# Rotationally-invariant slave-bosons for strongly correlated superconductors

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Royal Holloway, University of London, June 21 (2013)

# Outline

1. 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
2. Part II: Application to superconducting fullerides ($\mathrm{A_n C_{60}}$, $\mathrm{A} \equiv$ alkali metal)
3. Perspectives

# Kotliar-Ruckenstein's slave-bosons in multi-orbital models

## Auxiliary fields

- slave-bosons $\phi_n^\dagger$ for each *local* Fock state
  $|n\rangle_d \equiv \left(d_1^\dagger\right)^{n_1} \cdots \left(d_M^\dagger\right)^{n_M} |\text{vac}\rangle, \quad [n_\alpha = 0, 1]$
  $\alpha = 1, \ldots, M$ (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 $\underline{\mathcal{H}}$:

$$|n\rangle_d \longmapsto |\underline{n}\rangle \equiv \phi_n^\dagger |\text{vac}\rangle \otimes |n\rangle_f$$

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

$$\sum_n \phi_n^\dagger \phi_n n_\alpha = f_\alpha^\dagger f_\alpha$$

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## Density-density interactions

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

$$\mapsto \underline{H}_{\text{loc}} = \textstyle\sum_n E_n \phi_n^\dagger \phi_n, \qquad H_{\text{loc}}|n\rangle = E_n |n\rangle$$

free-boson Hamiltonian!

# Limitations of Kotliar-Ruckenstein's approach

Intrinsically *basis-dependent*

1. Unable to handle *arbitrary* forms of $H_{\rm loc}$
   - 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

$$H_{\rm loc} = \sum_{\alpha\beta} \epsilon^0_{\alpha\beta} d^\dagger_\alpha d_\beta + \sum_{\alpha\beta\gamma\delta} W_{\alpha\beta\gamma\delta}\, d^\dagger_\alpha d^\dagger_\beta d_\gamma d_\delta$$

- the eigenstates of $H_{\rm loc}$ are atomic *multiplets* $|\Gamma\rangle = \sum_n \mathcal{U}_{\Gamma n}|n\rangle$, $E_\Gamma = \sum_{nm} \mathcal{U}^*_{\Gamma n}\mathcal{U}_{\Gamma m} E_{nm}$

If we use $|\underline{n}\rangle \equiv \phi^\dagger_n|{\rm vac}\rangle \otimes |n\rangle_f$, the representation of $H_{\rm loc}$ is *no longer* a simple free-boson Hamiltonian:

$$H_{\rm loc} \longmapsto \underline{H}_{\rm loc} \stackrel{?}{=} \sum_{nm} E_{nm}\phi^\dagger_n \phi_m$$

# Limitations of Kotliar-Ruckenstein's approach (II)

- *Diagonal* relation between physical electron operators and auxiliary fermions (quasiparticles):

$$\underline{d}^\dagger_\alpha = \hat{r}_\alpha[\phi] f^\dagger_\alpha$$

$$\Downarrow$$

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

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

- $\langle d^\dagger_\alpha d^\dagger_\beta \rangle = 0 \quad \longrightarrow$ NO charge-symmetry breaking (superconductivity)
- $\langle d^\dagger_\alpha d_\beta \rangle = \delta_{\alpha\beta}\langle \hat{n}_\alpha \rangle \quad \longrightarrow$ NO off-diagonal spin/orbital magnetization

# Rotationally invariant formalism

A. I. and M. Capone, Phys. Rev. B **80**, 115120 (2009); Lechermann *et al.*, Phys. Rev. B **76** (2007)

## Representation of physical states

- $\{|A\rangle\} \quad \longrightarrow \quad$ basis set for the (physical) local Hilbert space $\mathcal{H}$, 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 $\underline{\mathcal{H}}$:

$$|A\rangle \;\longmapsto\; |\underline{A}\rangle \equiv \frac{1}{\sqrt{2^{M-1}}} \sum_n \phi_{An}^\dagger |\mathrm{vac}\rangle \otimes |n\rangle_f$$

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

$$[N_A - \textstyle\sum_\alpha n_\alpha] \bmod 2 = 0$$

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$\Rightarrow$

$(N_A - \sum_\alpha n_\alpha) \neq 0$ enables the *non-conservation* of the local quasiparticle number

# Rotationally invariant formalism

## Physical electron operator in $\underline{\mathcal{H}}$

- *definition*:
  $\underline{d}^\dagger_\alpha |\underline{B}\rangle = \sum_A \langle A| d^\dagger_\alpha |B\rangle\, |\underline{A}\rangle$
- $\underline{d}^\dagger_\alpha = \hat{R}^{(p)}_{\alpha\beta}[\phi]^* f^\dagger_\beta + \hat{R}^{(h)}_{\alpha\beta}[\phi] f_\beta$

## Constraints

$$\begin{aligned}
\sum_{An} \phi^\dagger_{An}\phi_{An} &= 1, \\
\sum_{Ann'} \phi^\dagger_{An}\phi_{An'} \langle n'| f^\dagger_\alpha f_{\alpha'} |n\rangle &= f^\dagger_\alpha f_{\alpha'} \\
\sum_{Ann'} \phi^\dagger_{An}\phi_{An'} \langle n'| f^\dagger_\alpha f^\dagger_{\alpha'} |n\rangle &= f^\dagger_\alpha f^\dagger_{\alpha'}
\end{aligned}$$

- $H = H_{\text{kin}} + \sum_i H_{\text{loc}}[i]$
- $H_{\text{loc}} \longmapsto \underline{H}_{\text{loc}} = \sum_{AB} \langle A| H_{\text{loc}} |B\rangle \sum_n \phi^\dagger_{An}\phi_{Bn} = \sum_\Gamma E_\Gamma \sum_n \phi^\dagger_{\Gamma n}\phi_{\Gamma n}$
- $H_{\text{kin}} \longmapsto \underline{H}_{\text{kin}} = \sum_{\mathbf{k},\,\alpha\beta} \epsilon_{\alpha\beta}(\mathbf{k})\, \underline{d}^\dagger_{\mathbf{k}\alpha} \underline{d}_{\mathbf{k}\beta}$

$$= \sum_{\mathbf{k},\,\alpha\beta} \left[ \hat{E}_{\alpha\beta}(\mathbf{k})[\phi]\, f^\dagger_{\mathbf{k}\alpha} f_{\mathbf{k}\beta} + \tfrac{1}{2}\left( \hat{\Delta}_{\alpha\beta}(\mathbf{k})[\phi]\, f^\dagger_{\mathbf{k}\alpha} f^\dagger_{-\mathbf{k}\beta} + \text{H.c.}\right)\right]$$

# Mean-field observables

## 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 $\{\mathcal{M}\}$

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## Local observables

- $\langle \hat{\mathcal{O}}_d \rangle = \sum_{AB} \langle A | \hat{\mathcal{O}}_d | B \rangle \sum_n \varphi^*_{An} \varphi_{Bn}$
- $\hat{\mathcal{O}}_d = d^\dagger_\alpha d^\dagger_\beta, \; d^\dagger_\alpha d_\beta, \; \ldots$

# Mean-field observables

## Physical electron propagator

- *definition* (Nambu-Gorkov formalism):

$$\mathbf{D}_d = -\langle T\Psi_d(\mathbf{k},\tau)\Psi_d^\dagger(\mathbf{k},0)\rangle, \qquad \Psi_d(\mathbf{k}) \equiv \begin{pmatrix} \{d_{\mathbf{k}\alpha}\} \\ \{d^\dagger_{-\mathbf{k}\alpha}\} \end{pmatrix}$$

- $\mathbf{D}_d(\mathbf{k},\omega) = \mathbf{R}\left[\omega - \mathbf{h}(\mathbf{k})\right]^{-1}\mathbf{R}^\dagger,$
  - $\mathbf{R}[\varphi] \;\longrightarrow\;$ matrix relating physical and quasiparticle operators: $\underline{\Psi}_d = \mathbf{R}\Psi_f$
  - $\mathbf{h}(\mathbf{k})[\varphi,\mathcal{M}] \;\longrightarrow\;$ quasiparticle energy matrix: $\underline{H}_f = \frac{1}{2}\sum_{\mathbf{k}} \Psi_f^\dagger(\mathbf{k})\,\mathbf{h}(\mathbf{k})\,\Psi_f(\mathbf{k})$

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

$$\begin{aligned}\mathbf{\Sigma}_d(\omega) &= \mathbf{D}_{d0}^{-1}(\mathbf{k},\omega) - \mathbf{D}_d^{-1}(\mathbf{k},\omega) \\ &= \omega\left(1 - [\mathbf{R}\mathbf{R}^\dagger]^{-1}\right) + \mathbf{\Sigma}_d(0)\end{aligned}$$

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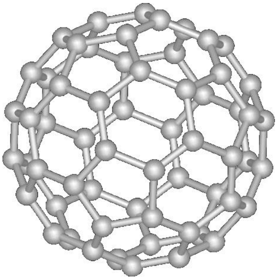
# A model for alkali-doped fullerides: $\mathrm{A_n C_{60}}$

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



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

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

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

Hund's rule is reversed!

# Slave-boson representation of the model

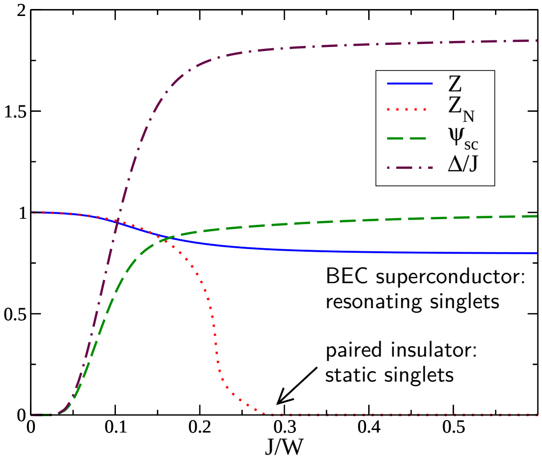
- eigenstates of $H_{\rm loc}$: $|\Gamma\rangle \equiv \big|n, (\ell, \ell_z), (s, s_z)\big\rangle$
- eigenvalues: $E_\Gamma = \frac{U}{2}n^2 + J\left[2s(s+1) + \frac{1}{2}\ell(\ell+1) + \frac{5}{6}(n-3)^2\right]$

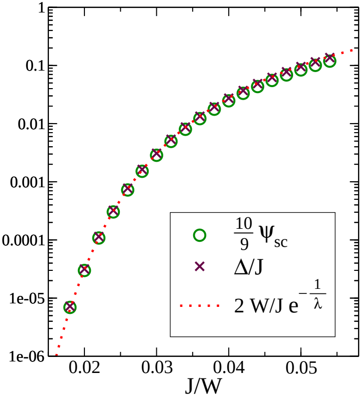
$J > 0$ (inverted Hund's rule) favors multiplets with *low* $s$ and $\ell$ $\Longrightarrow$ Cooper pairing in the spin- and orbital- *singlet* channel $(s = \ell = 0)$

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

- quasiparticle weight: $Z[\varphi]$
- $(s = \ell = 0)$ superconducting order parameter: $\psi_{sc}[\varphi] = \sum_{a=1}^{3} \left\langle d^\dagger_{a\uparrow} d^\dagger_{a\downarrow} \right\rangle$
- low-energy spectrum: $E_{\rm low}(\mathbf{k})[\varphi, \mathcal{M}] = \pm\sqrt{(Z\epsilon_{\mathbf{k}} + \lambda)^2 + |\tilde{\Delta}|^2}$

# $n_{\text{phys}} = 3$ (half-filling), $U = 0$ (attractive model)




- $W \longrightarrow$ bandwidth (flat density-of-states)

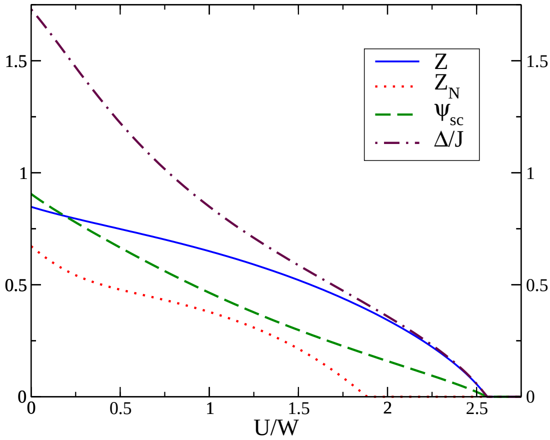
A. I. and M. Capone, Phys. Rev. B **80** (2009)

## BCS estimate

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

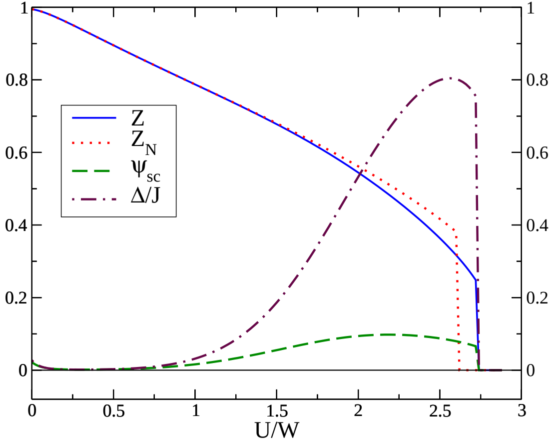
$\lambda = \frac{10}{3}(J/W)$

# $n_{\text{phys}} = 3$ (half-filling), $J/W = 0.2$ (large pair coupling)



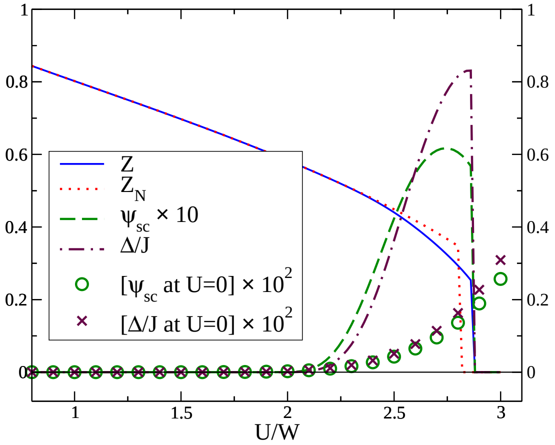

- $\Delta$ and $\psi_{sc}$ decrease *monotonically* with $U$
- $U > U_c^{(N,S)}$
  Mott-insulator:
  $\left\langle (\hat{n} - 3)^2 \right\rangle = 0$
- $Z > Z_N$: superconducting quasiparticles are *more coherent* than in normal metal

# $n_{\text{phys}} = 3$ (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 $\psi_{sc}$

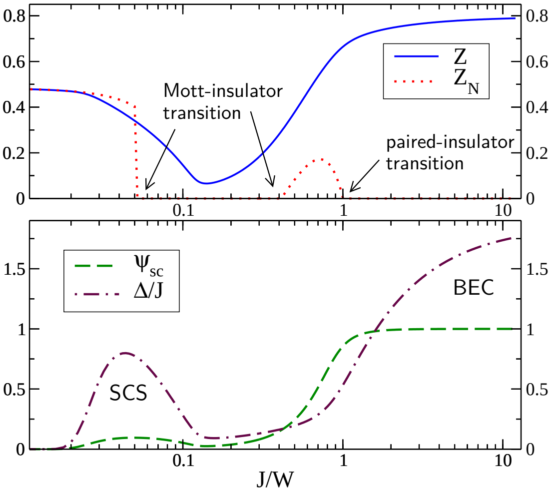
# $n_{\text{phys}} = 3$ (half-filling), $J/U = 0.01$ (small pair coupling)




- *non-BCS* superconductivity:
  - $\Delta/J \sim \mathcal{O}(1)$
  - $\Delta/J \sim 10 \times \psi_{sc}$
- large enhancement with respect to $U = 0$:

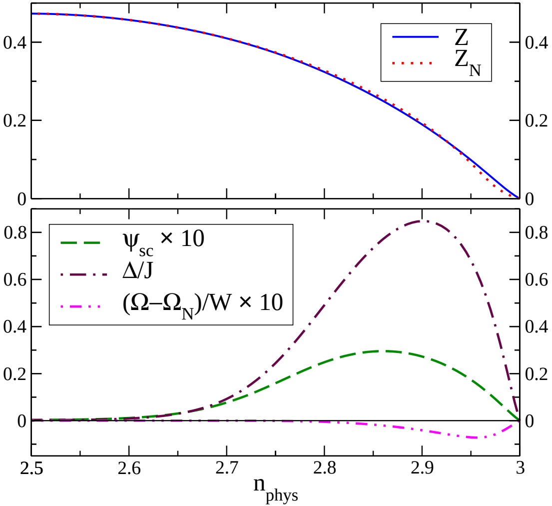
$$\Delta[J,\, U \lesssim U_c] \sim 10^3 \times \Delta[J,\, U = 0]$$

# $n_{\text{phys}} = 3$ (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:
  - $\frac{10}{3} J \gg U$

## $n_{\mathrm{phys}} = 3 - x$ (finite doping), $U/W = 5$, $J/W = 0.02$




- doping the Mott-insulator at $J/U \ll 1$
- superconducting *"dome"* as in cuprates, with optimal doping $x_{\mathrm{opt}} \approx 0.1$
- $\Delta/J \sim \mathcal{O}(1)$ at $x_{\mathrm{opt}}$
- underdoping $(x < x_{\mathrm{opt}})$: $Z > Z_N$
- overdoping $(x > x_{\mathrm{opt}})$: $Z < Z_N$

# Strongly Correlated Superconductivity

- 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: $\varphi \to \varphi(\mathbf{r}_i)$
  - 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