Heavy impurities in Fermi gases: A basis-change approach

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Abstract

- Unified framework that connects **Anderson's orthogonality catastrophe** [1] with the **quasiparticle picture** of mobile Fermi polarons.
- Recoil-induced **mass gap** generates an **in-gap state** ⓖ which is the microscopic origin of the **polaron-to-molecule transition**.
- **Mean-field treatment** and **basis change** yield accurate description of ground state and quasiparticle properties.

Fermi polaron problem

The Hamiltonian for a single impurity of mass M interacting with fermions of mass m in the Lee-Low-Pines (LLP) frame [2] with total momentum $\mathbf{P} = 0$ is

$$\hat{H} = \sum_{\mathbf{k}} \left(\frac{\mathbf{k}^2}{2m} + \frac{\mathbf{k}^2}{2M} \right) \hat{c}^\dagger_{\mathbf{k}} \hat{c}_{\mathbf{k}} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \hat{c}^\dagger_{\mathbf{k}} \hat{c}_{\mathbf{k}'} + \frac{1}{2M} \sum_{\mathbf{k},\mathbf{k}'} (\mathbf{k}\cdot\mathbf{k}')\, \hat{c}^\dagger_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}'} \hat{c}_{\mathbf{k}'} \hat{c}_{\mathbf{k}} \,.$$

Mass-gap description

Effective **quadratic** Hamiltonian $\hat{\mathcal{H}}_{\text{quad}}$ for heavy impurities,

$$\hat{\mathcal{H}}_{\text{quad}} = \sum_{\mathbf{k}} E_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}} \hat{c}_{\mathbf{k}} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\, \hat{c}^\dagger_{\mathbf{k}} \hat{c}_{\mathbf{k}'} \,,$$

with **gapped dispersion relation** $E_{\mathbf{k}}$ of the fermions,

$$E_{\mathbf{k}} = \begin{cases} \frac{\mathbf{k}^2}{2m} - \frac{\mathbf{k}^2}{2M} & \text{for} \quad |\mathbf{k}| < k_F \,, \\ \frac{\mathbf{k}^2}{2m} + \frac{\mathbf{k}^2}{2M} & \text{for} \quad |\mathbf{k}| > k_F \,. \end{cases}$$

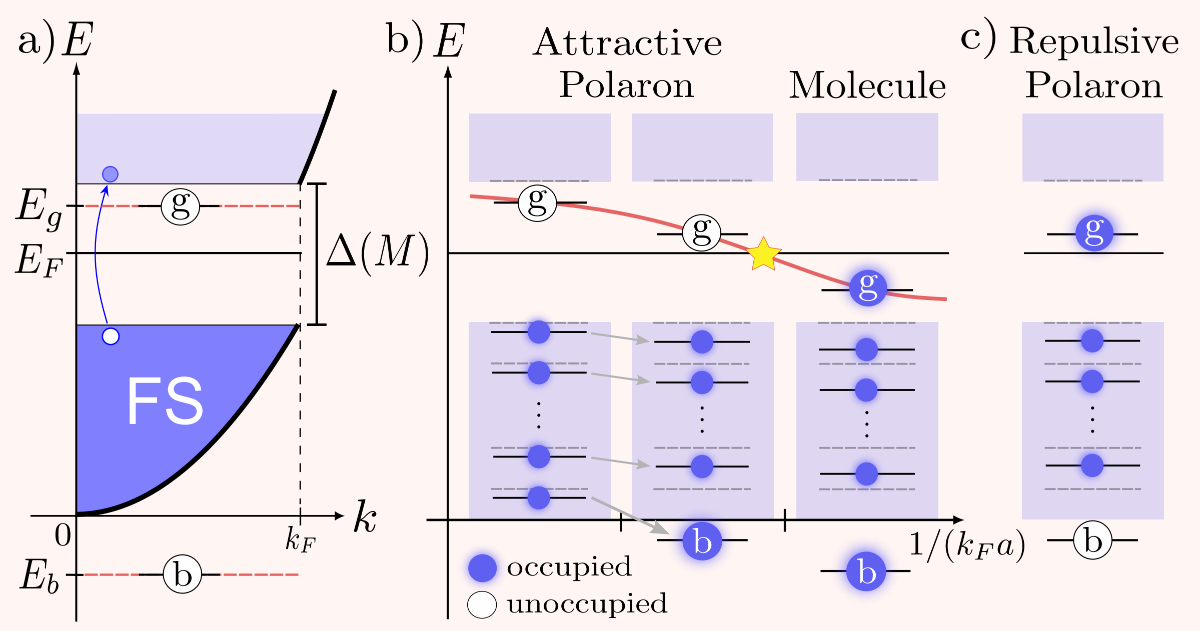

Figure 1. Gapped dispersion relation and physical interpretation of the in-gap state ⓖ.

Mean-field treatment (MFT)

Exact diagonalization of the gapped Hamiltonian $\hat{\mathcal{H}}_{\text{quad}}$ yields

$$\hat{\mathcal{H}}_{\text{quad}} = \sum_{\alpha} \omega_\alpha \hat{\gamma}^\dagger_\alpha \hat{\gamma}_\alpha \,,$$

with **single-particle spectrum** ω_α and corresponding eigenvectors $\hat{\gamma}^{(\dagger)}_\alpha$.

Functional determinant approach (FDA) to obtain the **many-body spectrum** $A(E)$,

$$S(t) = \langle e^{i\hat{\mathcal{H}}_0 t} e^{-i\hat{\mathcal{H}}_{\text{quad}} t} \rangle = \det[\hat{1} - \hat{n} + \hat{n} e^{i\hat{h}_0 t} e^{-i\hat{h}_{\text{quad}} t}] \,,$$

where the Ramsey signal $S(t)$ is the Fourier transform of the many-body spectrum,

$$A(E) = 2\text{Re} \int_0^\infty dt\, e^{iEt} S(t) \,.$$

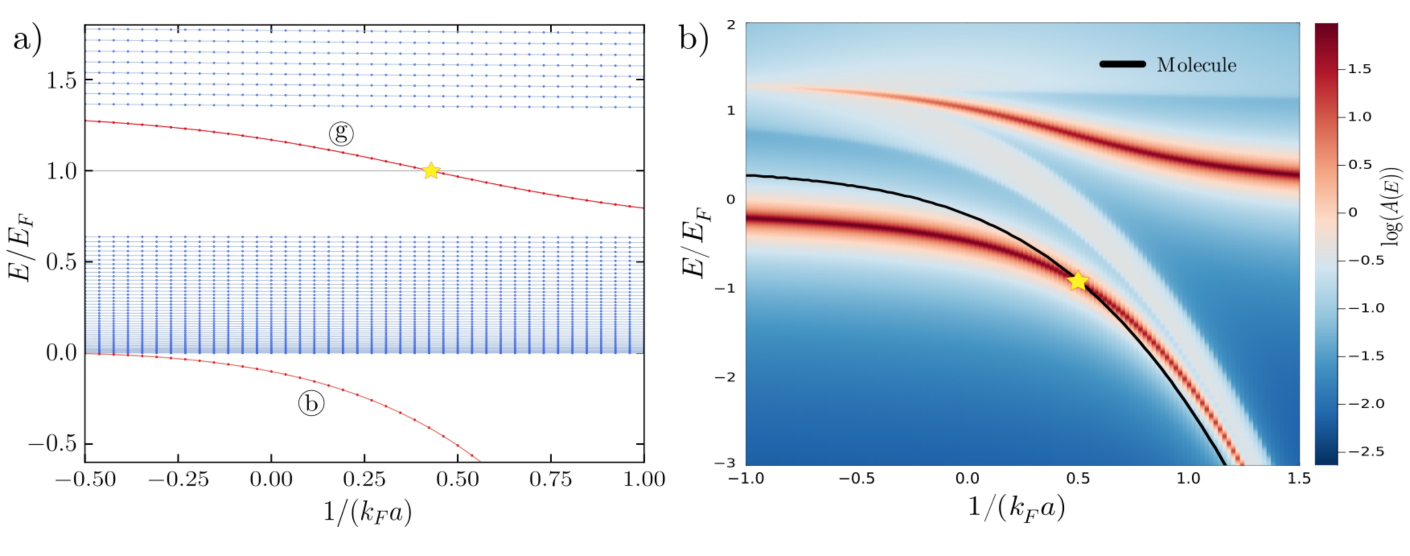

Figure 2. a) Single-particle spectrum ω_α and b) many-body spectrum $A(E)$ as function of $1/(k_F a)$.

Variational ansatz in the interacting basis (VAIB)

The **variational ansatz** in the basis-changed LLP frame has the general form

$$|\Psi\rangle = \phi_0 |\widetilde{\text{FS}}\rangle + \sum_{\alpha>,\beta<} \phi_{\alpha\beta}\, \hat{\gamma}^\dagger_\alpha \hat{\gamma}_\beta |\widetilde{\text{FS}}\rangle \,,$$

where $\beta <$ ($\alpha >$) denotes the occupied (unoccupied) states, and $|\widetilde{\text{FS}}\rangle = \prod_{\beta<} \hat{\gamma}^\dagger_\beta |0\rangle$ is the interacting Fermi sea. We can define three different variational ansätze for the **attractive polaron (AP)**, the **repulsive polaron (RP)** and the dressed **molecule (M)**.

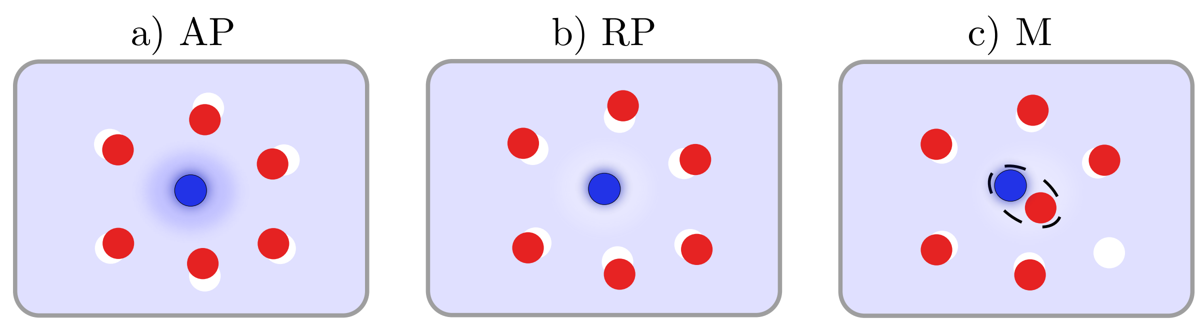

Figure 3. Illustration of the three excitations in the Fermi polaron problem: AP, RP and M.

Basis change

The new creation operators $\hat{\gamma}^\dagger_\alpha$ are related to the non-interacting fermions $\hat{c}^\dagger_{\mathbf{k}}$ via

$$\hat{\gamma}^\dagger_\alpha = \sum_{\mathbf{k}} \langle \mathbf{k} | \tilde{\alpha} \rangle \hat{c}^\dagger_{\mathbf{k}} \,.$$

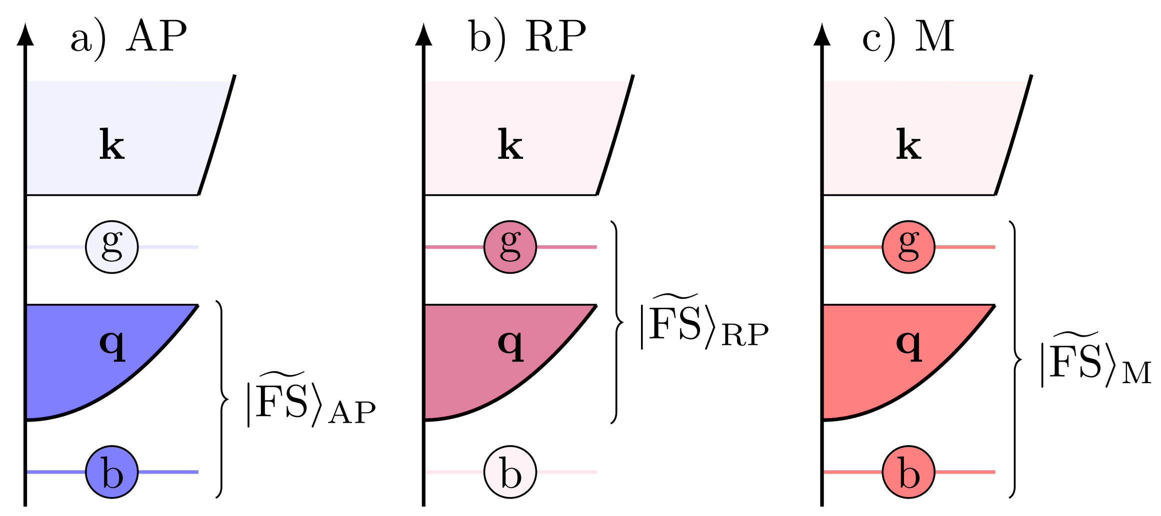

Figure 4. Definition of the modified Fermi sea $|\widetilde{\text{FS}}\rangle$ for the AP, RP and M.

Quasiparticle weight $Z = |\langle \text{FS}|\widetilde{\text{FS}}\rangle|^2$ and **ground state energy** $E = \langle \Psi | \hat{H} | \Psi \rangle$:

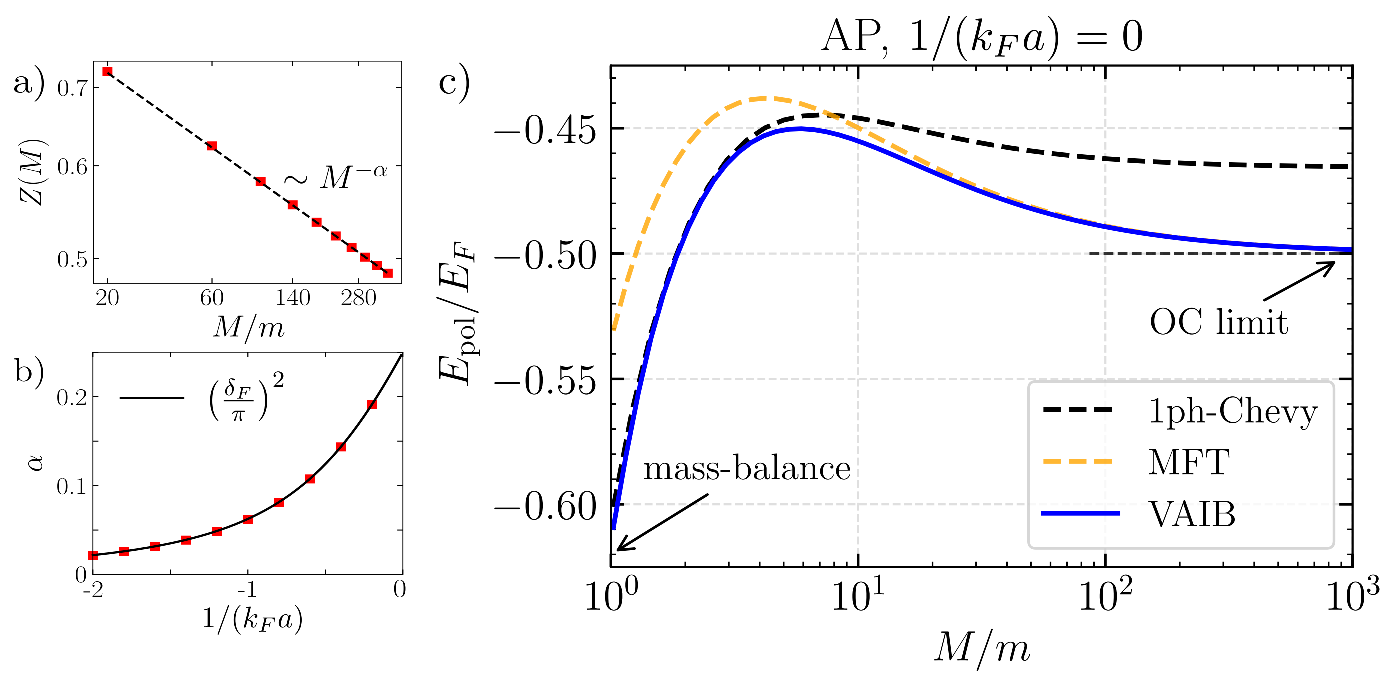

Figure 5. Quasiparticle weight and ground state energy at $1/(k_F a) = 0$ as function of mass-ratio M/m.

Method	MFT	HF	1ph-Chevy	2ph-Chevy	VAIB	DiagMC
E_{pol}/E_F	-0.534	-0.606	-0.6066	-0.6156	-0.616	-0.618

Table 1. Ground state energy for $M/m = 1$ and $1/(k_F a) = 0$ using different methods.

References

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