Novel Orbital Physics – Unconventional BEC, Ferromagnetism, and Curie-Weiss Metal

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Introduction

Orbital physics in optical lattices

Solid states orbital systems

New states: Unconventional BEC

Novel strongly correlated quantum “materials”
Electron orbitals: a degree of freedom independent of charge and spin

• Orbital degeneracy and **spatial anisotropy.**

**d-orbitals:** $d_{x^2-y^2}, d_{r^2-3z^2}, d_{xy}, d_{yz}, d_{xz}$

**p-orbitals:** $p_x, p_y, p_z$

**$e_g$**

**$t_{2g}$**

**$\sigma$-bond**

**$\pi$-bond**

$t_{//} >> t_{\perp}$

<table>
<thead>
<tr>
<th>Orbitals in solids</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>simple metal (s-orbital)</strong></td>
</tr>
<tr>
<td><strong>semiconductor (p-orbital)</strong></td>
</tr>
<tr>
<td><strong>transition metal (d-orbital)</strong></td>
</tr>
<tr>
<td><strong>Rare earth (f-orbital)</strong></td>
</tr>
</tbody>
</table>

For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.
Orbital physics in transition-metal oxides

- Important to magnetism, superconductivity, and transport properties.

Orbital stripe order:
Manganite: \( \text{La}_{1-x}\text{Sr}_{1+x}\text{MnO}_4 \)

Iron-pnictide Supercond.
LaOFeAs
BEC of cold alkali atoms

- Dilute and weakly interacting boson systems.

\[ T > T_c \quad T < T_c \quad T << T_c \]

Time-of-flight spectra measure momentum space distribution.


\[ T_{BEC} \sim 1 \mu K \quad n \sim 10^{14} \text{ cm}^{-3} \]
Optical lattices: a new era of cold atom physics

- Interaction effects tunable by varying laser intensity.

\[ t : \text{inter-site tunneling} \]
\[ U : \text{on-site interaction} \]
A new direction: optical lattice orbital physics!

- Bosons/fermions in high-orbital bands.

Orbitals: energy levels (e.g. s, p) of each optical site.
Atoms play the role of electrons.

Good timing: pioneering experiments on orbital-bosons.

Square lattice (Mainz); double well lattice (NIST, Hamburg); polariton lattice (Stanford)

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Novel strongly correlated quantum "materials"
**Conventional v.s. unconventional superconductivity**

- **Cooper pair wavefunctions (WF):**
  \[
  \Psi(r_1, r_2) = \psi[(r_1 + r_2) / 2] \Delta(r_1 - r_2)
  \]
  \[
  \Delta(r_1 - r_2) = \int d\vec{k} e^{i\vec{k}(\vec{r}_1 - \vec{r}_2)} \Delta(\vec{k})
  \]

- **Conventional:** s-wave pairing symmetry.

- **Unconventional:** high partial wave symmetries (e.g. p, d, etc).

  - **d-wave:** high $T_c$ cuprates.
Phase-sensitive detection – interference

- Corner-Josephson $\pi$-junction for $d_{x^2-y^2}$

D. Van Harlingen, RMP (1995)

\[
I_{\text{max}} = I_0 \frac{\sin(\pi \Phi / \Phi_0)}{\pi \Phi / \Phi_0}
\]

\[
I_{\text{max}} = I_0 \frac{\sin^2(\pi \Phi / 2 \Phi_0)}{\pi \Phi / \Phi_0}
\]
Conventional BEC: s-symmetry

- Conventional BEC (superfluid $^4$He, cold alkali atom BEC, etc) -- no-node, s-sym.

- "no-node" theorem in single-particle QM.

$$\psi_G(\vec{r}) \geq 0$$

Generalization to boson many-body ground states!

- No-go! Unconventional symmetry (e.g. p, d) forbidden in ground states – requiring nodes.
**Unconventional BECs in high-orbital bands**

**Meta-stable excited states:**
Novel properties not existing in the ground states

Unconventional condensation symmetry and time-reversal symmetry breaking


Already seen in experiments $(p_x \pm ip_y)$.


**matter-wave interference**
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Novel strongly correlated quantum "materials"
Strongly correlated p-orbitals

- Weakly correlated $p$-orbitals (e.g. semiconductors).

  Not many $p$-orbital Mott-insulators and ferromagnets.

- $p$-orbitals: the strongest anisotropy.

  - Combining strong correlation + strong anisotropy in optical lattices.

**Itinerant FM**, topological states, flat bands, unconventional Cooper pairing, frustrated orbital exchange…

$\sigma$-bond
Magnetism: local moments vs. itinerant fermions

• Local Moments: non-mobile, no Fermi surfaces.

\[ H = -J \sum_{ij} \sigma_i \sigma_j \]

\[ \chi = \frac{A}{T - T_c} \]

Curie-Weiss susceptibility

• Itinerant fermions: Fermi surfaces – much harder to form FM!

Pauli paramagnetism

\[ \chi = N_0 \left(1 - c \frac{T^2}{T_f^2}\right) \]

N_0: density of states at the Fermi level
Itinerant FM v.s. superconductivity: which is rarer?

Itinerant FM: A long-standing strong correlation problem
**Hund’s coupling ≠ global FM**

- Electron/hole spins add up when filling in degenerate orbitals.

- Most FM metals have orbital degeneracy and Hund’s coupling.

- Local vs. global:

  Hund’s rule usually cannot polarize the entire lattice!
Sufficient condition for Hund’s rule assisted itinerant FM

- Hund’s rule + quasi-1D bands (p-orbitals) \(\rightarrow\) 2D and 3D FM in the strong interaction regime.

• Orbital bosons (unconventional symmetry): $p_x \pm ip_y$
BECs beyond the “no-node” theorem – already observed!

• Orbital fermions: Itinerant FM, a long-standing problem – a non-perturbative study.
The “no-node” theorem (Perron-Frobenius)

• Many-body **ground-state wavefunctions** of bosons are positive-definite.

\[
\psi(r_1, r_2, \ldots r_n) \geq 0
\]

• A general property of the ground states:

Laplacian kinetic energy (no rotation).

Arbitrary single-particle potential (with lattice or not).

Coordinate-dependent interactions.

\[
H = \sum_{i=1}^{N} -\frac{\hbar^2 \nabla^2_i}{2M} + \sum_{i=1}^{N} U_{ex}(\vec{r}_i) + \sum_{i<j}^{N} V_{int}(\vec{r}_i - \vec{r}_j)
\]
Proof

Feynman, Statistical Mechanics

\[ \psi(r_1, r_2, \ldots r_n) \quad |\psi(r_1, r_2, \ldots r_n)| \quad \phi(r_1, r_2, \ldots r_n) > 0 \]

\[ \langle \psi | H | \psi \rangle = \int dr_1 \ldots dr_n \frac{\hbar^2}{2m} \sum_{i=1}^{n} |\nabla_i \psi(r_1, \ldots r_n)|^2 + |\psi(r_1, \ldots r_n)|^2 \sum_{i=1}^{n} U_{ex} (r_i) \]

\[ + |\psi(r_1, \ldots r_n)|^2 \sum_{i<j} V_{int} (r_i - r_j) \]

- Generally speaking not for fermions, but possible under certain conditions.
“no-node” consequences

• Valid for superfluid, Mott states, super-solids, etc.

• Constraint on bosons: Time-reversal symmetry cannot be spontaneously broken!

Complex-valued wavefunctions $\rightarrow$ positive-definite distr.

$$\text{TR: } \Psi(r_1, r_2 \ldots, r_n) \rightarrow \Psi^*(r_1, r_2 \ldots, r_n)$$

• Goal: Seek for unconventional BECs beyond “no-node” paradigm and breaking TR symmetry!

Unconventional (UBEC) – metastable states

- The condensate $\Psi(r)$ possesses a non-s-wave symmetry $\rightarrow$ Nodal lines or points beyond “no-node”.

- Complex, spontaneous time-reversal symmetry breaking.

- e.g. the $p$-orbital bands with degenerate minima.

$$
\Psi(\vec{r}) = \Psi_{K_1}(\vec{r}) + i\Psi_{K_2}(\vec{r})
$$

$$
R_{90^\circ} \Psi(\vec{r}) = \Psi_{-K_2}(\vec{r}) + i\Psi_{K_1}(\vec{r}) = -\Psi_{K_2}(\vec{r}) + i\Psi_{K_1}(\vec{r})
$$

$$
= i(\Psi_{K_1}(\vec{r}) + i\Psi_{K_2}(\vec{r}))
$$


p+ip UBEC:
Observed! Double-well lattice experiment

- Condensate wavevectors \((K_1, K_2)\): half values of reciprocal lattice vectors.

Experiment lattice – shallow (weakly interacting)

- Energy minima $K_{1,2} \equiv -K_{1,2}$ --- (mod reciprocal lattice vectors).

$$K_{1,2} = \left( \pm \frac{\pi}{2a}, \frac{\pi}{2a} \right)$$

- Real space distribution of $\Psi_{K_{1,2}}(r)$

- Standing waves (real).
- Nodal lines pass A-sites (p).
- Antinode B-sites (s).

Zi Cai, C. Wu, PRA, 84,033635 (2011)
Nodal points (complex) v.s. lines (real)

- Real $\Psi_{K_1} \pm \Psi_{K_2}$: nodal lines

- Complex $\Psi_{K_1} \pm i\Psi_{K_2}$: nodal points at crossings $\rightarrow$ more uniform (favored by repulsive interaction)

- Phase winding: vortex-anti-vortex lattice.

- Spontaneous TR symmetry breaking.
See the “i” -- Matter-wave interference
Hemmerich group PRL 114, 115301 (2015).

25ms expansion
Interference along the z-axis

Upper space

$$\Psi_{K_1} + i\Psi_{K_2} - K_1 - K_2$$

Lower space

$$\Psi_{K_1} - i\Psi_{K_2} - K_1 - K_2$$
• Orbital bosons (unconventional symmetry): \( p_x + i p_y \) BECs beyond the “no-node” theorem – already observed!

• Orbital Fermions (strong correlation): Itinerant FM, a long-standing problem – a Non-perturbative study.
The early age of ferromagnetism

The magnetic stone attracts iron.

慈 (ci) 石(shi) 召(zhao) 铁(tie)

---- Guiguzi (鬼谷子), (4th century BC)

慈 (loving, kind, merciful, gentle): the original Chinese character for magnetism

heart

磁 (magnetism, magnetic)

stone

World’s first compass: magnetic spoon: 1 century AD (司南 South-pointer)

“Slightly eastward, not directly south” (常微偏东,不全南也)- Kuo Shen (沈括)(1031-1095)

Thales says that a stone (lodestone) has a soul because it causes movement to iron.

---- De Anima, Aristotle (384-322 BC)
Origin of itinerant FM – fermion exchange

- **Fermi statistics** $\rightarrow$ **Slater determinant-like wavefunction** $\rightarrow$ **direct exchange.**

- **Stoner criterion:**

\[ UN_0 > 1 \]

$U$ – average interaction strength; $N_0$ – density of states at the Fermi level
Density functional (Kohn-Sham) theory

• Accurate on ground state magnetic polarization.

<table>
<thead>
<tr>
<th>Property</th>
<th>source</th>
<th>Fe (bcc)</th>
<th>Co (fcc)</th>
<th>Ni (fcc)</th>
<th>Gd (hcp)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M_{\text{spin}}$</td>
<td>LSDA</td>
<td>2.15</td>
<td>1.56</td>
<td>0.59</td>
<td>7.63</td>
</tr>
<tr>
<td>$M_{\text{spin}}$</td>
<td>GGA</td>
<td>2.22</td>
<td>1.62</td>
<td>0.62</td>
<td>7.65</td>
</tr>
<tr>
<td>$M_{\text{spin}}$</td>
<td>experiment</td>
<td>2.12</td>
<td>1.57</td>
<td>0.55</td>
<td></td>
</tr>
<tr>
<td>$M_{\text{tot.}}$</td>
<td>experiment</td>
<td>2.22</td>
<td>1.71</td>
<td>0.61</td>
<td>7.63</td>
</tr>
</tbody>
</table>

• Correlations partially contained in $V_{xc}(r)$, but wavefunctions remain Slater-determinant type.

• Thermal fluctuations difficult to handle -- Curie temperatures overestimated.
Correlations – Non-perturbative studies desired!

• Unpolarized but correlated WFs $\rightarrow$ less kinetic energy cost.

• **No go!** Two-electron ground states are non-magnetic.

\[
\begin{align*}
\text{triplet} & \quad \phi_{asym}(x_1 - x_2) \otimes |\uparrow\rangle_1 |\uparrow\rangle_2 \\
\text{nodal} & \quad (\text{ground state}) \text{ nodeless}
\end{align*}
\]

\[
\begin{align*}
\text{singlet} & \quad \phi_{sym}(x_1 - x_2) \otimes (|\uparrow\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |\uparrow\rangle_2)
\end{align*}
\]

• **No go!** Absence of itinerant FM in 1D – Lieb & Mattis theorem.
Previous exact results (e.g. Nagaoka FM, flat-band FM) do not really set up a stable phase of itinerant FM.

We need a **simple** and **quasi-realistic** model:

- A ground state FM **phase** of **itinerant fermions without ambiguity**.

- A controllable reference point for studying the **Curie-Weiss metal phase**.

- Hint for the driving force of itinerant FM?
Prediction for test: FM in p-orbitals (or $d_{xz}/d_{yz}$)

- p-orbital band: 1d-like band structure.
- Tunable interactions

Our prediction: itinerant FM phase appears at $t_\perp = 0$ in the strong coupling regime.
Multi-orbital onsite (Hubbard) interactions

- Intra-orbital repulsion $U \to \infty$.

  Intra-orbital singlet projected out

- Inter-orbital **Hund’s coupling** $J>0$, and repulsion $V$.

\[ E = J + V \]

\[ E = V \]
The orbital-assisted Itinerant FM

- **Theorem:** FM ground states at $U \to \infty$ (fully polarized and unique up to $2S_{\text{tot}}+1$-fold spin degeneracy).

- **An entire FM phase:** valid at any generic filling, any value for $J>0$, and $V$.

- Free of quantum Monte-Carlo (QMC) sign problem at any filling – a rare case for fermions.

A reliable reference point for analytic and numeric studies of FM in multi-orbital systems

Hund’s rule assisted global FM

- Intra-chain physics at $U \to \infty$: infinite degeneracy.
- Inter-chain physics ($J$): Hund’s coupling lifts the degeneracy by aligning spins $\rightarrow$ global FM.
- 2D FM coherence in spite of 1D band structure (the total spin in each chain is not conserved).
Open question: Curie-Weiss metal

Local-moment-like: Unnatural for metals with **Fermi surfaces**. \[ \chi = \frac{A}{1 - T / T_0} \quad T_0 < T \ll T_F \]

- The paramagnetic phase is NOT simple: domain fluctuations!

- Non-perturbative study – sign-problem free QMC simulations, asymptotically exact.
• Local moment-like: Curie-Weise (spin incoherent).

\[ \chi = \frac{C}{(T - T_0)} \quad T_0 \ll T_{ch} \]

• Metallic (itinerancy): \( K \) saturates at \( T < T_{ch} \), \( T_{ch} \) is roughly the kinetic energy scale.
QMC: Curie-Weiss temperature v.s filling (V=0)

\[ \chi = \frac{C}{T - T_0} \]

- \( T_0 \rightarrow 0 \) at both \( n \rightarrow 0 \) (particle vacuum), and \( n \rightarrow 2 \) (hole vacuum).
- \( T_0 \) reaches the maximum at \( n \sim 1 : T_{0,\text{max}} \approx 0.08t_\parallel \).
Deviation from the Curie-Weiss law (critical region)

- No long-range order at finite $T$ (Mermin-Wagner theorem)

- $O(3)$ NL$\sigma$-model: FM directional fluctuations

- As $T < T_0$, $\chi$ crosses over into an exponential growth.
Fermi distribution $n_F(k)$ — non-pertubative result

**Paramagnetic Curie-Weiss metal**

$$n_F(k) = n_{\uparrow}(k) + n_{\downarrow}(k)$$

- At $k \to 0$, $n_{\uparrow}(k) = n_{\downarrow}(k) \approx 0.54 \ll 1$
- Large entropy (the $k$-space picture)
- Strongly correlated Curie-Weiss metal phase

Reference: polarized fermion with $k_F^0 = \frac{\pi}{2}$
Hints for mechanism for itinerant FM

• Why is FM difficult? Large kinetic energy cost to polarize the ideal Fermi distribution.

• Hund J is the key, but by itself, it is insufficient!

• Hubbard U mostly favors anti-FM, but brutal enough to distort the Fermi distribution.

• Apply J on top of U ➔ FM with less kinetic energy cost and even gain kinetic energy (c.f. J. Hirsch’s works).
Summary: orbital physics with cold atoms

• Novel orbital physics not easily accessible in solid state systems.

• Unconventional BEC beyond the “no-node” theorem.

• A novel system for itinerant ferromagnetism – a non-perturbative study.