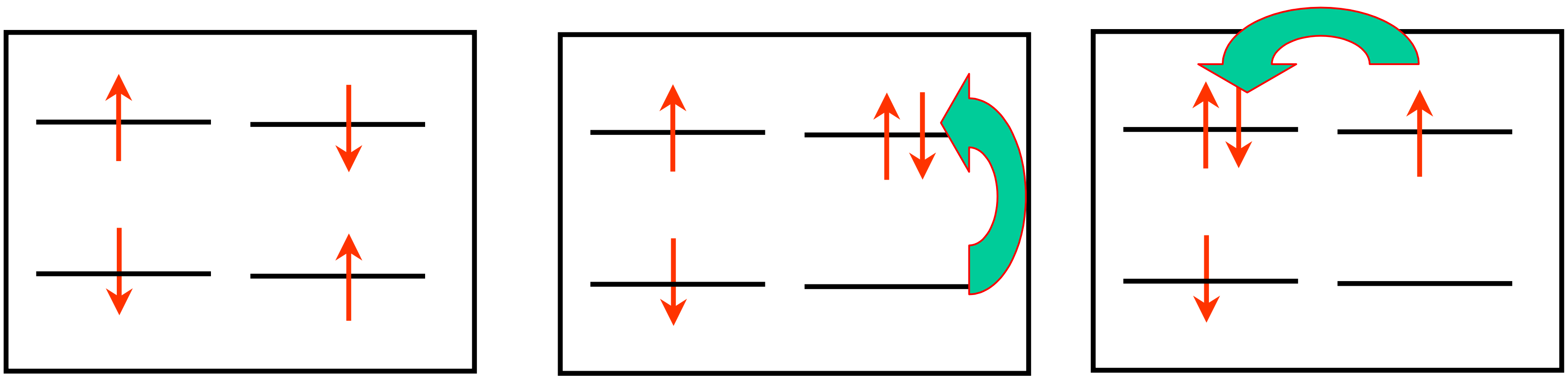
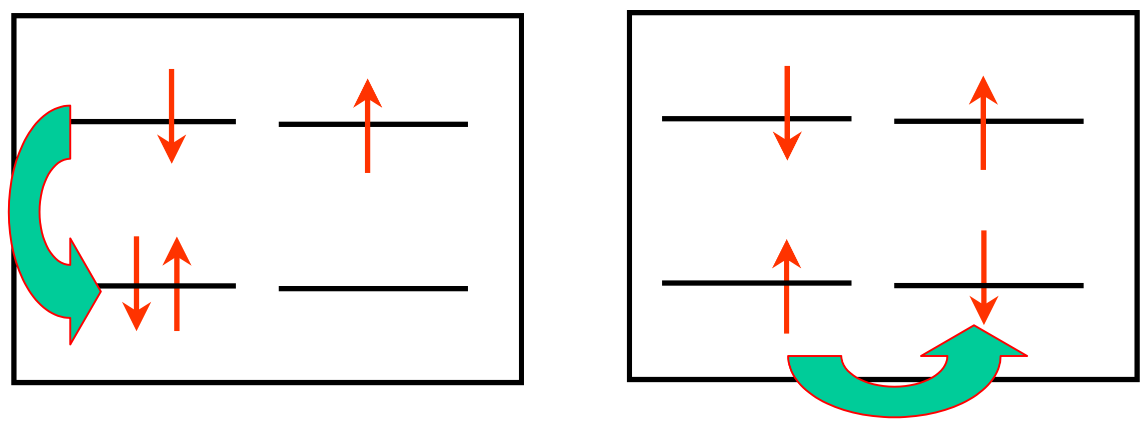


Effective model: Heisenberg: $J = 4t^2/U$



Ring exchange

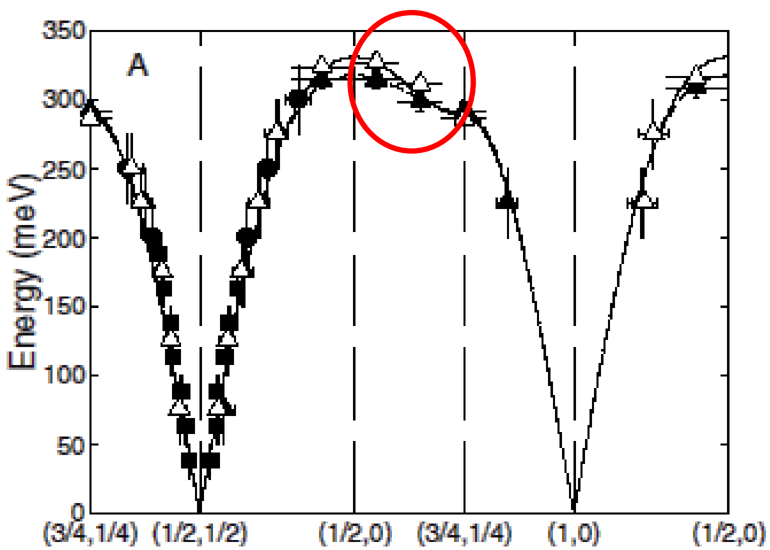


$J_c = 80t^4/U^3$

and second-neighbor hopping

Experimental approach and analysis

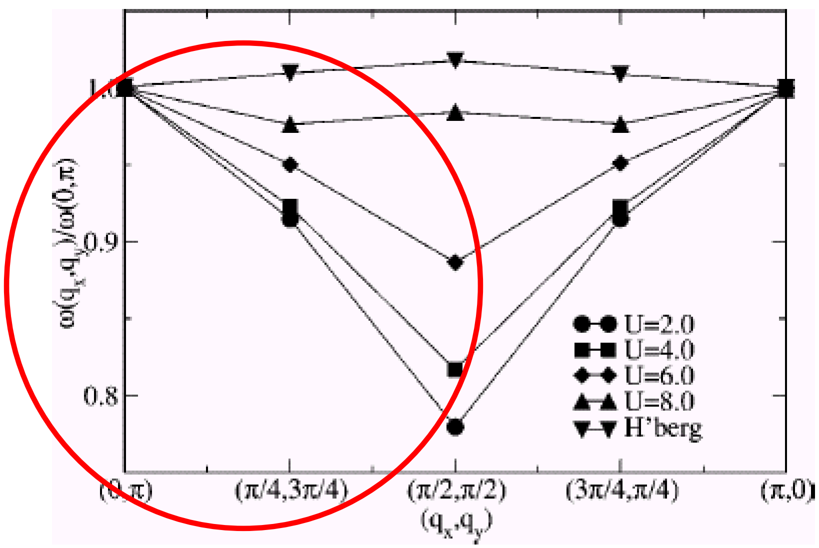
Experimental spin-wave dispersion



R. Coldea PRL **86**, 5377 (2001)

- Fitting the dispersion, knowing $J = 4t^2 /U$ and $J_c = 80t^4 /U^3$ determines both t and U.
- Find $U = 7.3\ t$.
  - Beyond limit of validity of expansion in t/U
  - Use linear spin-wave analysis.

Some earlier theoretical work



P. Sengupta *et al.* Phys. Rev. B **66**, 144420 (2002)

- Quantum Monte Carlo simulations include quantum corrections (beyond linear spin waves)
- Limitation, SMA
- Find $U = 6t$
  - In agreement with RPA
  - Too small to fit optical gap at half-filling
  - Band structure effects should become more important.

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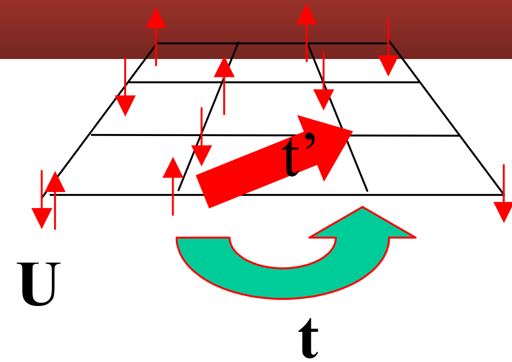
What we do here



$t' = -0.35\ t$

- Quantum Monte Carlo with SMA for

$$H = -t \sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma} \left(c^{\dagger}_{\mathbf{i},\sigma} c_{\mathbf{j},\sigma} + c^{\dagger}_{\mathbf{j},\sigma} c_{\mathbf{i},\sigma}\right) - t' \sum_{\langle\langle \mathbf{i},\mathbf{j}\rangle\rangle,\sigma} \left(c^{\dagger}_{\mathbf{i},\sigma} c_{\mathbf{j},\sigma} + c^{\dagger}_{\mathbf{j},\sigma} c_{\mathbf{i},\sigma}\right) + U \sum_{\mathbf{i}} n_{\mathbf{i},\uparrow} n_{\mathbf{i},\downarrow}$$

- Second-neighbor hopping, $t' = -0.35\ t$

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What is the method?

Quantum Monte Carlo calculations, including *t'*

Single Mode Approximation

$$\omega(\mathbf{q}) = 2S(\mathbf{q})/\chi(\mathbf{q})$$

How QMC works

Compute statistical averages with $\mathrm{Tr}[e^{-\beta(H-\mu N)}]$

$$k_B = 1,\ t = 1,\ \beta = 1/T$$

Problem for importance sampling

$$H = K + V$$

$$[K, V] \neq 0$$

Trotter decomposition

$$e^{-\beta(H-\mu N)} = e^{-\Delta\tau(H-\mu N)} e^{-\Delta\tau(H-\mu N)} \ldots e^{-\Delta\tau(H-\mu N)}$$

$$e^{-\Delta\tau(H-\mu N)} = e^{-\Delta\tau K} e^{-\Delta\tau(V-\mu N)} + O(\Delta\tau^2)$$

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QMC, continued

Hubbard-Stratonovich transformation :

$$e^{-\Delta\tau U\left(n_{\mathbf{i},\uparrow}-\frac{1}{2}\right)\left(n_{\mathbf{i},\downarrow}-\frac{1}{2}\right)} = e^{-\Delta\tau U/4}\,\frac{1}{2}\sum_{x_i=\pm 1} e^{\lambda x_i (n_{\mathbf{i},\uparrow}-n_{\mathbf{i},\downarrow})}$$

$$\cosh(\lambda) = e^{\Delta\tau U/2}$$

Quantum Mechanical trace can be performed : gives a determinant

Determinant as a Boltzmann weight gives « sign problem ».

Put sign in observables.

Parameters for QMC calculations

- Imaginary time discretization :

  $\Delta\tau = 1/10$ but same results as $\Delta\tau = 1/8$
- Gram-Schmidt every 5 time slices
- Estimator, $\langle S_z S_z \rangle$
- Measurements, 1.25×10^5
- Block size for statistical error estimation, *250*

Technical details

- Fortran 90
- ifc
- Scaling of computation time $L^6 N_\tau$
- One job for *12 X 12* with 10^5 measurements, 10^4 warmups takes *33 MB* and 20 days on one CPU of elix 2 (*P IV, 2.5 GHz*)
- If distribute job on 10 nodes for *8 X 8* lattice, one run at fixed parameters takes one day on elix 1 (*P III, 667 MHz*).

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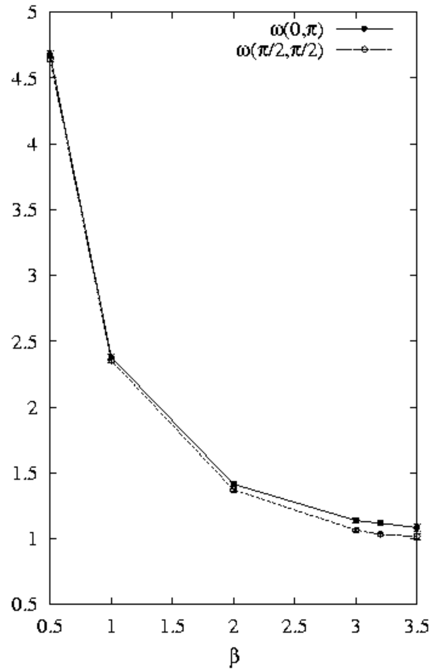
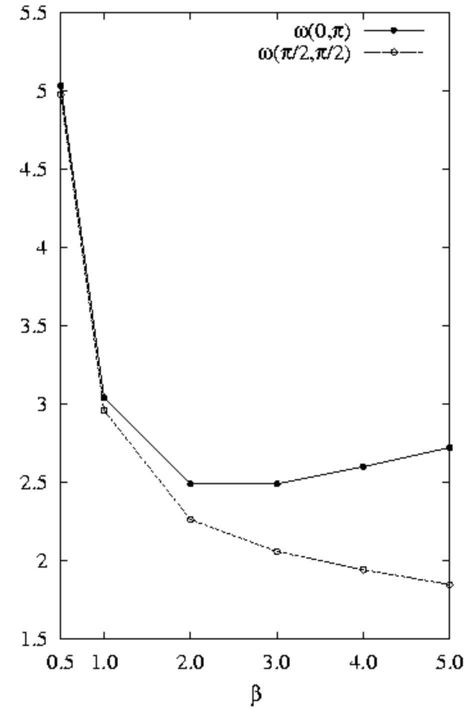
Single-mode approximation

$$\omega(\mathbf{q}) = 2S(\mathbf{q})/\chi(\mathbf{q})$$





U = 6

U = 0

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What are the results ?

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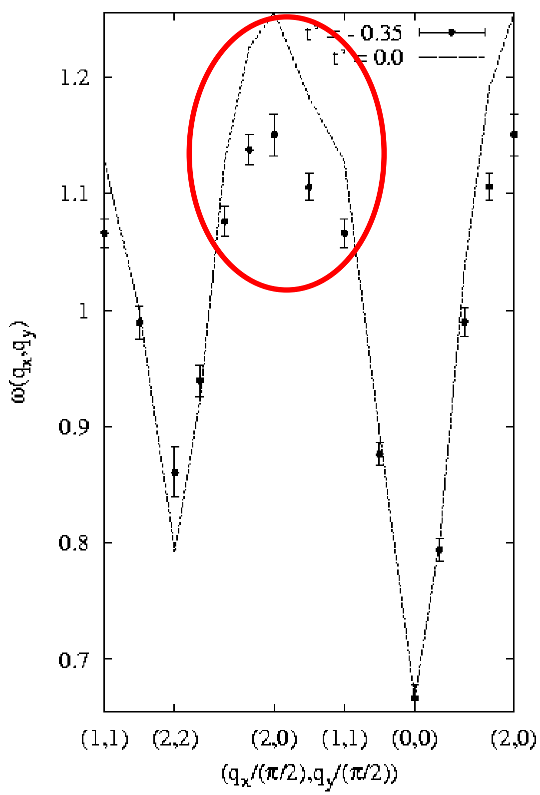
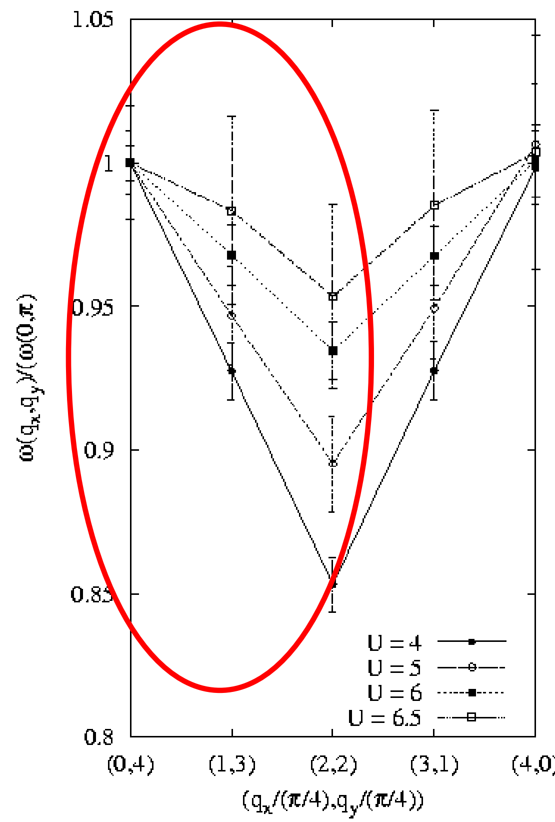
What are the results ?



Spin-wave dispersion,

U = 6, *t'*=0 and *t'* = -0.35



Various values of *U*

Results

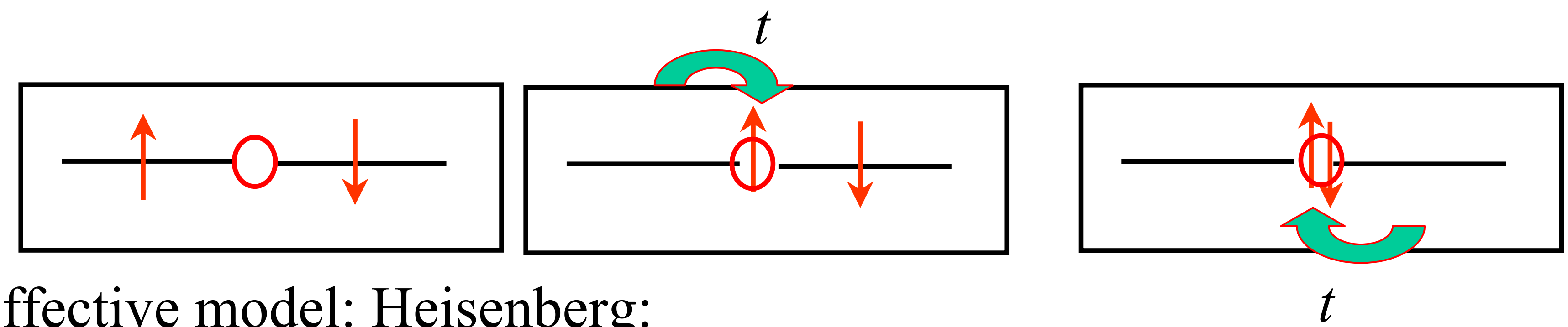
- $U = 5.0\ t\ \ \pm 0.5\ t$ (*cf* $U = 6\ t$ when $t' = 0$)
- In agreement with RPA
  - Singh Goswami, Phys. Rev. B **66,** *92402 (2002)*.
  - Peres, Araujo, Phys. Stat. Sol. **236**, 523 (2003).
- Correction in the wrong direction but this is expected at strong coupling:
  - t' induces antiferromagnetic second-neighbor interaction.
  - Should be ferro. according to linear spin waves

Perspectives

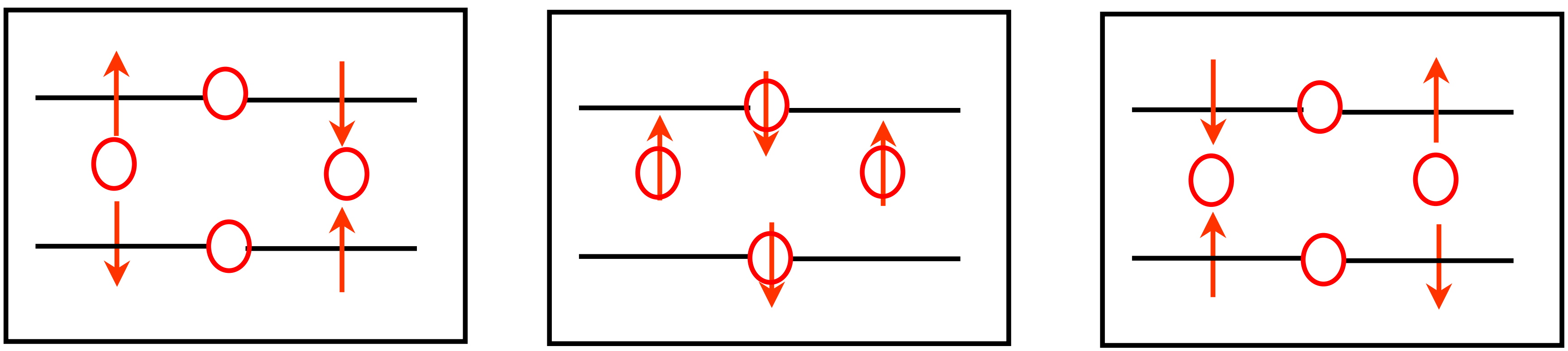
- Single-mode approximation invalid ?

- Should go back to three-band model where link between J and J_c is different.
  - E. Müller-Hartmann and A. Reischl, Eur. Phys. J. B 28, 173 (2002).

- Same Hamiltonian (Hubbard one-band) cannot describe both spin and charge (optical gap) excitations.



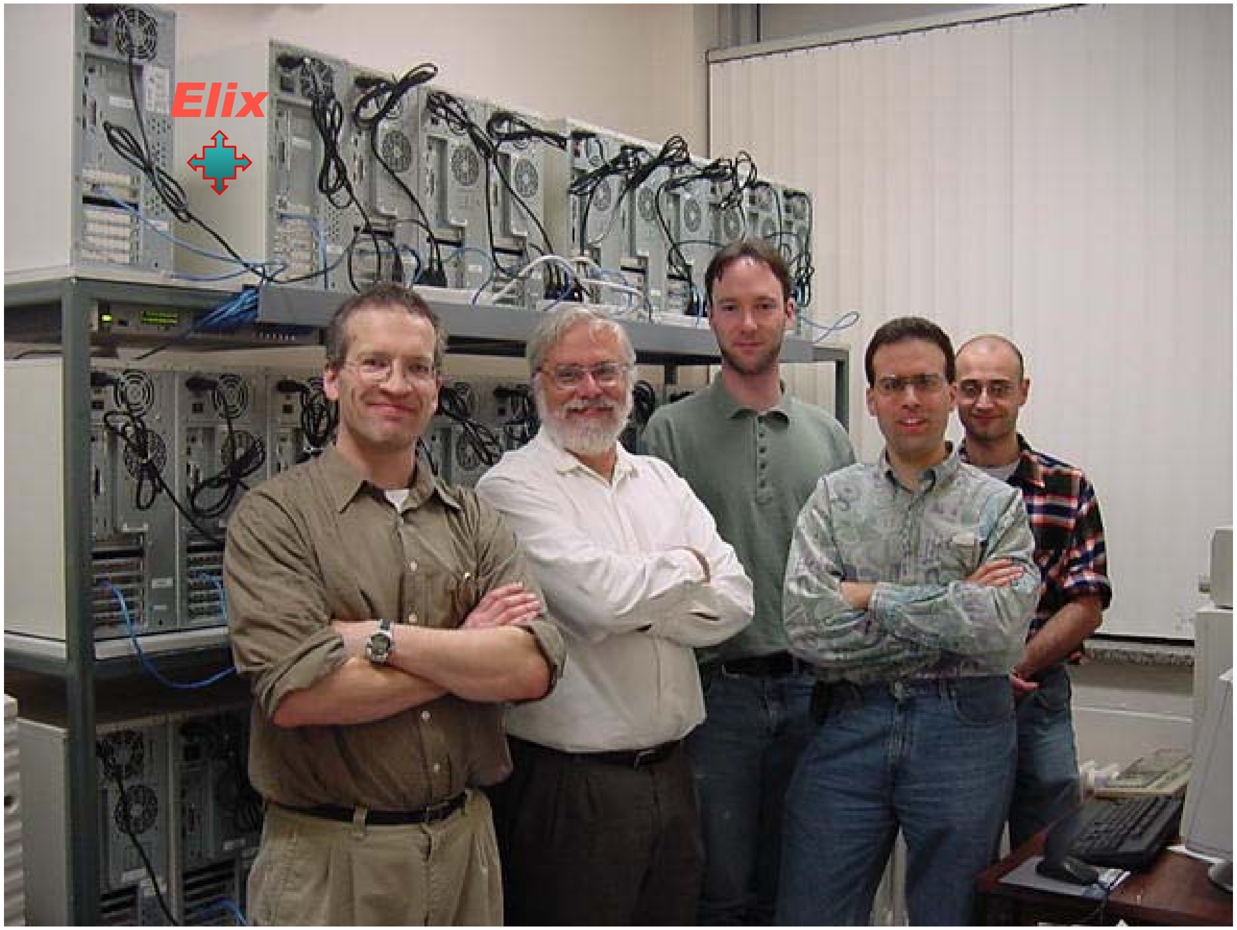
Effective model: Heisenberg:



Ring
exchange

and second-neighbor hopping

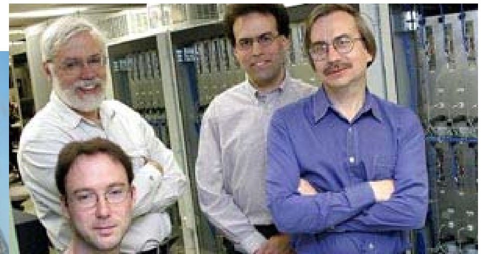
Michel Barrette Mehdi Bozzo-Rey

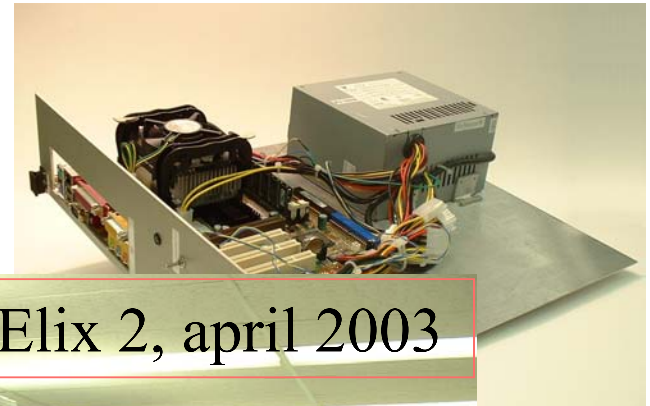


David Sénéchal A.-M.T. Alain Veilleux

Elix 2, april 2003

Carol Gauthier, analyste en Calcul du CCS en plein machinage d'un noeud d'Elix2





Un noeud d'Elix2

Elix2 vu de profil

De gauche à droite: Alain Veilleux, Michel Barrette, Jean-Phillipe Turcotte, Carol Gauthier, Patrick Vachon et le 1er noeud d'Elix

Equipe du CCS devant Elix2. Al'arrière: Patrick Vachon, Minh-Nghia Nguyen, David Lauzon, Michel Barrette, Mehdi Bozzo-Rey, Simon Lessard, Alain Veilleux. A l'avant: Patrice Albaret, Karl Gaven-Venet, Benoît des Ligneris, Francis Giraldeau. Etait absent de la photo: Jean-Philippe Turcotte, Carol Gauthier, Xavier Barnabé Thériault et Mathieu Lutfy

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A-M.T. Alexandre Blais Vasyl Hankevych

Sébastien Roy Sarma Kancharla

Bumsoo Kyung Maxim Mar'enko

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C'est fini. . .

enfin