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Outline

1. CompFUSE — Introduction
2. Some highlights
3. Bond-stretching phonons in $\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$
4. Two pairing domes in cuprates
5. Acknowledgments
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CompFUSE: Computational framework for unbiased studies of correlated electron systems

Advanced simulations of correlated quantum materials, including unconventional superconductors and quantum spin liquids.

Development of accelerated algorithms based on DQMC, DCA and DMRG and efficient implementations on leadership class supercomputers.

Development of new approaches for analytic continuation of QMC results to extract real time dynamics from imaginary time data.

Focus: Dynamics, excited states, finite temperatures, mechanisms
Dynamical and thermal magnetic properties of $\alpha$-RuCl$_3$

Failure of available spin models for $\alpha$-RuCl$_3$

- Derived a spin model for RuCl$_3$ and studied several available models from the literature
- Using exact diagonalization based methods, calculated the specific heat and the inelastic neutron scattering response
- All existing models fail to completely explain the experiments

Research Details

- DFT calculation of RuCl$_3$, Wannier transformation to Ru-t$_{2g}$ states
- Interaction parameters from constrained Random Phase Approximation
- Spin-only model from perturbation theory

For details see poster by Satoshi Okamoto

Eichstaedt et al., arXiv:1904.01523
Laurell & Okamoto, arXiv:1906.07579
AI to accelerate determinantal lattice quantum Monte Carlo simulations

Neural networks to speed up DQMC

- Artificial neural networks (ANNs) can predict with near-perfect accuracy moves in quantum Monte Carlo (QMC) simulations of many-body Hamiltonians and obtain an order of magnitude reduction in the run time.
- Demonstration that machines can learn to perform efficient QMC simulations—without an underlying physics model and given only limited information about the configuration space—means the method can be easily generalized even to other challenging models, such as the Fermi-Hubbard model.

Research Details

- ANNs were designed to predict the acceptance probabilities of local and global moves in determinantal QMC simulations of the Holstein model.
- This development in artificial intelligence (AI) granted access to large systems at low-temperatures, overcame long autocorrelation times for the model, and facilitated a thermodynamic scaling analysis.

Thermodynamic scaling analysis of the charge density wave structure factor of the half-filled two-dimensional Holstein model in proximity to the metal-to-CDW insulator transition $T_c$

For details see poster by Steve Johnston

Li et al., arXiv:1905.10430
Analytic continuation of noisy data using multistep neural network

New data-driven framework

\[
G(\tau) = \int K(\tau, \omega)A(\omega)d\omega; \quad K(\tau, \omega) = \frac{e^{-\omega \tau}}{1 + e^{-\beta \omega}}
\]

- Use **novel linear multi-step residual neural network (ResNet)** to learn the inverse of the kernel
- Generate training data set as a sum of \( R \) uncorrelated Gaussians
- 100k training data set, 1000 samples for validation and testing

**Compared to Maximum Entropy**

- 2-step ResNet gives similar results for high-quality data, and much better results at high noise levels.

For details see poster by Xuping Xie

Xie et al., arXiv:1905.10430
Accelerating DCA++ on Summit

DCA++ code
- Two kernels: (1) Coarse-graining of momentum space to map lattice problem onto effective cluster problem, (2) quantum Monte Carlo cluster (QMC) solver
- Two-level parallelization (MPI internode + std::threads intranode)

Several optimizations
- Extensive profiling (in collaboration with RAPIDS institute)
- Coarse-graining: Improved multi-threading and intra-process scheduling
- QMC solver: (1) Improved asynchronous CPU-GPU communication
  (2) GPU support for measurement accumulation of observables
  (3) Improved (direct) walker - accumulator communication
  (4) Dynamic intra-node workload distribution
  (5) Overlapping computation and communication
  (6) Mixed precision – Double precision (walker), single precision (two-particle vertex accumulation)

Speedup & Performance on Summit
- ~ 100 x speedup
- ~ 75 PFlops

Chatterjee et al., submitted to PACT ‘19
Accelerating DMRG++ for dynamics and finite temperatures

Targeting multiple states in DMRG
- **Multiple states** are needed in density matrix matrix for **finite temperature calculations and dynamics**
- Replacing the density matrix by a **singular value decomposition (SVD)** increases **performance** significantly and enables multiple targeting

Optimized GPU support for Summit
- Use of **multiple GPUs** for larger problems (more states)
- Use of **atomic updates in MAGMA** library to take advantage of symmetry of Hamiltonian to reduce HBM storage on GPU
- Calculation of spectral functions is embarrassingly parallel and thus can take full advantage of parallelization on Summit, significantly increasing frequency resolution


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**Table I: Wall times in seconds of typical runs depending**

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<tr>
<th>ω</th>
<th>fullRunSVD</th>
<th>fullRunDM</th>
<th>fullRunSVD</th>
<th>fullRunDM</th>
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<td>1402</td>
<td>1757</td>
<td>2014</td>
</tr>
</tbody>
</table>

Run-time in seconds on a Volta GPU on x86 Linux workstation. Note all SVD performed on CPU.
DMRG: $S(Q,\omega)$ for telephone ladder cuprates

\[ \langle n \rangle = 1 \]

\[ \langle n \rangle = 0.9375 \]

Parameters:
2-leg Hubbard ladder; 64 x 2; intermediate to strong coupling
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DQMC study of bond phonons in Ba$_{1-x}$K$_x$BiO$_3$

**Ba$_{1-x}$K$_x$BiO$_3$**

- Negative charge transfer regime
- Holes self-dope from cation to ligand oxygen atoms
- Hybridization between cation and oxygen atom leads to sizable electron-phonon coupling
- **Charge-ordered insulator** for $x=0$
- **Superconductor** ($T_c \sim 30$ K) at finite $x$

3-orbital Su-Schrieffer-Heger (SSH) model

\[
H_0 = -t_{sp} \sum_{(r,\delta),\sigma} (P_{\delta,r,\sigma}^+ P_{r,\delta,\sigma} + \text{h.c.}) + t_{pp} \sum_{(r,\delta),\delta'} P_{\delta,r,\sigma}^+ P_{r,\delta',\sigma} + \sum_{r,\sigma} \left[ (\varepsilon_s - \mu) \hat{n}_{r,\sigma}^s + (\varepsilon_p - \mu) (\hat{n}_{r,\sigma}^p + \hat{n}_{r,\sigma}^p) \right]
\]

\[
H_{\text{lat}} = \sum_r \left( \frac{\hat{P}_{r,x}^2}{2M} + K\hat{X}_{r,x}^2 + \frac{\hat{P}_{r,y}^2}{2M} + K\hat{X}_{r,y}^2 \right)
\]

Phonon frequency $\Omega = \sqrt{2t_{sp}}$

\[
H_{\text{e-ph}} = \alpha t_{sp} \sum_{(r,\delta),\sigma} (\hat{u}_{r,\delta,\sigma}^s \hat{n}_{r,\sigma}^s + \text{h.c.})
\]

e-ph coupling strength $\alpha = 4a^{-1}$

**Sign-problem free DQMC algorithm!**
**First non-perturbative treatment in > 1D!**
Bond disproportionated, charge ordered state at half-filling

Displacement correlation functions

(a) $s$  \hspace{1cm} $p_x, (p_y)$

(b) $< \hat{X}_{x,x} \hat{X}_{0,x}>$

(c) $< \hat{X}_{r,y} \hat{X}_{0,y}>$

(d) $< \hat{X}_{r,y} \hat{X}_{0,y}>$

In (a), the unit cells are indexed by $O_2$. The orbital basis consists of a Bi 6$t$ orbitals, as shown in Fig. 1(a). We freeze the $h_{sp}$ orbitals, as shown in Fig. 1(a).

Panel (d) plots the real-space displacement correlation function $t$ respectively. The nearest Bi atom in the undistorted square structure is $0.3\,/\,M$. Here, $\beta G(r=0=r=0/2)$.

dc conductivity and spectral weight at $E_F$

(a) $<\hat{n}> = 1$

(b) $\beta G(r=0=r=0/2)$

CDW susceptibility

(b) $\chi_C(\pi, \pi) = 0.3$

Li et al., arXiv:1901.07612
Polaronic liquid and superconductivity at finite doping

- Bipolaronic state at half-filling that melts into a polaron-liquid-like metallic state with a superconducting ground state upon doping.

Li et al., arXiv:1901.07612
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Two pairing domes as \( \text{Cu}^{2+} \) varies to \( \text{Cu}^{3+} \)

**Highly (hole) overdoped curates**

- \( \text{Sr}_2\text{CuO}_4-\delta \) (\( T_c \sim 95 \text{ K} \); isostructural to 214 \( \text{La}_2\text{CuO}_4 \))
- \( \text{Cu}_{0.75}\text{Mo}_{0.25}\text{Sr}_2\text{YC}_{0.2}\text{O}_{7.54} \) (\( T_c \sim 84 \text{ K} \))
- \( \text{Ba}_2\text{CuO}_4-\delta \) (\( T_c \sim 70 \text{ K} \))
- Monolayer \( \text{CuO}_2 \) films (\( T_c \sim 100 \text{ K} \))
- High pressure oxidized synthesis
- Reduced Cu - apical O spacing
- \( d_{3z^2-r^2} \) orbital important, in addition to \( d_{x^2-y^2} \) orbital

**Two-orbital tight-binding Hubbard-Hund model**

\[
H_0(x) = \sum_{k\alpha} \sum_{\ell\ell'} \left( \xi_{\ell\ell'}(k) + (\varepsilon_{\ell}(x) - \mu) \delta_{\ell\ell'} \right) d_{\ell\alpha}^+(k)d_{\ell'\alpha}^-(k)
\]

\[
H_1 = U \sum_{i,\ell} n_{i\ell\uparrow}n_{i\ell\downarrow} + U' \sum_{i,\ell < \ell'} n_{i\ell\uparrow}n_{i\ell'\downarrow} + J \sum_{i,\ell < \ell',\sigma,\sigma'} d_{i\ell\sigma}^+d_{i\ell'\sigma}^+d_{i\ell\sigma'}d_{i\ell'\sigma'} + J' \sum_{i,\ell \neq \ell'} d_{i\ell\sigma}^+d_{i\ell'\sigma}^+d_{i\ell'\sigma'}d_{i\ell\sigma'}
\]

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Maier, Berlijn & Scalapino, PRB ‘19

From Geballe & Marezio, Physica C ‘09
Two pairing domes

- **First dome at small doping** $x$ describes superconductivity in usual, lightly doped cuprates
- **Second dome at much larger doping** describes recently observed superconductivity in highly overdoped cuprates
- **Second dome has much larger pairing strength**
- For large doping, mixing of different $d$-orbitals allows for strong nesting between electron and hole Fermi surfaces
- Possibility of Bardassis-Schrieffer mode in Raman scattering due to near degeneracy of $d$- and $s^\pm$ pairing channels
Dynamic Cluster Quantum Monte Carlo results: $\langle n \rangle = 2.85$ ($x = 0.15$)

Parameters: 4 x 4 cluster; $U = 4$, $U' = 2$, $J = J' = 0$; Doping $x = 0.15$
Dynamic Cluster Quantum Monte Carlo results: $\langle n \rangle = 2.0 \ (x = 1)$

Fermi surface ($\mid \nabla n(k) \mid$)

Leading eigenvalue of Bethe-Salpeter equation)

$\chi_d(T) \sim (1 - \lambda_d(T))^{-1}$

Parameters: $4 \times 4$ cluster; $U = 4, U' = 2, J = J' = 0$; Doping $x=1$
Pairing in 2-orbital model for cuprates

- Pairing is stronger in heavily overdoped region with hole and electron Fermi surface pockets
- $d$-wave and $s^\pm$- pairing almost degenerate in heavily overdoped region

\[ \chi_d(T) \sim (1 - \lambda_d(T))^{-1} \]

- $\lambda_d (x=1.0)$
- $\lambda_{s^\pm} (x=1.0)$
- $\lambda_d (x=0.15)$

$T \ [eV]$
Acknowledgments

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