Nagaoka physics in kinetically frustrated electronic models

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Collaborators: Cintia Sposetti, Barbara Bravo, Franco Lisandrilni
Luis Manuel, Adolfo Trumper (Rosario)

Introduction: Hubbard model and Nagaoka ferromagnetism, and kinetic energy frustration
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Outlines

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We have found the generic existence of classical kinetic antiferromagnetism in kinetically frustrated (KF) models.
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🌟 We propose a new itinerant antiferromagnetism mechanism: **Release of the kinetic energy frustration** (non trivial spin Berry Phases or vanishing of frustrating loops)
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Calculations: DMRG on triangular and frustrated square lattices.
Interpretation: slave-fermion mean-field approximation,
Itineracy and Magnetism

Generic magnetic phase diagram of the Hubbard model on a bipartite lattice

virtual kinetic processes

real kinetic processes

\[ \hat{H}_{Hubbard} = - \sum_{\langle ij \rangle \sigma} t_{ij} (\hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \hat{c}^\dagger_{j\sigma} \hat{c}_{i\sigma}) + U \sum_i \hat{c}^\dagger_{i\uparrow} \hat{c}_{i\uparrow} \hat{c}^\dagger_{i\downarrow} \hat{c}_{i\downarrow} \]
Saturated Nagaoka's ferromagnetism

One of the few exact results:
Saturated Nagaoka's ferromagnetism

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Conditions

✧ Hubbard $U=\infty$ ($J=0$)
✧ One hole $N = N - 1$
✧ Connectivity $e^{\sum_i (-t_{ij})^n} > 0$
✧ minimum $n \leq 4$

Claudio Gazza,
Instituto de Física Rosario
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Y. Nagaoka, Phys. Rev. 147, 392 (1966)

Unique saturated ferromagnetic ground state (total spin $S = N_e / 2$)

Origin: constructive interference between processes in which the hole reaches a given lattice site via different routes.
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Bipartite lattice: particle-hole transformations can absorb $t$ sign, so it is irrelevant.

Non bipartite lattices: particle-hole asymmetry, $t$ sign is relevant

When the connectivity condition is not fulfilled the kinetic energy is frustrated, and Nagaoka's theorem is not valid.
Kinetic energy frustration

Three-site toy model
Kinetic energy frustration

Three-site toy model

**Magnetic frustration:**
classical and/or quantum
Kinetic energy frustration

Three-site toy model

**Magnetic frustration:**
classical and/or quantum

![Diagram](triangle)

**But there is also a kinetic energy frustration: quantum origin**

Consider one toy model: a tight-binding model on a triangle
Kinetic energy frustration

Three-site toy model

**Magnetic frustration:**
classical and/or quantum

But there is also a kinetic energy frustration: quantum origin
Consider one toy model: a tight-binding model on a triangle

For one electron, we expect

\[ E_{\text{min}} = -z |t| \]

where \( z = 2 \), however →

<table>
<thead>
<tr>
<th>Unfrustrated</th>
<th>Frustrated</th>
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<tbody>
<tr>
<td>For ( t &gt; 0 ):</td>
<td>For ( t &lt; 0 ):</td>
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Kinetic energy frustration and magnetism

Another toy model: 3-site Hubbard with 4 electrons
Kinetic energy frustration and magnetism

Another toy model: 3-site Hubbard with 4 electrons

\[ U > 0, \ t > 0 : \]

\begin{align*}
\text{triplet} \\
t > 0: \text{triplet} \rightarrow \text{Nagaoka ferromagnetism}
\end{align*}
Kinetic energy frustration and magnetism

Another toy model: 3-site Hubbard with 4 electrons

$U > 0, t > 0$:

$U > 0, t < 0$:

$\cos(\theta)\left(\begin{array}{c}+\end{array}\right)$

$sin(\theta)\left(\begin{array}{c}+\end{array}\right)$

triplet

t>0: triplet $\rightarrow$ Nagaoka ferromagnetism

t<0: singlet $\rightarrow$ resonating valence bond state

Figure taken from J. Merino et al., PRB 73, 235107 (2006)
What happens when theorem is not valid?

... little is known
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In a seminal work, Haerter and Shastry [PRL 95, 087202 (2005)] proposed a $120^\circ$ Neel order in the triangular lattice $\rightarrow$ Kinetic antiferromagnetism
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We study the infinite U Hubbard model, with one hole doped away half filling, on two kinetically frustrated lattices:

★ Triangular lattice with $t > 0$
★ Square lattice with second neighboor hopping $t_2 = t_1 > 0$
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We study the infinite U Hubbard model, with one hole doped away half filling, on two kinetically frustrated lattices:

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- Square lattice with second neighbour hopping $t_2 = t_1 > 0$

![Diagram showing lattice configurations](image)

Number of states retained
$m=200$ to $m=300 \rightarrow P_m \sim O(10^{-7})$

Clusters size used: 18, 36, 54, 72 and 90

$L_x=3, 6, 9, 12$ and $15$  $L_y=6$

cylindrical boundary conditions
(open in x, periodic in y)

White and Chernyshev, PRL 99, 127004 (2007),
$S^{zz}(k) = \frac{1}{N} \sum_{ij} \langle S^z_i S^z_j \rangle e^{ik(R_i - R_j)}$

Ground state has an AF 120° Neel order, as the triangular Heisenberg
Local magnetization: triangular lattice $t>0$

$$M_s = \sqrt{(1/N) \sum_\alpha \langle \sum_{i \in \alpha} (S_i)^2 \rangle} = \sqrt{(4/N) S^{zz}(q^*)}$$

- Local magnetization extrapolates to the classical value
- Heisenberg model: strong quantum spin fluctuations

- △ Hubbard
- ○ Heisenberg
Local magnetization: triangular lattice \( t > 0 \)

\[
M_s = \sqrt{\frac{1}{N}} \sum_\alpha \left( \sum_{i \in \alpha} (S_i)^2 \right) = \sqrt{\frac{4}{N}} S^{zz} (q^*)
\]

- Local magnetization extrapolates to the classical value
- Heisenberg model: strong quantum spin fluctuations
- \( \triangle \) Hubbard
- \( \triangle \) Hubbard \( (B=0.1t) \)
- \( \bigcirc \) Heisenberg
- \( \bullet \) Heisenberg \( (B=0.1t) \)
- B: small magnetic field applied in one sublattice to pin the classical order
Local magnetization: square lattice

\[ t_2 = t_1 > 0 \]

- Local magnetization extrapolates to its classical value
  - \( \square \) Hubbard (B=0)
  - \( \blacksquare \) Hubbard (B=0.1t)

\[ M_s \]

\[ N^{-1/2} \]

Antiferromagnetic \( (\pi, \pi) \) Neel classical order!

The frustrated J1-J2 Heisenberg model, with J1=J2, has a collinear ground state, \( Q = (\pi, 0) \)
Origin of this kinetic magnetism

Which is the origin of this kinetic antiferromagnetism?

Hole motion in antiferromagnetic backgrounds can release its kinetic energy frustration
Slave-fermions - mean field approximation
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Slave-fermion representation:
charge $\rightarrow$ spinless fermion
spin $\rightarrow$ Schwinger bosons

$$\hat{c}_{i\sigma} = \hat{f}_{i}^{\dagger} \hat{b}_{i\sigma}.$$  
L. Manuel, et al,  
PRB 61, 3470 (2000)

$$\hat{H}_{t,J}^{MF} = \sum_{\mathbf{k}} \varepsilon_{f\mathbf{k}} \hat{f}_{\mathbf{k}}^{\dagger} \hat{f}_{\mathbf{k}} + \sum_{\mathbf{k}\sigma} \left[ \varepsilon_{\mathbf{k}} \hat{b}_{\mathbf{k}\sigma}^{\dagger} \hat{b}_{\mathbf{k}\sigma} + \sigma \gamma_{\mathbf{k}} \hat{b}_{\mathbf{k}\sigma}^{\dagger} \hat{b}_{-\mathbf{k}\bar{\sigma}}^{\dagger} + \sigma \tilde{\gamma}_{\mathbf{k}} \hat{b}_{\mathbf{k}\sigma} \hat{b}_{-\mathbf{k}\bar{\sigma}} \right] + \text{Cte.}$$

hole motion on magnetic background
exchange interactions: spin fluctuations $\rightarrow 0$ with $J/t$
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hole motion on magnetic background
exchange interactions: spin fluctuations $\rightarrow 0$ with J/t

$$\varepsilon_{f\mathbf{k}} = 4t \left[ B_{1} \cos k_{x} + B_{2} \cos \left( \frac{k_{x}}{2} + \frac{\sqrt{3}k_{y}}{2} \right) + B_{3} \cos \left( -\frac{k_{x}}{2} + \frac{\sqrt{3}k_{y}}{2} \right) \right] + \mu$$

Hole (slave fermion) band dispersion

$$B_{R} = \langle \frac{1}{2} \sum_{\sigma} \hat{b}_{i\sigma}^{\dagger} \hat{b}_{i+R\sigma} \rangle \sim B_{R}^{2} = S \cos \frac{Q_{R}}{2}$$

B complex phase around a closed loop $\sim$ spin Berry phases
Slave-fermions - mean field approximation

Slave-fermion representation:
charge → spinless fermion
spin → Schwinger bosons

\[ \hat{c}_{i\sigma} = \hat{f}_{i}^{\dagger} \hat{b}_{i\sigma}. \]

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\[ \hat{H}_{MF}^{tJ} = \sum_{\mathbf{k}} \varepsilon_{f\mathbf{k}} \hat{f}_{\mathbf{k}}^{\dagger} \hat{f}_{\mathbf{k}} + \sum_{\mathbf{k}\sigma} \left[ \varepsilon_{\mathbf{k}} \hat{b}_{\mathbf{k}\sigma}^{\dagger} \hat{b}_{\mathbf{k}\sigma} + \sigma \gamma_{\mathbf{k}} \hat{b}_{\mathbf{k}\sigma}^{\dagger} \hat{b}_{-\mathbf{k}\sigma}^{\dagger} + \sigma \tilde{\gamma}_{\mathbf{k}} \hat{b}_{\mathbf{k}\sigma} \hat{b}_{-\mathbf{k}\sigma} \right] + \text{Cte.} \]

hole motion on magnetic background
exchange interactions: spin fluctuations → 0 with J/t

\[ \varepsilon_{f\mathbf{k}} = 4t \left[ B_1 \cos k_x + B_2 \cos \left( \frac{k_x^2}{2} + \frac{\sqrt{3} k_y}{2} \right) + B_3 \cos \left( -\frac{k_x}{2} + \frac{\sqrt{3} k_y}{2} \right) \right] + \mu \]

Hole (slave fermion) band dispersion

Tight-binding like dispersion with renormalized hoppings

\[ \tilde{t}_R \rightarrow \tilde{t}_R B_R \]

i) Bandwidth reduction |B| <= 1/2 (like in double exchange processes)

ii) B can change the kinetic energy frustration of the hole motion, through its sign or modulus.
Release of the kinetical energy frustration
Release of the kinetical energy frustration

**Triangular lattice \( t > 0 \)**

Ferromagnetic phase:
all B's \( > 0 \) → the magnetic order does not change the kinetic frustration

\[ B_3 = B > 0 \quad B_2 = B > 0 \]
\[ B_1 = -B < 0 \]

120° Neel phase:
one B \( < 0 \), the other 2 B's \( > 0 \) →
the sign of B's (\( \pi \) spin Berry phase)
allows the release of the kinetic frustration
Release of the kinetical energy frustration

**Triangular lattice t>0**

Ferromagnetic phase:
all B's >0 → the magnetic order does not change the kinetic frustration

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120° Neel phase:
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Release of the kinetic energy frustration

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Ferromagnetic phase:
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\[ B_3 = B > 0 \quad B_2 = B > 0 \]

\[ B_1 = -B < 0 \]

120° Neel phase:
one B < 0, the other 2 B's > 0 → the sign of B's (π spin Berry phase) allows the release of the kinetic frustration

**Square lattice t2>0**

\[ t_R = t_R |B_R| \exp(i\phi_R) \]

\[ B_R \sim S \cos \left( \frac{Q \cdot R}{2} \right) \]

(π,π) Neel phase
vanishing of the effective hopping amplitude along the frustrating loops releases the kinetic frustration
Finite U: local magnetization vs J/t

DMRG and mean-field results

Triangular lattice, doping=0.0185

For all $J/t$ the ground state has 120° Neel order
$J/t \rightarrow 0$ Classical order parameter
$J/t \rightarrow$ infinite Heisenberg order parameter.

synergy between exchange and kinetic mechanism

\[
\hat{H}_{t,J} = -\sum_{iR\sigma} t_R \hat{c}_{i\sigma}^{\dagger} \hat{c}_{i+R\sigma} + \frac{1}{2} \sum_{iR} J_R \mathbf{S}_i \cdot \mathbf{S}_{i+R}
\]
Here we study anisotropic triangular lattice

\[ \frac{t'}{t} = 0 \quad Q = (0,0) \]

\[ \frac{t'}{t} = 1 \quad Q = \left( \frac{4\pi}{3}, 0 \right) \]

Magnetic wave vector vs spatial anisotropy
Kinetic magnetism transition

Here we study anisotropic triangular lattice

$t'/t=0$ $t'/t=1$

$Q=(0,0)$ $Q=(\frac{4\pi}{3},0)$

Magnetic wave vector vs spatial anisotropy

Square lattice:
abrupt transition between ferromagnetism and Neel order for
$t_2/t_1 \approx 0.22$
Conclusions
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- We propose a new itinerant antiferromagnetism mechanism: **Release of the kinetic energy frustration** driven by i) the spin Berry phase acquired by the hole or ii) the vanishing of effective hopping amplitude along the frustrating loops.
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Kagome lattice: Work in progress!
Thanks for your attention