A novel ground state of KOs$_2$O$_6$ lattice?

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Why $\text{AOs}_2\text{O}_6$? 

- Physics on the triangular lattice:
  - superconductivity - $\text{LiTi}_2\text{O}_4$, $\text{LiV}_2\text{O}_4$, $\text{Na}_x\text{CoO}_2\cdot\text{H}_2\text{O}$, $\text{Cd}_2\text{Re}_2\text{O}_7$;
  - charge ordering - $\text{CuIr}_2\text{S}_4$, $\text{Tl}_2\text{Ru}_2\text{O}_7$.

- $\text{KOs}_2\text{O}_6$ vs $\text{RbOs}_2\text{O}_6$, $\text{CsOs}_2\text{O}_6$ - isoelectronic materials with surprisingly different physical properties (superconductivity, transport and low temperature thermodynamics).

Why?
### Superconductivity

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a$ (Å)</th>
<th>$T_c$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>KOs$_2$O$_6$</td>
<td>10.101</td>
<td>9.6</td>
</tr>
<tr>
<td>RbOs$_2$O$_6$</td>
<td>10.114</td>
<td>6.3</td>
</tr>
<tr>
<td>CsOs$_2$O$_6$</td>
<td>10.149</td>
<td>3.2</td>
</tr>
</tbody>
</table>

KOSO - non-s-wave pairing (T$_1$ NMR, muons), $H_c^2$ above Pauli limit

ROSO, COSO - BCS type superconductivity

Superconductivity suppressed by pressure $\sim$ 5 GPa (suppression of $N(E_F)$ - Saniz private commun.)


Muramatsu \textit{et al.} cond-mat/0407610
Conductivity

KOSO - non-Fermi liquid behavior vs. FL behavior in ROSO and COSO

KOs$_2$O$_6$  

CsOs$_2$O$_6$
Specific heat

- Large enhancement of linear specific heat coefficient ($\lambda \sim 4$ ROSO, COSO; $\lambda \sim 12$ KOSO)
- Einstein modes identified in ROSO, COSO
- Large D-W factors associated with A
- Second peak in KOSO

Z. Hiroi et al. cond-mat/0502043
Lattice structure

O: Os-O-Os bonds

Os: OsO$_6$ octahedra
   Os pyrochlore lattice

A: cavities inside the pyrochlore cage
   A - diamond lattice
Density of states

Formal valency: $A^+\text{Os}_2^{5.5+}\text{O}_6^{2-} \implies d^{2.5}$
Density of states

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Formal valency: $A^+\text{Os}_2^{5.5+}\text{O}_6^{2-} \rightarrow d^{2.5}$
Bandstructure
Na, K, Rb, Cs - symmetric mode
Stability of alkali site

Site symmetry: \( l=0, 3, 4, 6, \ldots \)

\[ E(\Delta) \] - polynomial fit (exp. \( \geq 2 \))

- On-site potential = Os-O cage + average K-K interaction
- K-K correlation
Single site K dynamics
Single site K dynamics
Single site K dynamics
Single site K dynamics
Single site K dynamics
**K-K interaction**

Calculated force acting of a static K ion, while its neighbors are displaced.

\[ V(x) = \frac{\exp(-x/\Lambda)}{x} \]

Force (mRy/a.u.) vs. Displacement of neighbors (a.u.)
- No on-site term => anisotropic generalized Potts model $q=4$ on bipartite lattice (classical)
- On-site singlet-triplet splitting => off-diagonal terms (quantum)
Summary

- Dynamics of alkali ion is strongly size dependent
- K dynamics is anharmonic
- On-site ground state is a singlet-triplet split ($\Delta \sim 8$ K) => Schottky anomaly in specific heat
- K motion survives to low temperatures:
  - NFL conductivity
  - large D-W factor (anomalous T dependence)
  - quadrupolar contribution to nuclear spin relaxation

Future outlook

Is there a phase transition in our model?
What type?

- Find classical ground state (degeneracy)
  => identify the order parameter.

- Mean field solution.

- Classical Monte-Carlo simulation.