Rotationally-invariant slave-bosons for strongly correlated superconductors

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Part I: Slave-boson formulations

- Barnes (1976), Coleman (1984), Kotliar and Ruckenstein (1986), Frésard and Wölfle (1992), Lechermann et al. (2007)
- Limitations of old approaches
- Rotationally invariant formalism

Part II: Application to superconducting fullerides \((A_nC_{60}, A \equiv \text{alkali metal})\)

Perspectives
Kotliar-Ruckenstein’s slave-bosons in multi-orbital models

**Auxiliary fields**

- slave-bosons $\phi_n^{\dagger}$ for each local Fock state
  \[
  |n\rangle_d \equiv \left( d_1^{\dagger} \right)^{n_1} \cdots \left( d_M^{\dagger} \right)^{n_M} |\text{vac}\rangle, \quad [n_\alpha = 0, 1] \quad \alpha = 1, \ldots, M \quad \text{(local electronic species: orbitals and spin)}
  \]
- auxiliary fermions $f_\alpha^{\dagger}$ to retain Fermi-liquid properties

Representation of physical states in the *enlarged* Hilbert space $\mathcal{H}$:

\[
|n\rangle_d \quad \longrightarrow \quad |n\rangle \equiv \phi_n^{\dagger} |\text{vac}\rangle \otimes |n\rangle_f
\]
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$$|n\rangle_d \mapsto |n\rangle \equiv \phi_n^\dagger |\text{vac}\rangle \otimes |n\rangle_f$$

**Constraints**

$$\sum_n \phi_n^\dagger \phi_n = 1$$

$$\sum_n \phi_n^\dagger \phi_n n_\alpha = f_\alpha^\dagger f_\alpha$$
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Density-density interactions

$$H_{\text{loc}} = \sum_\alpha \epsilon_\alpha^0 \hat{n}_\alpha + \sum_{\alpha\beta} W_{\alpha\beta} \hat{n}_\alpha \hat{n}_\beta, \quad \hat{n}_\alpha = d_\alpha^\dagger d_\alpha$$

$$\mapsto \quad H_{\text{loc}} = \sum_n E_n \phi_n^\dagger \phi_n, \quad H_{\text{loc}} |n\rangle = E_n |n\rangle$$

free-boson Hamiltonian!
Limitations of Kotliar-Ruckenstein’s approach

Intrinsically *basis-dependent*

1. Unable to handle *arbitrary* forms of $H_{\text{loc}}$
   - non density-density interactions
   - inter-orbital hybridization
   - ...

2. Unable to describe, at mean-field level, phases with *off-diagonal* order parameters
   - superconductivity
   - spin/orbital ordering off the quantization axis
   - ...
**Limitations of Kotliar-Ruckenstein’s approach (I)**

**Arbitrary local Hamiltonian**

\[
H_{\text{loc}} = \sum_{\alpha\beta} \epsilon_{\alpha\beta} d_\alpha^\dagger d_\beta + \sum_{\alpha\beta\gamma\delta} W_{\alpha\beta\gamma\delta} d_\alpha^\dagger d_\beta^\dagger d_\gamma d_\delta
\]

- the eigenstates of \(H_{\text{loc}}\) are atomic *multiplets* \(|\Gamma\rangle = \sum_n U_{\Gamma n} |n\rangle\),

\[
E_\Gamma = \sum_{nm} U_{\Gamma n}^* U_{\Gamma m} E_{nm}
\]

If we use \(|n\rangle \equiv \phi_n^\dagger |\text{vac}\rangle \otimes |n\rangle_f\), the representation of \(H_{\text{loc}}\) is *no longer* a simple free-boson Hamiltonian:

\[
H_{\text{loc}} \longrightarrow H_{\text{loc}} \overset{?}{\Rightarrow} \sum_{nm} E_{nm} \phi_n^\dagger \phi_m
\]
Limitations of Kotliar-Ruckenstein’s approach (II)

- Diagonal relation between physical electron operators and auxiliary fermions (quasiparticles):
  \[ d_\alpha^\dagger = \hat{r}_\alpha [\phi] f_\alpha^\dagger \]

\[ \downarrow \]

At mean-field level the (local) self-energy is diagonal:

\[ \Sigma(\omega)_{\alpha\beta} = \delta_{\alpha\beta} \Sigma_\alpha(\omega) \]

- \( \langle d_\alpha^\dagger d_\beta^\dagger \rangle = 0 \quad \rightarrow \quad \text{NO charge-symmetry breaking (superconductivity)} \)

- \( \langle d_\alpha^\dagger d_\beta \rangle = \delta_{\alpha\beta} \langle \hat{n}_\alpha \rangle \quad \rightarrow \quad \text{NO off-diagonal spin/orbital magnetization} \)
Representation of physical states

- \{ |A\rangle \} \rightarrow \text{basis set for the (physical) local Hilbert space } \mathcal{H}, \text{ eigenstates of the local particle number: } \sum_{\alpha=1}^{M} d_{\alpha}^{\dagger} d_{\alpha} |A\rangle = N_{A} |A\rangle \\
  (e.g., \{ |A\rangle \} = \{ |n\rangle \}, \{ |\Gamma\rangle \}, \ldots )

- Mapping onto the enlarged Hilbert space \( \mathcal{H} \):

\[ |A\rangle \leftrightarrow |A\rangle \equiv \frac{1}{\sqrt{2^{M-1}}} \sum_{n} \phi_{An}^{\dagger} |\text{vac}\rangle \otimes |n\rangle_{f} \]

\( \phi_{An}^{\dagger} \) are introduced for each pair of physical and quasiparticle states with the same statistics (\( |A\rangle, |n\rangle_{f} \)):

\[ [N_{A} - \sum_{\alpha} n_{\alpha}] \mod 2 = 0 \]
Representation of physical states

- \{ |A\rangle \} \longrightarrow \text{basis set for the (physical) local Hilbert space } \mathcal{H},
  \text{eigenstates of the local particle number: } \sum_{\alpha=1}^{M} d^\dagger_{\alpha} d_{\alpha} |A\rangle = N_A |A\rangle
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- Mapping onto the enlarged Hilbert space \overline{\mathcal{H}}:

  |A\rangle \iff |A\rangle \equiv \frac{1}{\sqrt{2^{M-1}}} \sum_n \phi_A^\dagger \phi_{An} \langle \text{vac} | \otimes |n\rangle_f

\phi_{An}^\dagger \text{ are introduced for each pair of physical and quasiparticle states with the same statistics } (|A\rangle, |n\rangle_f):

\left[ N_A - \sum_{\alpha} n_{\alpha} \right] \text{ mod } 2 = 0 \quad \Rightarrow \quad (N_A - \sum_{\alpha} n_{\alpha}) \neq 0 \text{ enables the non-conservation of the local quasiparticle number}
Rotational invariant formalism

Physical electron operator in $\mathcal{H}$

- **Definition:**
  \[
  d_{\alpha}^\dagger |B\rangle = \sum_A \langle A|d_{\alpha}^\dagger |B\rangle |A\rangle
  \]
  \[
  d_{\alpha}^\dagger = \hat{R}_{\alpha\beta}^{(p)}[\phi]^*f_{\beta}^\dagger + \hat{R}_{\alpha\beta}^{(h)}[\phi]f_{\beta}
  \]

- $H = H_{\text{kin}} + \sum_i H_{\text{loc}}[i]$

- $H_{\text{loc}} \mapsto \tilde{H}_{\text{loc}} = \sum_{AB} \langle A|H_{\text{loc}}|B\rangle \sum_n \phi_{An}^\dagger \phi_{Bn} = \sum_\Gamma E_\Gamma \sum_n \phi_{\Gamma n}^\dagger \phi_{\Gamma n}$

- $H_{\text{kin}} \mapsto \tilde{H}_{\text{kin}} = \sum_{\mathbf{k}, \alpha\beta} \epsilon_{\alpha\beta}(\mathbf{k})d_{\mathbf{k}\alpha}^\dagger d_{\mathbf{k}\beta}$
  \[
  = \sum_{\mathbf{k}, \alpha\beta} \left[ \hat{E}_{\alpha\beta}(\mathbf{k})[\phi] f_{\mathbf{k}\alpha}^\dagger f_{\mathbf{k}\beta} + \frac{1}{2} \left( \hat{\Delta}_{\alpha\beta}(\mathbf{k})[\phi] f_{\mathbf{k}\alpha}^\dagger f_{-\mathbf{k}\beta}^\dagger + \text{H.c.} \right) \right]
  \]

Constraints

- $\sum_{An} \phi_{An}^\dagger \phi_{An} = 1$
- $\sum_{Ann'} \phi_{An}^\dagger \phi_{An'}\langle n'|f_{\alpha}^\dagger f_{\alpha}|n\rangle = f_{\alpha}^\dagger f_{\alpha}$
- $\sum_{Ann'} \phi_{An}^\dagger \phi_{An'}\langle n'|f_{\alpha}^\dagger f_{\alpha}^\dagger|n\rangle = f_{\alpha}^\dagger f_{\alpha}^\dagger$
Saddle-point solution

- **condensation** of slave-boson fields into *static* amplitudes:
  \[ \phi_{An} \to \langle \phi_{An} \rangle \equiv \varphi_{An} \]

- **minimization** of the free-energy functional
  \[ \Omega[\{\varphi\}, \{\mathcal{M}\}] = -\frac{1}{\beta} \ln \mathcal{Z} \]
  with respect to \( \varphi \)'s and Lagrange multipliers \( \{\mathcal{M}\} \)
Mean-field observables

**Saddle-point solution**

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**Local observables**

- \[ \langle \hat{O}_d \rangle = \sum_{AB} \langle A | \hat{O}_d | B \rangle \sum_n \varphi_{An}^* \varphi_{Bn} \]

- \( \hat{O}_d = d_{\alpha}^\dagger d_{\beta}, \ d_{\alpha}^\dagger d_{\beta}, \ldots \)
Mean-field observables

**Physical electron propagator**

- **definition** (Nambu-Gorkov formalism): 
  \[ D_d = - \langle T \Psi_d(k, \tau) \Psi_d^\dagger(k, 0) \rangle, \quad \Psi_d(k) \equiv \left( \begin{array}{c} \{ d_{k\alpha} \} \\ \{ d^\dagger_{-k\alpha} \} \end{array} \right) \]

- \[ D_d(k, \omega) = R[\omega - h(k)]^{-1} R^\dagger, \]

- \[ R[\varphi] \rightarrow \text{matrix relating physical and quasiparticle operators: } \Psi_d = R \Psi_f \]

- \[ h(k)[\varphi, M] \rightarrow \text{quasiparticle energy matrix: } \]

\[ H_f = \frac{1}{2} \sum_k \Psi_f^\dagger(k) h(k) \Psi_f(k) \]

**NON-DIAGONAL** self-energy matrix in orbital and particle-hole space:

\[ \Sigma_d(\omega) = D_{d0}^{-1}(k, \omega) - D_d^{-1}(k, \omega) \]
\[ = \omega \left( 1 - [RR^\dagger]^{-1} \right) + \Sigma_d(0) \]
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Part II: Application to superconducting fullerides ($A_nC_{60}$, $A \equiv$ alkali metal)

Perspectives
A model for alkali-doped fullerides: $A_nC_{60}$

$$H_{\text{loc}} \left[ C_{60}^{n-} \right] = \frac{U}{2} \hat{n}^2 + J \left[ 2 \mathbf{S} \cdot \mathbf{S} + \frac{1}{2} \mathbf{L} \cdot \mathbf{L} + \frac{5}{6} (\hat{n} - 3)^2 \right]$$

- $\hat{n} = \sum_{a\sigma} \hat{d}^\dagger_{a\sigma} \hat{d}_{a\sigma}$,
  - $\sigma = \uparrow, \downarrow$
  - $a = 1, 2, 3$  $t_{1u}$ orbitals (valence electrons)
- $\mathbf{S}$, $\mathbf{L}$  spin and orbital angular momentum
- $J = -J_{\text{Hund}} + J_{\text{JT}} > 0$

**Jahn-Teller coupling $J_{\text{JT}}$**

$$J_{\text{JT}} \propto \sum_{\nu=1}^{8} \frac{g^2_{\nu}}{\omega_{\nu}} \text{ effective electron-electron interaction mediated by intramolecular vibrational modes of } C_{60}$$

Hund’s rule is reversed!
Slave-boson representation of the model

- eigenstates of $H_{\text{loc}}$: $|\Gamma\rangle \equiv |n, (\ell, \ell_z), (s, s_z)\rangle$

- eigenvalues: $E_{\Gamma} = \frac{U}{2} n^2 + J \left[ 2s(s+1) + \frac{1}{2} \ell(\ell+1) + \frac{5}{6} (n-3)^2 \right]$

$J > 0$ (inverted Hund’s rule) favors multiplets with low $s$ and $\ell$ $\Rightarrow$ Cooper pairing in the spin- and orbital- singlet channel ($s = \ell = 0$)

Mean-field observables (degenerate bands: $\epsilon_{ab}(k) = \delta_{ab}\epsilon_k$)

- quasiparticle weight: $Z[\varphi]$

- $(s = \ell = 0)$ superconducting order parameter: $\psi_{sc}[\varphi] = \sum_{a=1}^{3} \langle d_{a\uparrow}^\dagger d_{a\downarrow}^\dagger \rangle$

- low-energy spectrum: $E_{\text{low}}(k)[\varphi, M] = \pm \sqrt{(Z\epsilon_k + \lambda)^2 + |\tilde{\Delta}|^2}$
\( n_{\text{phys}} = 3 \) (half-filling), \( U = 0 \) (attractive model)

\[
\frac{\Delta}{J} = \frac{10}{9} \psi_{sc} = \frac{W}{J} e^{-\frac{1}{\lambda}},
\]

\[
\lambda = \frac{10}{3} \left(\frac{J}{W}\right)
\]

A. I. and M. Capone, Phys. Rev. B 80 (2009)
$n_{\text{phys}} = 3$ (half-filling), $J/W = 0.2$ (large pair coupling)

- $\Delta$ and $\psi_{sc}$ decrease monotonically with $U$
- $U > U_{c}^{(N,S)}$ Mott-insulator: $\langle (\hat{n} - 3)^2 \rangle = 0$
- $Z > Z_{N}$: superconducting quasiparticles are more coherent than in normal metal

\[ Z \]
\[ Z_{N} \]
\[ \psi_{sc} \]
\[ \Delta/J \]
$n_{\text{phys}} = 3$ (half-filling), $J/W = 0.04$ (small pair coupling)

- **non-monotonic** behaviour of $\Delta$ and $\psi_{sc}$ as functions of $U$
- $U/W \ll 1$
  - Coulomb repulsion *destroys* BCS-like superconductivity
- $W \lesssim U \lesssim U_c$
  - superconductivity *re-emerges*, with enhanced values of $\Delta$ and $\psi_{sc}$
\( n_{\text{phys}} = 3 \) (half-filling), \( J/U = 0.01 \) (small pair coupling)

- non-BCS superconductivity:
  \[ \Delta/J \sim \mathcal{O}(1) \]
  \[ \Delta/J \sim 10 \times \psi_{\text{sc}} \]

- large enhancement with respect to \( U = 0 \):
  \[ \Delta[J, U \lesssim U_c] \sim 10^3 \times \Delta[J, U = 0] \]
$n_{\text{phys}} = 3$ (half-filling), $U/W = 2.5$ (strong repulsion)

- Strongly correlated superconductivity (SCS):
  - $U \sim U_c^{(N)}$
  - $\frac{10}{3} J \ll U$

- BEC superconductivity:
  - $\frac{10}{3} J \gg U$
\( \mathit{n}_{\text{phys}} = 3 - x \) (finite doping), \( U/W = 5, \quad J/W = 0.02 \)

- doping the Mott-insulator at \( J/U \ll 1 \)
- superconducting “dome” as in cuprates, with optimal doping \( x_{\text{opt}} \approx 0.1 \)
- \( \Delta/J \sim \mathcal{O}(1) \) at \( x_{\text{opt}} \)
- underdoping \( (x < x_{\text{opt}}) \): \( Z > Z_N \)
- overdoping \( (x > x_{\text{opt}}) \): \( Z < Z_N \)
Superconductivity is mediated by local phonons (molecular-vibrations).

Strong correlation enhances superconductivity:
- charge fluctuations are suppressed
- on-site pairing remains unscreened

Slave-bosons vs. DMFT

A similar scenario is found using Dynamical Mean-Field Theory:
M. Capone et al., Rev. Mod. Phys. 81 (2009)

- the different kinds of interactions are accurately treated on the same footing
- compared to DMFT, the computational effort is much smaller, allowing a more detailed study over a larger range of parameters
Conclusions and Perspectives

- powerful analytical tool to describe the low-energy physics of strongly correlated systems with non-trivial multiplet structure

- qualitative agreement with Dynamical Mean-Field Theory, but lower computational cost

- generalization to finite-size *mesoscopic* systems:
  - spatially dependent slave-boson amplitudes: $\varphi \to \varphi(r_i)$
  - non-homogeneous order parameters

- generalization to systems *out-of-equilibrium*:
  - time-dependent slave-boson amplitudes: $\varphi \to \varphi(t)$

  M. Behrmann, M. Fabrizio, and F. Lechermann, arXiv:1304.6013