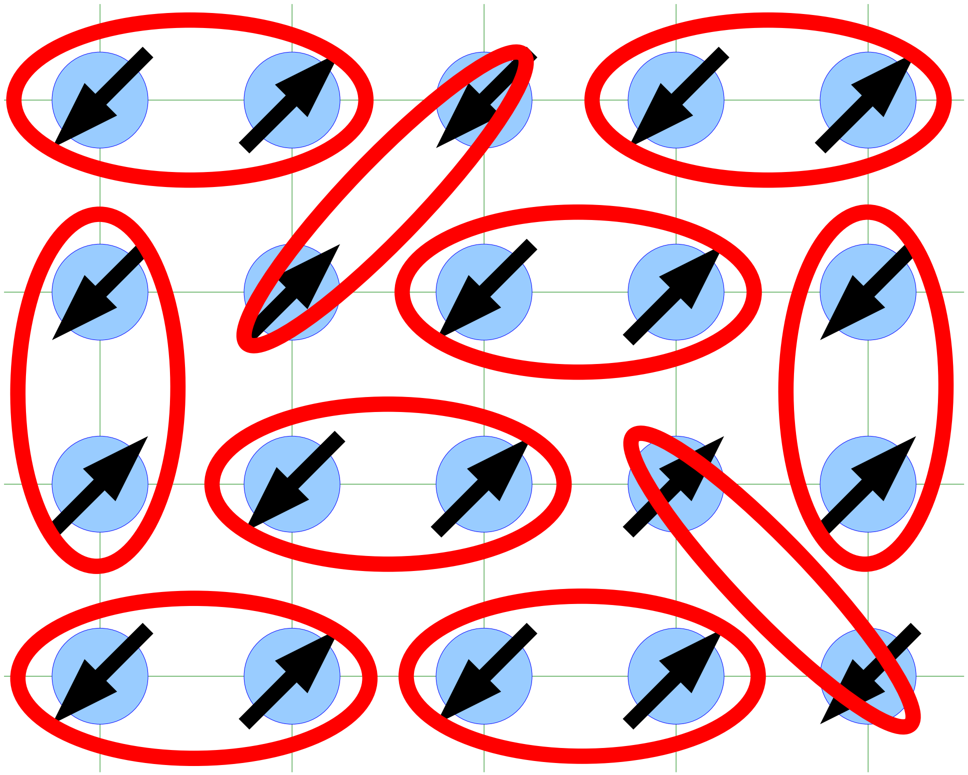
Resonating-valence-bond physics and topological order in two dimensions: from dimer models to high-temperature superconductivity

D. Ivanov, EPFL

Collaboration with:

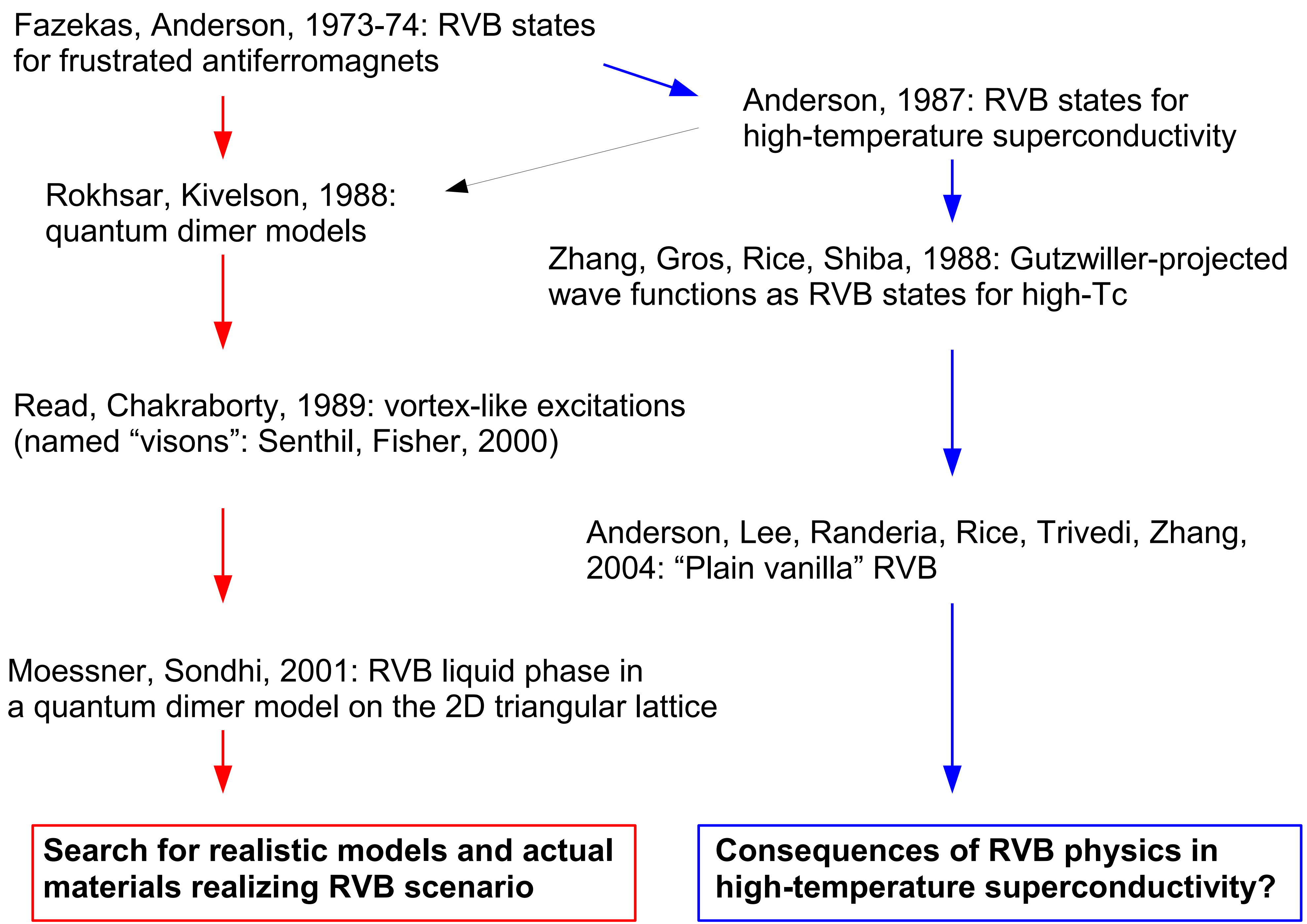
P.A.Lee, T. Senthil – MIT
M.Feigelman, A. Ioselevich – Landau Institute
F.Mila, A.Ralko – EPFL
F.Becca, M.Ferrero – SISSA, Trieste

Resonating-valence-bond (RVB) state:



Electrons on the lattice
(half-integer spin per unit cell)
form <u>short-range singlets</u>
(fluctuating = linear superposition
of different singlet configurations)

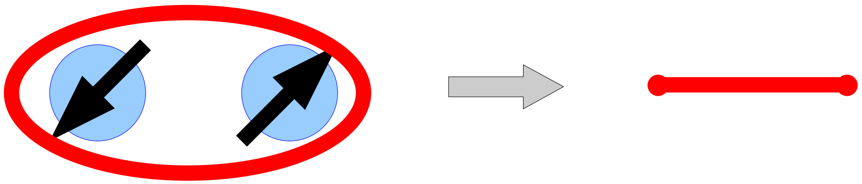
<u>No symmetry breaking:</u>
(1) the wave function is a spin singlet (no <u>spin</u> symmetry breaking)
(2) no preferred positions of singlets (no <u>translational</u> symmetry breaking)


Fazekas, Anderson, 1973-74: RVB states for frustrated antiferromagnets
Anderson, 1987: RVB states for high-temperature superconductivity
Rokhsar, Kivelson, 1988: quantum dimer models
Zhang, Gros, Rice, Shiba, 1988: Gutzwiller-projected wave functions as RVB states for high-Tc
Read, Chakraborty, 1989: vortex-like excitations (named “visons”: Senthil, Fisher, 2000)
Anderson, Lee, Randeria, Rice, Trivedi, Zhang, 2004: “Plain vanilla” RVB
Moessner, Sondhi, 2001: RVB liquid phase in a quantum dimer model on the 2D triangular lattice
Search for realistic models and actual materials realizing RVB scenario
Consequences of RVB physics in high-temperature superconductivity?

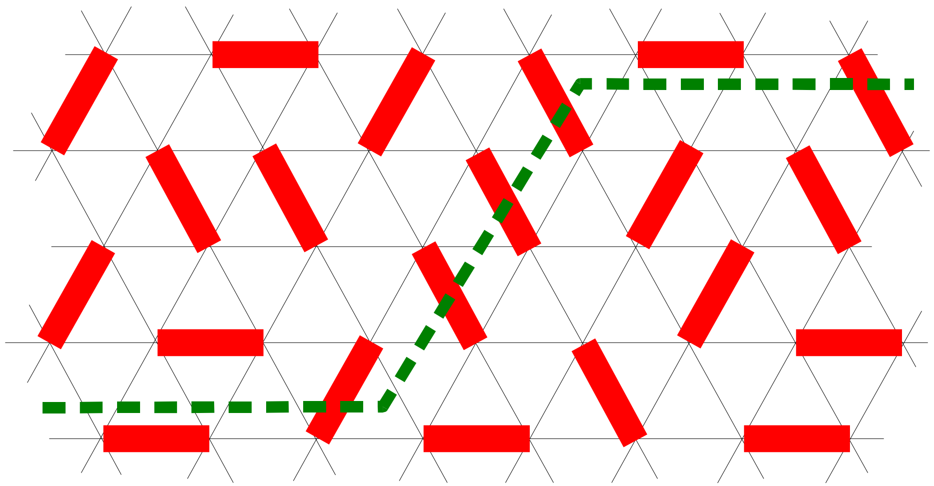
Outline:

1. Z_2 topological order and vortex-like excitations (“visons”)
2. Visons in dimer models
3. Visons in Gutzwiller-projected wave functions
4. Generalization of the RVB construction: loop path integral
5. Summary, comments, and questions.

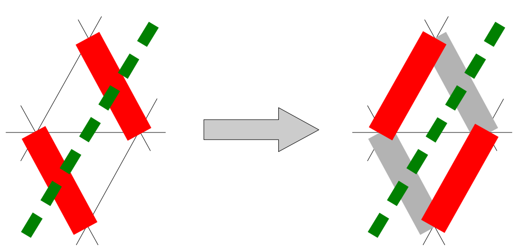
Z_2 topological order



From singlets – to dimers
(neglecting the overlap!!!)



New type of conservation law emerges: for any contour, local rearrangement of dimers does not change the parity of the number of intersecting dimers (Z_2 index)



this conservation law does not depend on the properties of the lattice or on the type of local rearrangement

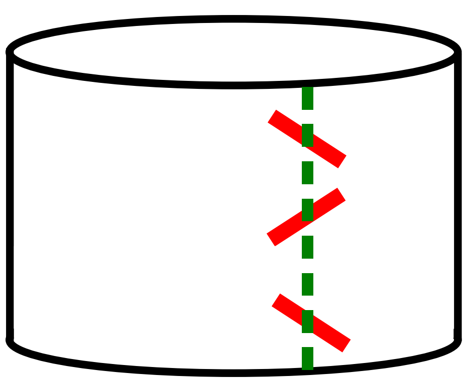
[for bipartite lattices, additional conservation laws, $Z_2 \rightarrow U(1)$]

Topological degeneracy on multiply connected domains

For multiply connected domains (cylinder, torus, plane with holes, etc.), this conservation law implies decomposition of the Hilbert space into several disconnected subspaces

Assuming the absence of dimer crystallization (all correlations are exponentially decaying), this leads to a topological degeneracy in the thermodynamic limit (system size $L \longrightarrow \infty$)

Example: cylinder



Two topological sectors: even / odd with identical properties (ground state and excitations)

Criteria of topological order for RVB states

On a multiply connected domain:

Degenerate states $|A\rangle$ and $|B\rangle$ should obey

1. identical local properties: $\langle A|X|A\rangle = \langle B|X|B\rangle$

   for any local operator X (in the limit $L \to \infty$)

2. orthogonality: $\langle A|X|B\rangle = 0$

   again, for any local operator X (in the limit $L \to \infty$)

For dimer models, the condition 2. is <u>automatically satisfied</u>, the condition 1. is related to the <u>absence of crystallization</u>.

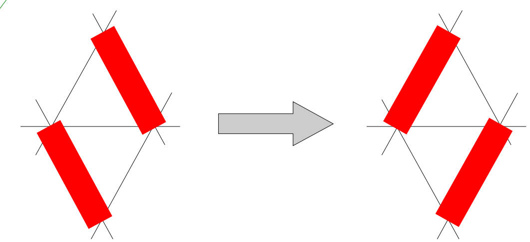
For RVB states with spin, the condition 2. is nontrivial (related to the <u>absence of spin ordering</u>).

Example: Rokhsar-Kivelson model on the triangular lattice

$$H_{RK} = \sum \left(-t \,|\, = \,\rangle\langle\, \| \,| + v \,|\, = \,\rangle\langle\, = \,| \right)$$

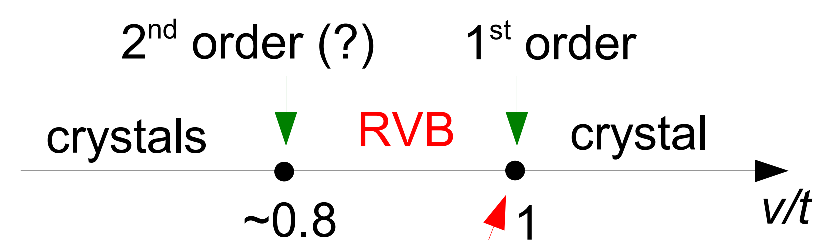
sum over all rhombi of the triangular lattice

flips



potential term

Phase diagram [Moessner, Sondhi, 2001; Ralko, Ferrero, Becca, D.I., Mila, 2005-06]:

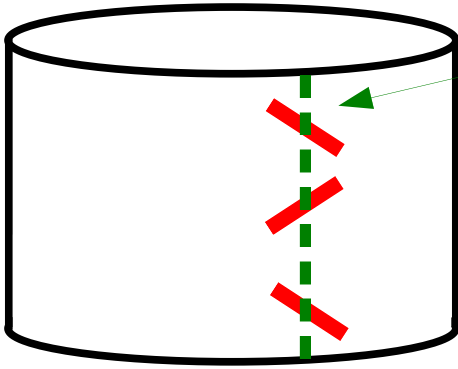


Topological order explicitly proven [Ioselevich, D.I., Feigelman]:

$$\langle A|X|A\rangle - \langle B|X|B\rangle \propto e^{-L/\xi}$$

A special "RK point" (ground state is exactly known and correlations can be computed)

Topological order → vortex-like excitations



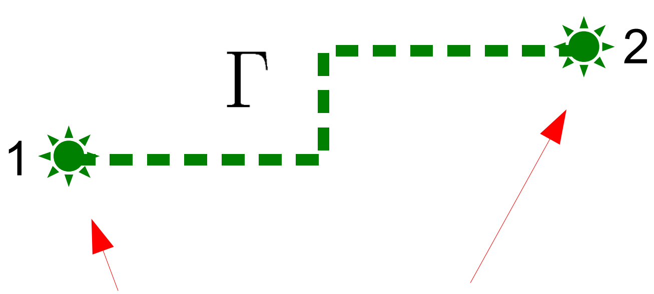
N_Γ – number of intersections with the contour Γ

"vison" operator: $V = (-1)^{N_\Gamma}$

$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ in the even-odd basis

The topological degeneracy implies a new type of excitations: Z_2 vortices ("visons")

A prototype of a vison:

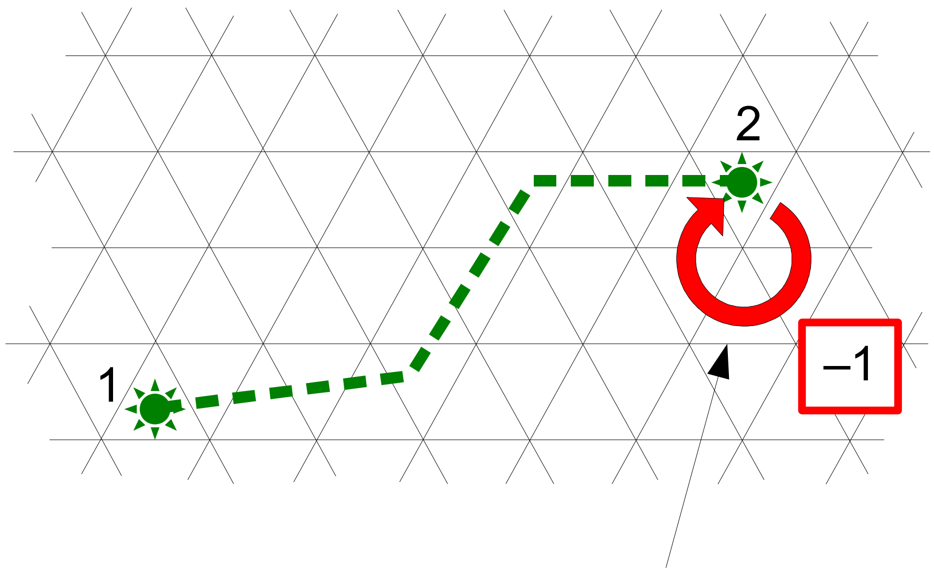


Now end points are inside two lattice plaquettes (triangles)

$$V_1 \cdot V_2 = (-1)^{N_\Gamma}$$

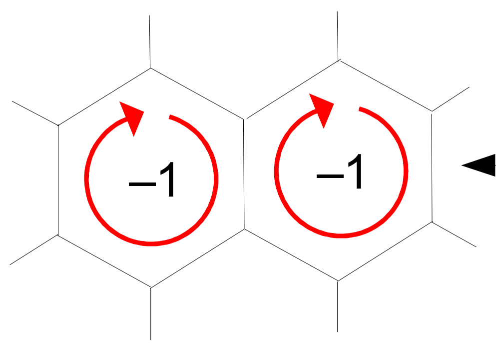
Two vortices (nonlocal) should be "dressed" with local dimer operators to become eigenstates

Example: visons in the RK dimer model on the triangular lattice



At the RK point (v=t), the excitation spectrum may be computed by using the equivalence between quantum mechanics in imaginary time and a classical stochastic process (modeling a classical 2D system instead of a quantum 2+1D) [C.Henley, 2003]

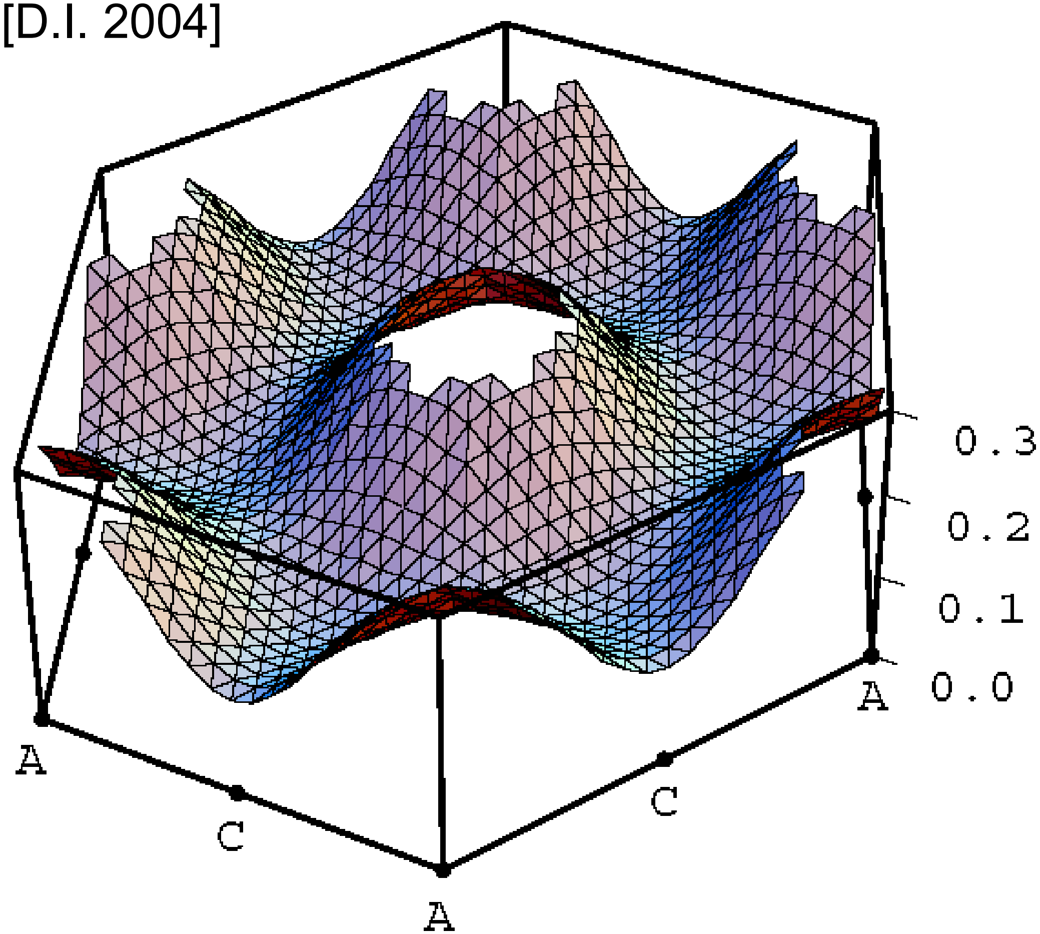
Note that because of the contour attached, visons live on a dual lattice (hexagonal) with frustration.

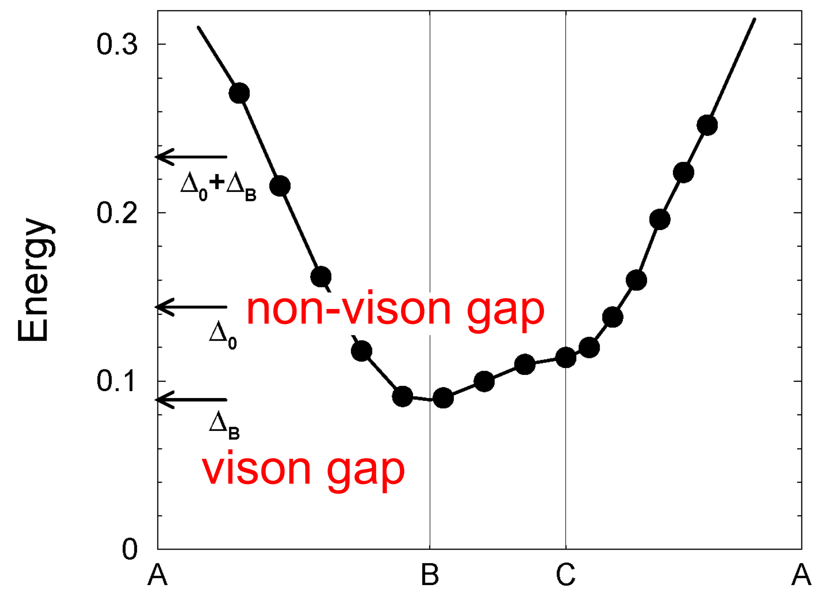


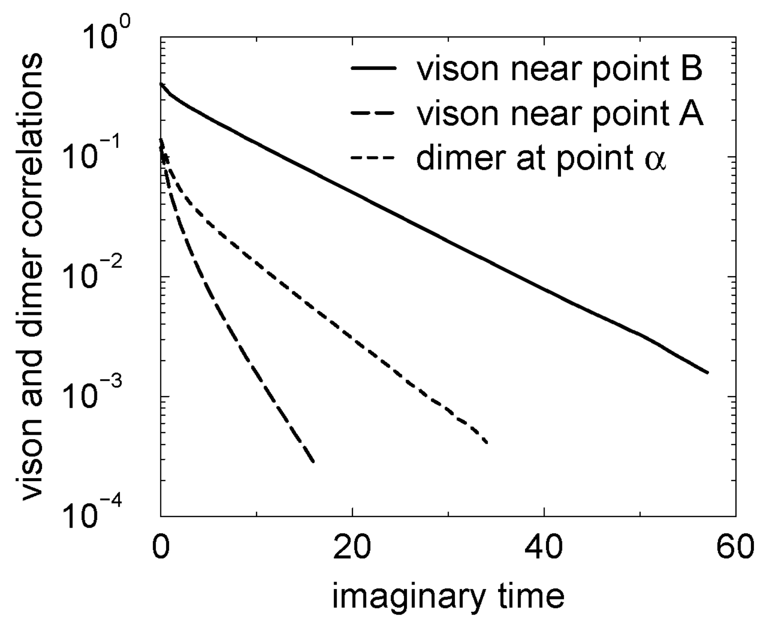
Half flux per hexagon for visons

Vison gap and spectrum at the RK point

[D.I. 2004]







1. Non-trivial vison dispersion
2. Visons are indeed elementary (lowest) excitations [non-vison gap is higher]

Summary 1:

1. In the RVB state, visons are elementary excitations which carry no spin and no charge.
2. Visons appear as a consequence of topological order (degeneracy depending on the connectivity of the cluster).
3. Visons can be conveniently modeled in quantum dimer systems.

Question:

Can we find visons in systems with spin and charge degrees of freedom?

Hint: possibly in Gutzwiller-projected wave functions

Gutzwiller-projected (GP) construction for [doped] Mott insulators

Physical Hamiltonian: spin or t-J (on a lattice)

<u>t-J model</u> [for high-temperature superconductivity]:

$$H_{\text{phys}} = P_G \left(-t \sum_{ij} (c_i^\dagger c_j + c_j^\dagger c_i) \right) P_G + J \sum_{ij} (\vec{S}_i \vec{S}_j - \frac{1}{4} n_i n_j)$$

Projectors onto no-double-occupancy states
(two electrons on one lattice site are prohibited)

hopping

spin interaction

reduces to a <u>Heisenberg spin Hamiltonian</u> at “half filling”:

$$H_{\text{phys}} = \sum_{ij} J_{ij} \vec{S}_i \vec{S}_j$$

(possibly frustrated, depending on the couplings J_{ij})

For frustrated antiferromagnets (either Heisenberg frustration or effective frustration by mobile holes), Gutzwiller projection often provides a good variational ground-state ansatz

GP construction:

1. Take a BCS wave function: $\Psi_{\mathrm{BCS}} = \prod_k \left(u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \right) |0\rangle$
2. Project onto no-double-occupancy states: $\Psi_{\mathrm{GP}} = P_G \Psi_{\mathrm{BCS}}$
3. Calculate (numerically) energy $E(\chi, \Delta) = \langle \Psi_{\mathrm{GP}} | H_{\mathrm{phys}} | \Psi_{\mathrm{GP}} \rangle$
4. Optimize variational parameters (χ, Δ) to minimize it.

Gutzwiller-projected states are:

(1) known to provide a good variational ansatz for systems with magnetic frustration (t-J model, J1-J2 Heisenberg model, Heisenberg model on the kagome lattice, etc.)

(2) suggested to have a RVB structure [Anderson, 1987]

Do they also have topological order and visons?

Testing for topological order in GP wave functions

[D.I., Senthil, 2002]

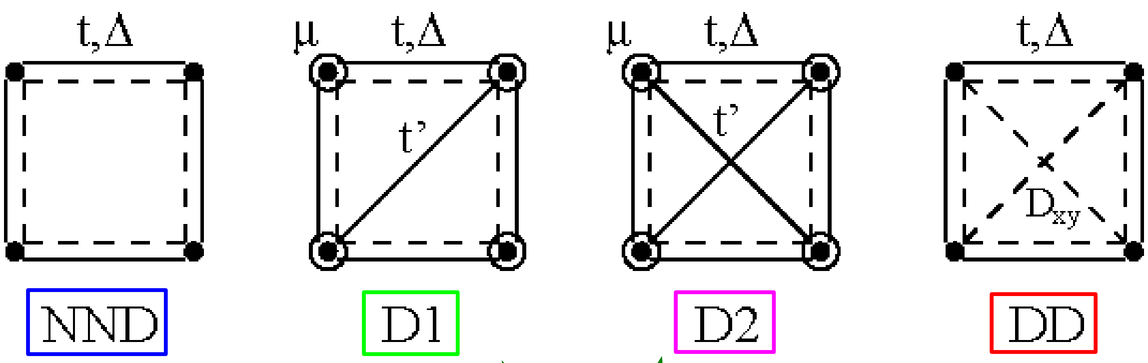
Instead of even-odd sectors (for dimers), the topological sectors (if any) are realized by projecting BCS states with periodic or antiperiodic boundary conditions for fermions.

For the spin system (undoped), this produces two wave functions $|+\rangle$ and $|-\rangle$ for the same spin Hamiltonian (the spin system have the same boundary conditions).

Both criteria of the topological order must be checked:

1. $\langle + | X | - \rangle \to 0$
2. $\langle + | X | + \rangle - \langle - | X | - \rangle \to 0$

Numerically testing four wave functions [D.I., Senthil, 2002]:



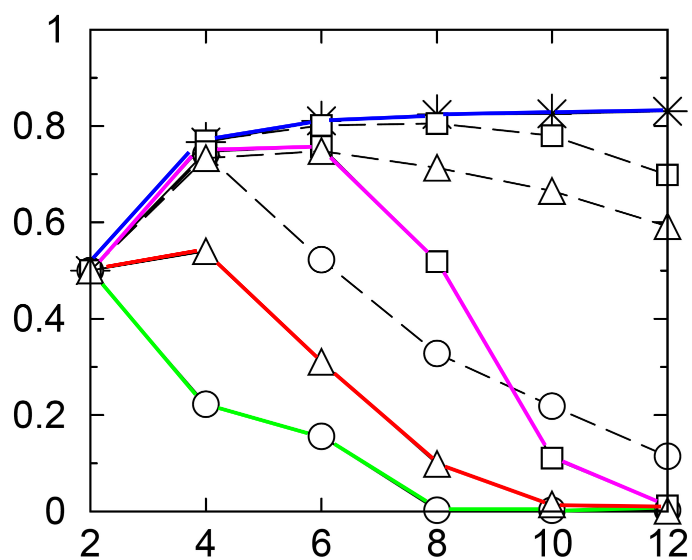
All these wave functions have nodes in the spectrum

nearest-neighbor d-wave BCS

+n-n-n hopping

$d_{x^2-y^2} + d_{xy}$ BCS [proposed for J_1-J_2 model by Capriotti, Becca, Parola, Sorella, 2001]

Test 1: overlaps $\langle + | - \rangle$

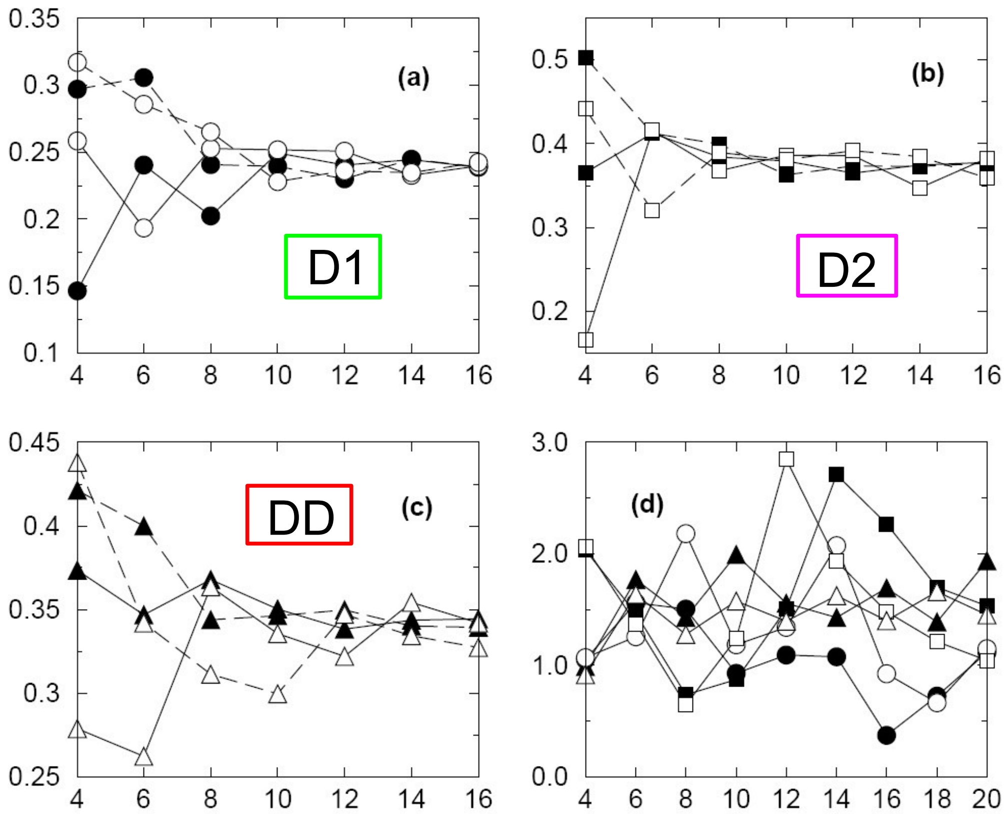


(linear system size)

NND does not pass the test, the other three wave functions do!

Test 2: nearest-neighbor correlations in different topological sectors

Spin correlations: $\langle S_i S_j \rangle_{\text{top. sector}}$



(four topological sectors on a torus)

Mean-square deviation among four sectors

$$\Delta S \cdot L^2$$

(linear system size)

Convergence between topological sectors is only algebraic

– because of nodes in the wave functions:

$$\langle + | S_i S_j | + \rangle - \langle - | S_i S_j | - \rangle \propto L^{-\alpha}\,, \qquad \alpha \sim 2$$

Summary 2:

1. Gutzwiller-projected wave functions may exhibit topological order (depending on the symmetries of the wave function ?)
2. For projected BCS states with nodes, the topological order is “weak” (algebraic).
3. Visons are projected BCS vortices [on doping into a superconducting state, they should become superconducting vortices]

Comment:

The RVB structure of GP wave functions may be conveniently described in terms of a “loop path integral”

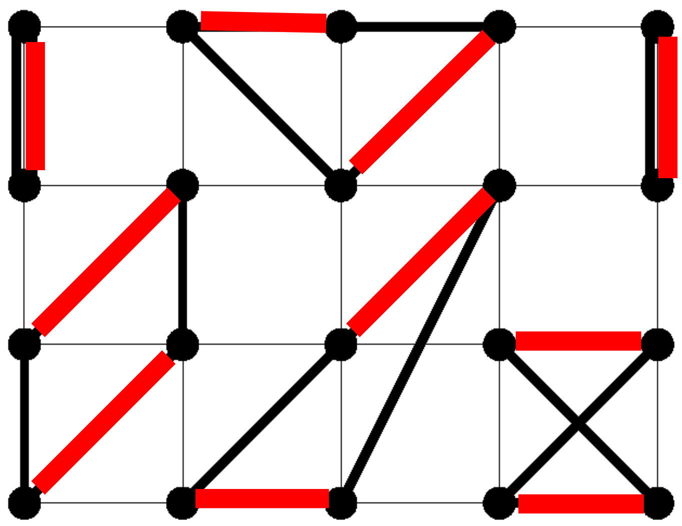
Loop path integral: RVB states

For wave functions composed of singlets with range-dependent amplitudes, the expectation values may be written in terms of a “loop path integral”:

“partition function”: $$\langle \Psi | \Psi \rangle = \sum_{\{C_n\}} \prod_n A(C_n)$$

loop amplitudes

sum over all loop coverings



(overlap of two singlet configurations)

For RVB construction (overlaps of spin singlets):

$$A(C) = -2\; a_{12}\; a_{23} \ldots a_{k1}$$

fermionic minus sign (for “fermionic” RVB)

singlet amplitudes

The "loop path integral" has a wider range of validity.
It unifies all RVB-like constructions of wave functions:

$$\boxed{\langle\Psi|\Psi\rangle = \sum_{\{C_n\}} \prod_n A(C_n)}$$

1. RVB state composed of singlets: $A(C) = -2\, a_{12}\, a_{23} \ldots a_{k1}$

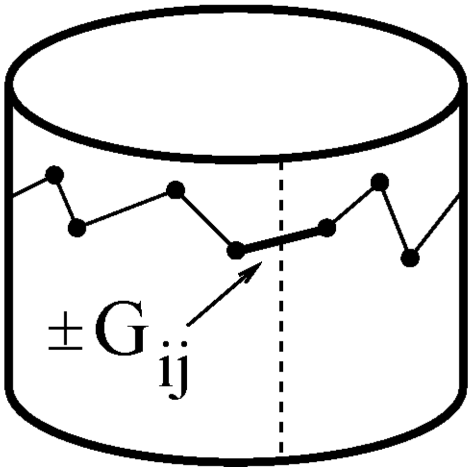
2. Rokhsar-Kivelson dimer state: $A(C) = \begin{cases} 1 & \text{for length-two loops} \\ 0 & \text{otherwise} \end{cases}$

3. Gutzwiller-projected BCS wave functions (possibly with nodes) [D.I. 2005]:

$$A(C) = -\mathrm{Tr}\, G_{12} G_{23} \ldots G_{k1}$$

2x2 matrices: equal-time BCS Green functions

Topological order may be formulated in terms of loop behavior (topological sectors ↔ assigning ± sign for globally winding loops)



The two conditions of topological order may be understood as
(1) loops are short ranged and
(2) loops do not crystallize

Algebraic G_{ij} ➡ Algebraic decay of loop size: $|G_{ij}|^2$ or slower! ➡ Algebraic topological order

Analytic study of loop correlations is difficult because of the close-packing constraint

RVB state in doped systems

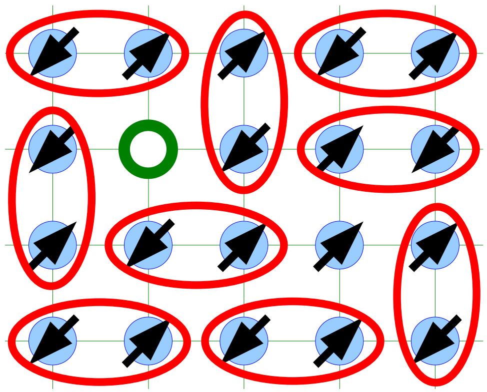
(with charge and spin degrees of freedom)

???

spin-charge separation

or

Gutzwiller-projected quasiparticles
(renormalized BCS)



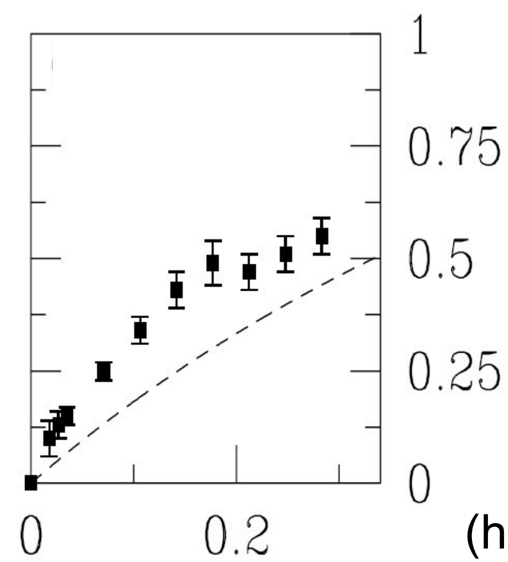
$$|\Psi_k\rangle = P_G\,\gamma_k\,|\mathrm{BCS}\rangle$$

Have reduced spectral weight
[Paramekanti, Randeria, Trivedi, 2001]

Static monomer correlation function
in the RK dimer model on the triangular
lattice indicates hole deconfinement
[Fendley, Moessner, Sondhi, 2002]

partition function with two holes

$$\lim_{|x_1-x_2|\to\infty} \frac{Z(x_1,x_2)}{Z} > 0$$



quasiparticle
spectral
weight

(hole doping)

Summary and outlook

1. RVB states are characterized by the Z_2 topological order (topological degeneracy + vortex-like excitations).

2. Quantum dimer models can be used as toy models for studying chargeless and spinless degrees of freedom of RVB.

3. Gutzwiller-projected wave functions have a RVB-like structure even when projecting BCS states with nodes, but the topological order, if present, is only "algebraic".

Questions:

1. What happens to topological order upon doping? Are there any traces of Z_2 topological order in high-T_c superconductors?
   [conjecture by Senthil and Fisher, 2001: visons in the pseudogap state
   → not observed so far]

2. Can realistic spin models (e.g. frustrated Heisenberg models) have RVB phase?