

Rotationally-invariant slave-bosons for strongly correlated superconductors

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- 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 fullerenes ($A_n C_{60}$, $A \equiv$ alkali metal)
- 3 Perspectives

Auxiliary fields

- slave-bosons ϕ_n^\dagger for each *local* Fock state

$$|n\rangle_d \equiv \left(d_1^\dagger\right)^{n_1} \cdots \left(d_M^\dagger\right)^{n_M} |\text{vac}\rangle, \quad [n_\alpha = 0, 1]$$

$\alpha = 1, \dots, M$ (local electronic species: orbitals and spin)

- auxiliary fermions f_α^\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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Constraints

$$\sum \phi_n^\dagger \phi_n = 1$$

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

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Density-density interactions

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

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

free-boson Hamiltonian!

Limitations of Kotliar-Ruckenstein's approach

Intrinsically *basis-dependent*

- 1 Unable to handle *arbitrary* forms of H_{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

$$H_{\text{loc}} = \sum_{\alpha\beta} \epsilon_{\alpha\beta}^0 d_{\alpha}^{\dagger} d_{\beta} + \sum_{\alpha\beta\gamma\delta} W_{\alpha\beta\gamma\delta} d_{\alpha}^{\dagger} d_{\beta}^{\dagger} d_{\gamma} d_{\delta}$$

- the eigenstates of H_{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 $|\underline{n}\rangle \equiv \phi_n^{\dagger} |\text{vac}\rangle \otimes |n\rangle_f$, the representation of H_{loc} is *no longer* a simple free-boson Hamiltonian:

$$H_{\text{loc}} \mapsto \underline{H}_{\text{loc}} \stackrel{?}{=} \sum_{nm} E_{nm} \phi_n^{\dagger} \phi_m$$

Limitations of Kotliar-Ruckenstein's approach (II)

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

$$\underline{d}_\alpha^\dagger = \hat{r}_\alpha[\phi] f_\alpha^\dagger$$



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

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

- $\langle d_\alpha^\dagger d_\beta^\dagger \rangle = 0 \quad \longrightarrow \quad$ NO charge-symmetry breaking (superconductivity)
- $\langle d_\alpha^\dagger d_\beta \rangle = \delta_{\alpha\beta} \langle \hat{n}_\alpha \rangle \quad \longrightarrow \quad$ 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

- $\{|A\rangle\}$ \longrightarrow 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., $\{|A\rangle\} = \{|n\rangle\}, \{|\Gamma\rangle\}, \dots$)
- Mapping onto the enlarged Hilbert space $\underline{\mathcal{H}}$:

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

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

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

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

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

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

Rotationally invariant formalism

Physical electron operator in \mathcal{H}

- *definition:*

$$\underline{d}_\alpha^\dagger |B\rangle = \sum_A \langle A | d_\alpha^\dagger |B\rangle |A\rangle$$

- $\underline{d}_\alpha^\dagger = \hat{R}_{\alpha\beta}^{(p)}[\phi]^* f_\beta^\dagger + \hat{R}_{\alpha\beta}^{(h)}[\phi] f_\beta$

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

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

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

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:

$$\phi_{An} \rightarrow \langle \phi_{An} \rangle \equiv \varphi_{An}$$

- minimization of the free-energy functional $\Omega[\{\varphi\}, \{\mathcal{M}\}] = -\frac{1}{\beta} \ln \mathcal{Z}$ with respect to φ 's and Lagrange multipliers $\{\mathcal{M}\}$

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Local observables

- $\langle \hat{O}_d \rangle = \sum_{AB} \langle A | \hat{O}_d | B \rangle \sum_n \varphi_{An}^* \varphi_{Bn}$
- $\hat{O}_d = d_\alpha^\dagger d_\beta^\dagger, d_\alpha^\dagger d_\beta, \dots$

Physical electron propagator

- *definition* (Nambu-Gorkov formalism):

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

- $\mathbf{D}_d(\mathbf{k}, \omega) = \mathbf{R} [\omega - \mathbf{h}(\mathbf{k})]^{-1} \mathbf{R}^\dagger$
 - $\mathbf{R}[\varphi] \rightarrow$ matrix relating physical and quasiparticle operators: $\underline{\Psi}_d = \mathbf{R} \Psi_f$
 - $\mathbf{h}(\mathbf{k})[\varphi, \mathcal{M}] \rightarrow$ 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:

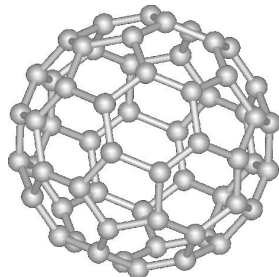
$$\begin{aligned} \Sigma_d(\omega) &= \mathbf{D}_{d0}^{-1}(\mathbf{k}, \omega) - \mathbf{D}_d^{-1}(\mathbf{k}, \omega) \\ &= \omega (1 - [\mathbf{R}\mathbf{R}^\dagger]^{-1}) + \Sigma_d(0) \end{aligned}$$

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A model for alkali-doped fullerenes: A_nC_{60}

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

- $\hat{n} = \sum_{a\sigma} d_{a\sigma}^\dagger d_{a\sigma}$,
 $\sigma = \uparrow, \downarrow$
 $a = 1, 2, 3$ 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_{JT}

$$J_{\text{JT}} \propto \sum_{\nu=1}^8 \frac{g_\nu^2}{\omega_\nu} \quad \text{effective electron-electron interaction}$$

mediated by intramolecular vibrational modes of C_{60}

Hund's rule
is reversed!

Slave-boson representation of the model

- eigenstates of H_{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 ℓ



Cooper pairing in the
spin- and orbital- *singlet*
channel ($s = \ell = 0$)

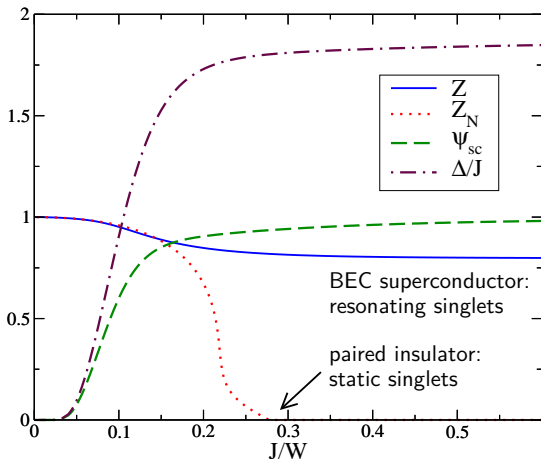
Mean-field observables (degenerate bands: $\epsilon_{ab}(\mathbf{k}) = \delta_{ab}\epsilon_{\mathbf{k}}$)

- quasiparticle weight: $Z[\varphi]$

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

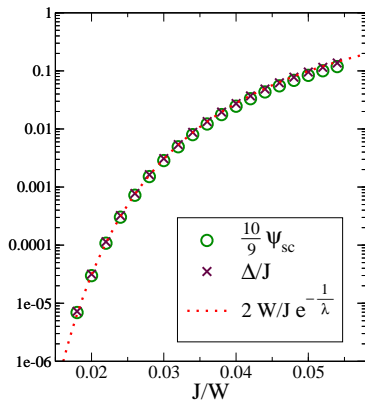
- low-energy spectrum: $E_{\text{low}}(\mathbf{k})[\varphi, \mathcal{M}] = \pm \sqrt{(Z\epsilon_{\mathbf{k}} + \lambda)^2 + |\tilde{\Delta}|^2}$

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



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

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

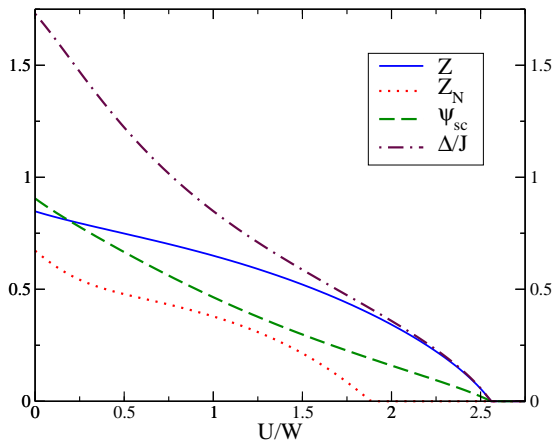


BCS estimate

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

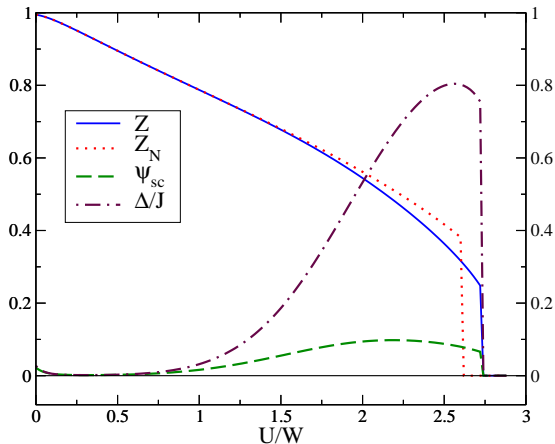
$$\lambda = \frac{10}{3} (J/W)$$

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



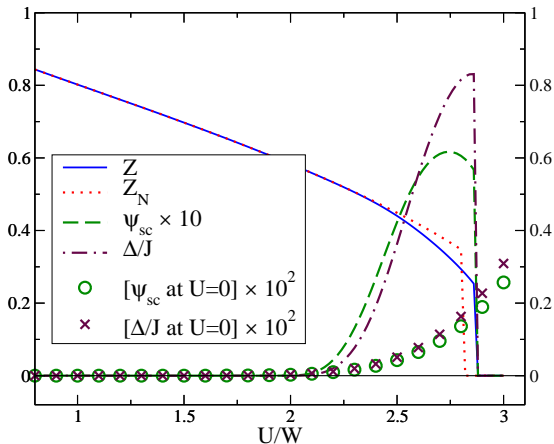
- Δ and ψ_{sc} decrease *monotonically* with U
- $U > U_c^{(N,S)}$
Mott-insulator:
 $\langle (\hat{n} - 3)^2 \rangle = 0$
- $Z > Z_N$: superconducting quasiparticles are *more coherent* than in normal metal

$n_{\text{phys}} = 3$ (half-filling), $J/W = 0.04$ (small pair coupling)



- *non-monotonic* behaviour of Δ and ψ_{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 Δ and ψ_{sc}

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



- *non-BCS*

superconductivity:

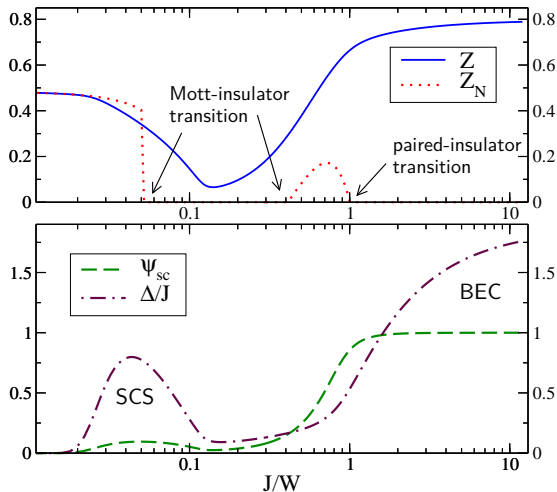
- $\Delta/J \sim \mathcal{O}(1)$

- $\Delta/J \sim 10 \times \psi_{\text{sc}}$

- 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)



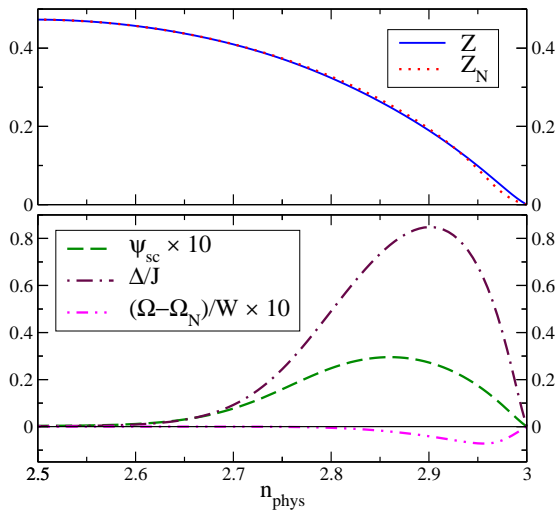
- strongly correlated superconductivity (SCS):

- $U \sim U_c^{(N)}$
- $\frac{10}{3} J \ll U$

- BEC superconductivity:

- $\frac{10}{3} J \gg U$

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



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

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: $\varphi \rightarrow \varphi(\mathbf{r}_i)$
 - non-homogeneous order parameters
 - generalization to systems *out-of-equilibrium*:
 - time-dependent slave-boson amplitudes: $\varphi \rightarrow \varphi(t)$
- M. Behrmann, M. Fabrizio, and F. Lechermann, arXiv:1304.6013