Precision Thermodynamics of the Fermi Polaron at Strong Coupling

Shasta Ramachandran

Scott Jensen

Yoram Alhassid

Center for Theoretical Physics, Yale University

LUX ET VERITAS

Yoram Alhassid
Yale University

Scott Jensen
University of Louisville

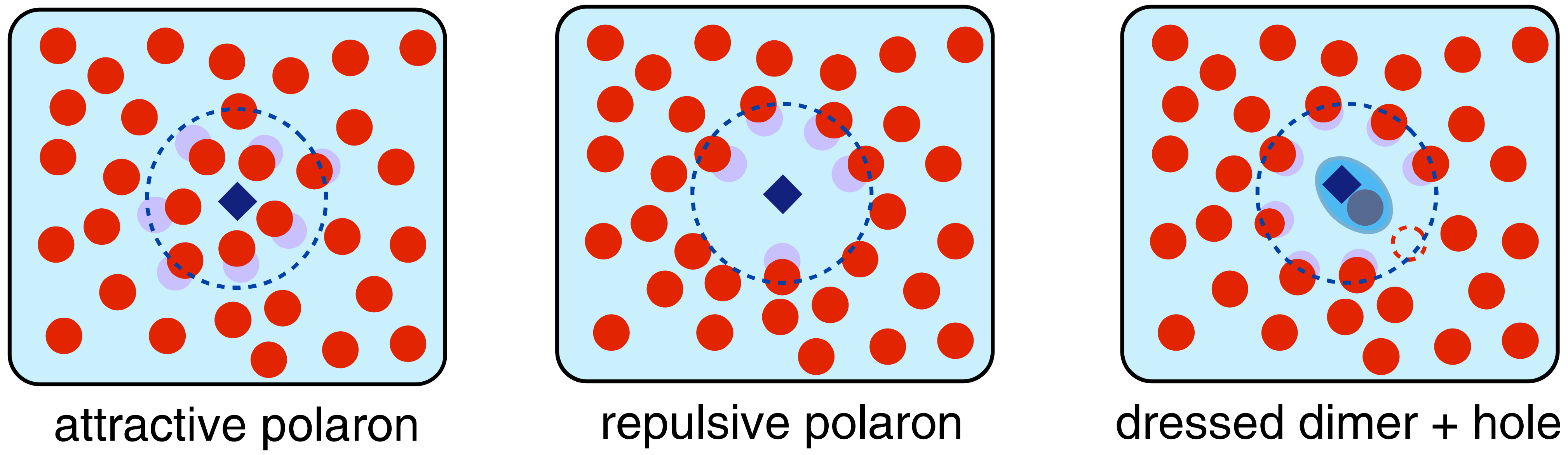
Outline

- Introduction: the Fermi polaron problem
- Canonical-ensemble auxiliary field quantum Monte Carlo
- Monte Carlo sign problem
- The contact
- Impurity free energy and spectroscopy
- Conclusions + Outlook

S. Ramachandran, S. Jensen, and Y. Alhassid, arXiv:2410.00886, in press (2025)

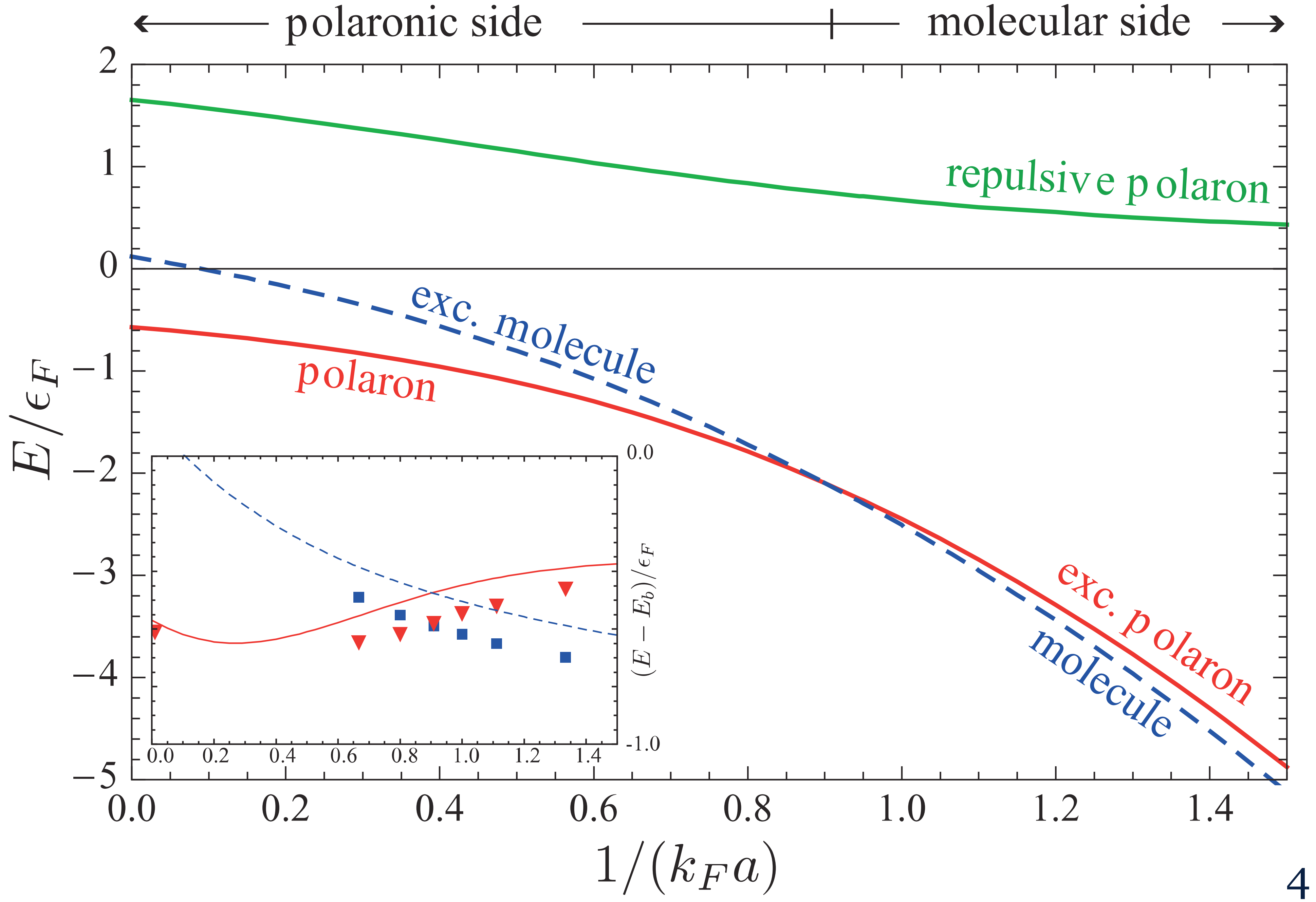
Introduction: the Fermi polaron problem

- A mobile impurity interacting with a spin-polarized medium (Fermi sea) - a fundamental problem first described by Landau and Pekar (1948)
- Quasiparticle excitations: attractive and repulsive Fermi polarons, dimer molecule



Massignan et al (2014)

Schmidt et al (2011)



- Interaction: can be tuned to reproduce the two-particle scattering length a
- Unitary limit of $k_F a \to \infty$: crossover to a Fermi polaron at low temperatures
- Transition from polaron to dressed dimer at $\frac{1}{k_F a} \sim 1$
- Recently realized in cold atom experiments

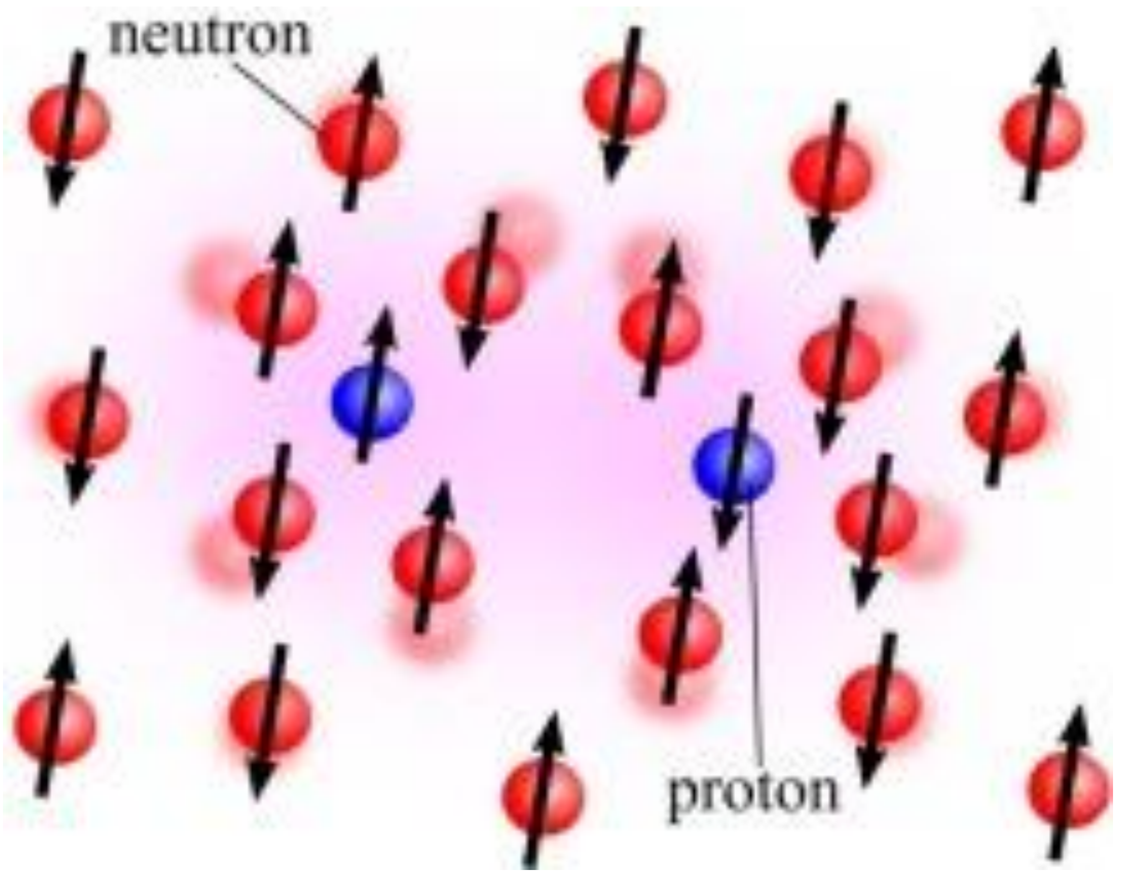
Introduction: the polaron problem in nuclear matter

- The polaron is a paradigm system for impurity physics in nuclear matter

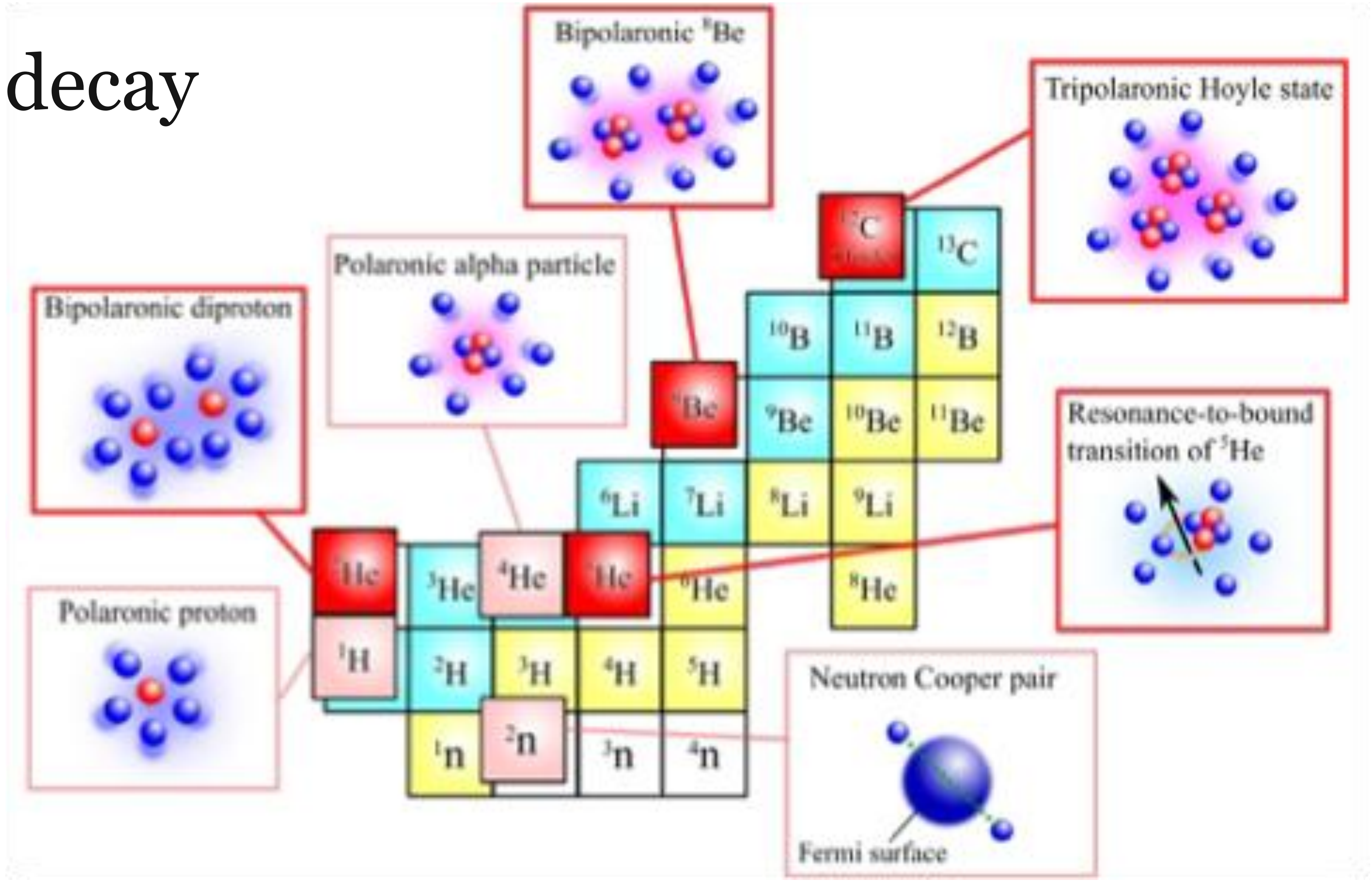
- Neutron stars: impurities in neutron matter

  - Protons, He^3 nuclei, Tritons, Alpha Particles, and Hyperons

- Polaron ejection spectroscopy: model for alpha particle decay



Tajima et al (2024)



Tajima et al (2025)

Model Hamiltonian

We consider the two-species Fermi gas (spin 1/2) with a contact interaction at near-total spin polarization, $N_\uparrow = N$ (Fermi sea) and $N_\downarrow = 1$ (impurity)

- Continuum Hamiltonian

$$\hat{H} = \int d^3\mathbf{r} \sum_{s_z} \hat{\psi}^\dagger_{s_z}(\mathbf{r}) \left(-\frac{\hbar^2 \nabla^2_{\mathbf{r}}}{2m} \right) \hat{\psi}_{s_z}(\mathbf{r}) + V_0 \int d^3\mathbf{r}\ \hat{\psi}^\dagger_\uparrow(\mathbf{r}) \hat{\psi}^\dagger_\downarrow(\mathbf{r}) \hat{\psi}_\downarrow(\mathbf{r}) \hat{\psi}_\uparrow(\mathbf{r})$$

- Lattice Model: we use a discrete lattice of size N_L^3 with spacing δx

$$\hat{H} = \sum_{\mathbf{k}, s_z} \frac{\hbar^2 k^2}{2m} \hat{a}^\dagger_{\mathbf{k}, s_z} \hat{a}_{\mathbf{k}, s_z} + \frac{V_0}{(\delta x)^3} \sum_{\mathbf{x}_i} \hat{n}_{\mathbf{x}_i, \uparrow} \hat{n}_{\mathbf{x}_i, \downarrow}$$

- The coupling strength V_0 is determined to reproduce the scattering length a on the lattice
- Two important limits must be taken
  - Continuum limit $\delta x \to 0$ at fixed N
  - Thermodynamic limit of large N

Canonical-ensemble auxiliary-field quantum Monte Carlo (AFMC) method

- We performed the first controlled calculation of the polaron problem at finite temperature with AFMC

- AFMC is based on the Hubbard-Stratonovich Transformation, which describes the thermal propagator as a path integral over imaginary-time dependent auxiliary fields $\sigma(\mathbf{x}, \tau)$

$$e^{-\beta \hat{H}} = \int D[\sigma] G_\sigma \hat{U}_\sigma$$

G_σ is a Gaussian weight and $\hat{U}_\sigma$ is the thermal propagator for *non-interacting* particles moving in external auxiliary fields $\sigma(\mathbf{x}, \tau)$; the integrand can be evaluated using matrix algebra in the single-particle space

- We use Monte Carlo sampling to select the important configurations of the auxiliary fields

- We perform an exact particle number projection, enabling canonical-ensemble calculations

For a recent review, see Y. Alhassid, Emergent Phenomena in Atomic Nuclei from Large-Scale Modeling (2017)

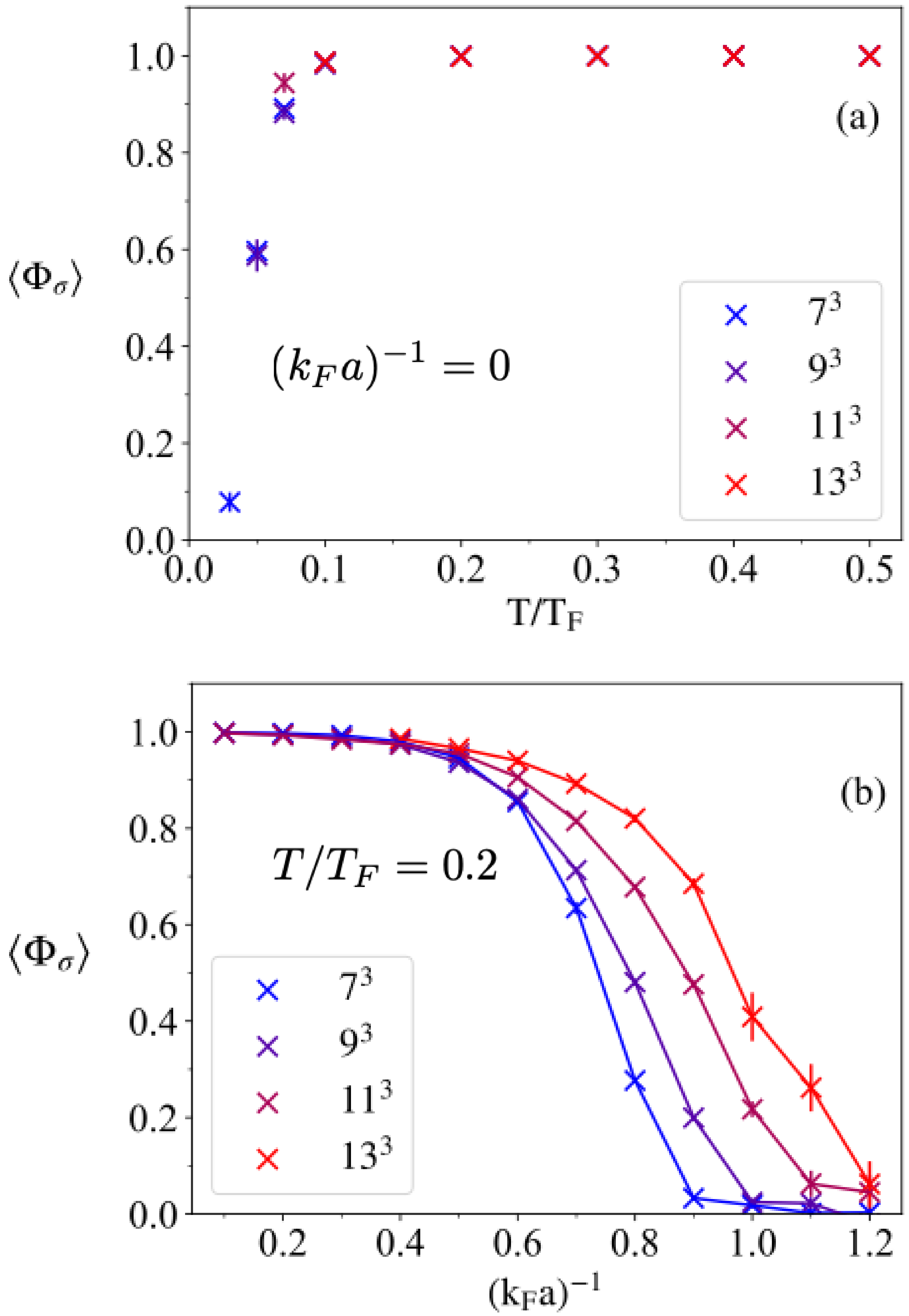
S. Jensen, C. N. Gilbreth, and Y. Alhassid, Phys. Rev. Lett. 125 (2020)

The Monte Carlo sign

- Spin-imbalanced systems are prone to a Monte Carlo sign problem

- We find that for a single impurity, the Monte Carlo sign $\langle \Phi_\sigma \rangle$ is good or moderate at experimentally accessible temperatures and interaction strengths

- The Monte Carlo sign worsens near the polaron-molecule transition, but still manageable



The contact

- The contact C is defined through the two-body correlation function at short distance:

$$\langle \hat{n}_\uparrow(\mathbf{r})\hat{n}_\downarrow(0)\rangle \sim \frac{C}{4\pi r^2}$$

- A fundamental property of quantum many-body systems with short range interactions

- The universal Tan relations relate the contact to other properties of the system

- Characterizes the tail of momentum distribution: $n_\sigma(\mathbf{k}) \sim \dfrac{C}{k^4}$

- Describes the derivative of the energy with respect to the interaction strength

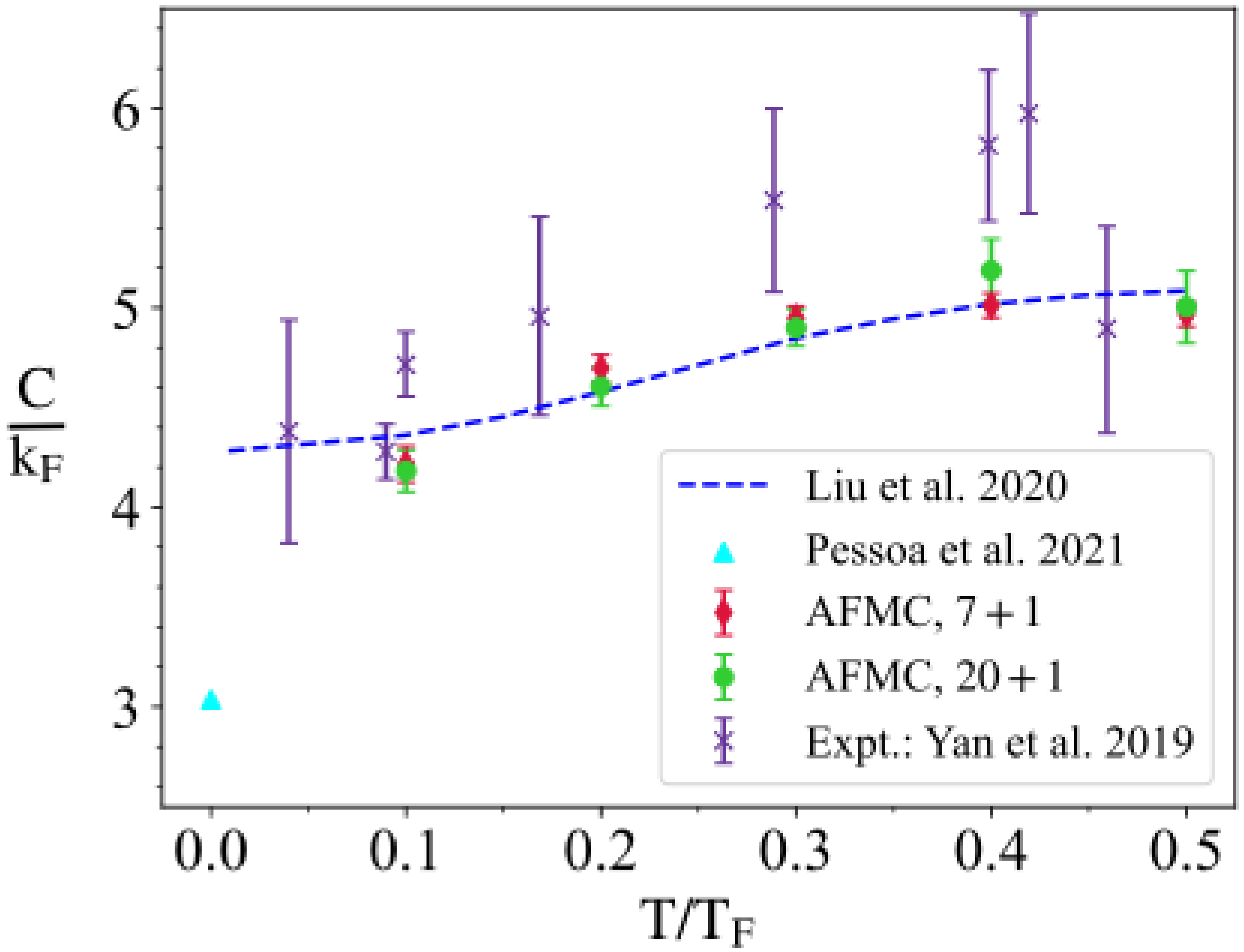
$$C = \frac{4\pi m}{\hbar^2} \left.\frac{\partial E}{\partial(-1/a)}\right|_S$$

Contact vs. temperature at unitarity

- Our results are in overall agreement with the experimental results of the MIT group

- Our results are in good agreement with the variational one-particle hole results of Liu et. al.

- The monotonic increase in the contact reflects the increased population of the molecular continuum, where pair correlations are larger

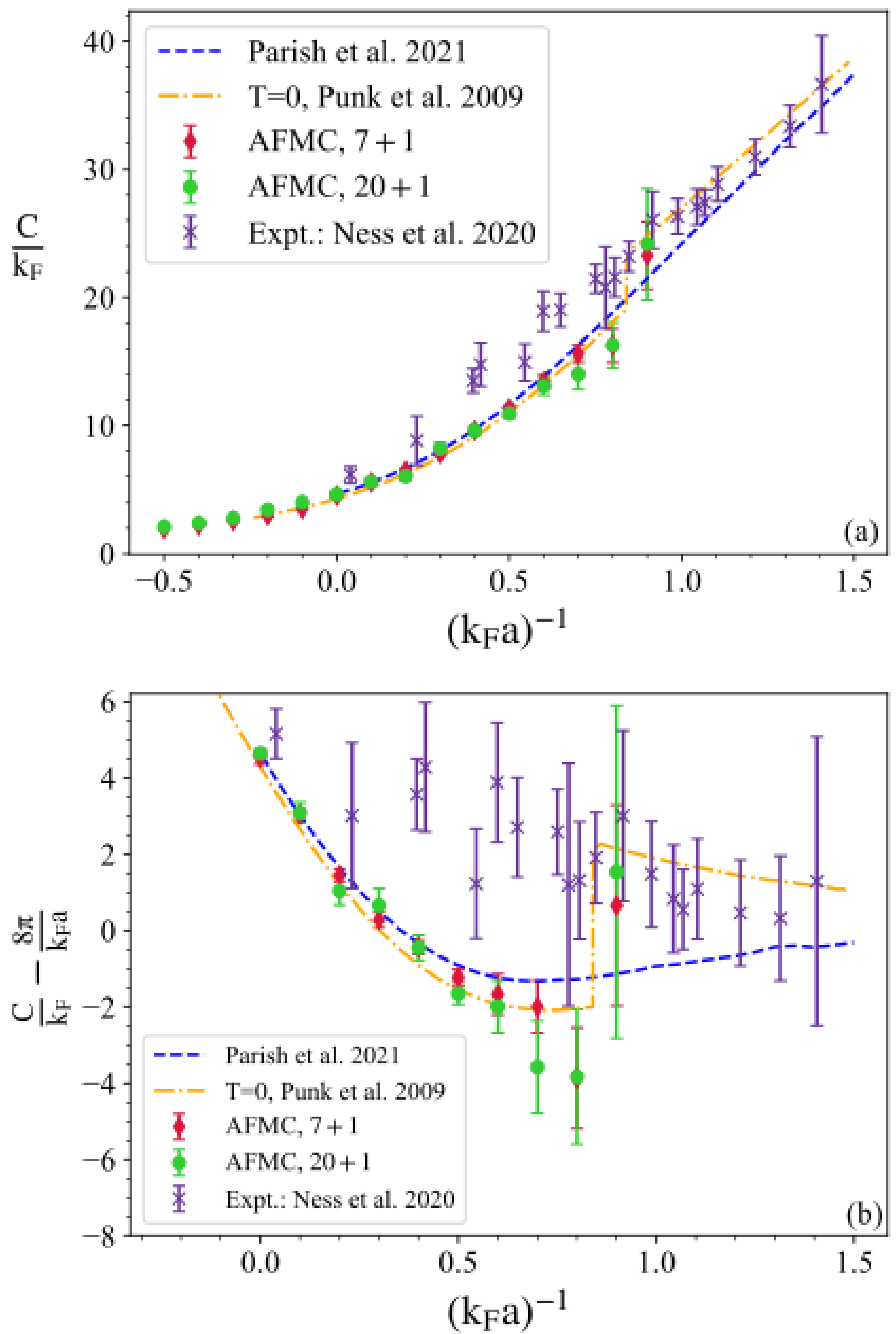


Contact vs. $\frac{1}{k_F a}$ at $T = 0.2\ T_F$

- As a function of $(k_F a)^{-1}$, the leading term arises from the two-particle binding energy, so we also plot $C - \frac{8\pi}{a}$ (lower panel)

- Our results are in between Punk et al and Parish et al

- We see a significant deviation from experiment for $\frac{1}{k_F a} \sim 0.2 - 0.7$



Impurity free energy

- The impurity free energy $\Delta F = F - F_{\text{med}} - F_{\text{imp}}$ relates the ejection (1 -> 0 impurity transition) and injection (0 -> 1 transition) spectral functions through the detailed balance condition

$$A_{\text{ej}}(\mathbf{p}, \omega) = e^{\beta \Delta F} e^{\beta \omega} n_B(\mathbf{p}) A_{\text{inj}}(\mathbf{p}, -\omega)$$

- Calculating real-time observables like these spectral functions with AFMC requires the use of numerical analytic continuation

- However, we can calculate the impurity free energy as a thermodynamic observable, without the use of analytic continuation

Impurity free energy vs. temperature at unitarity

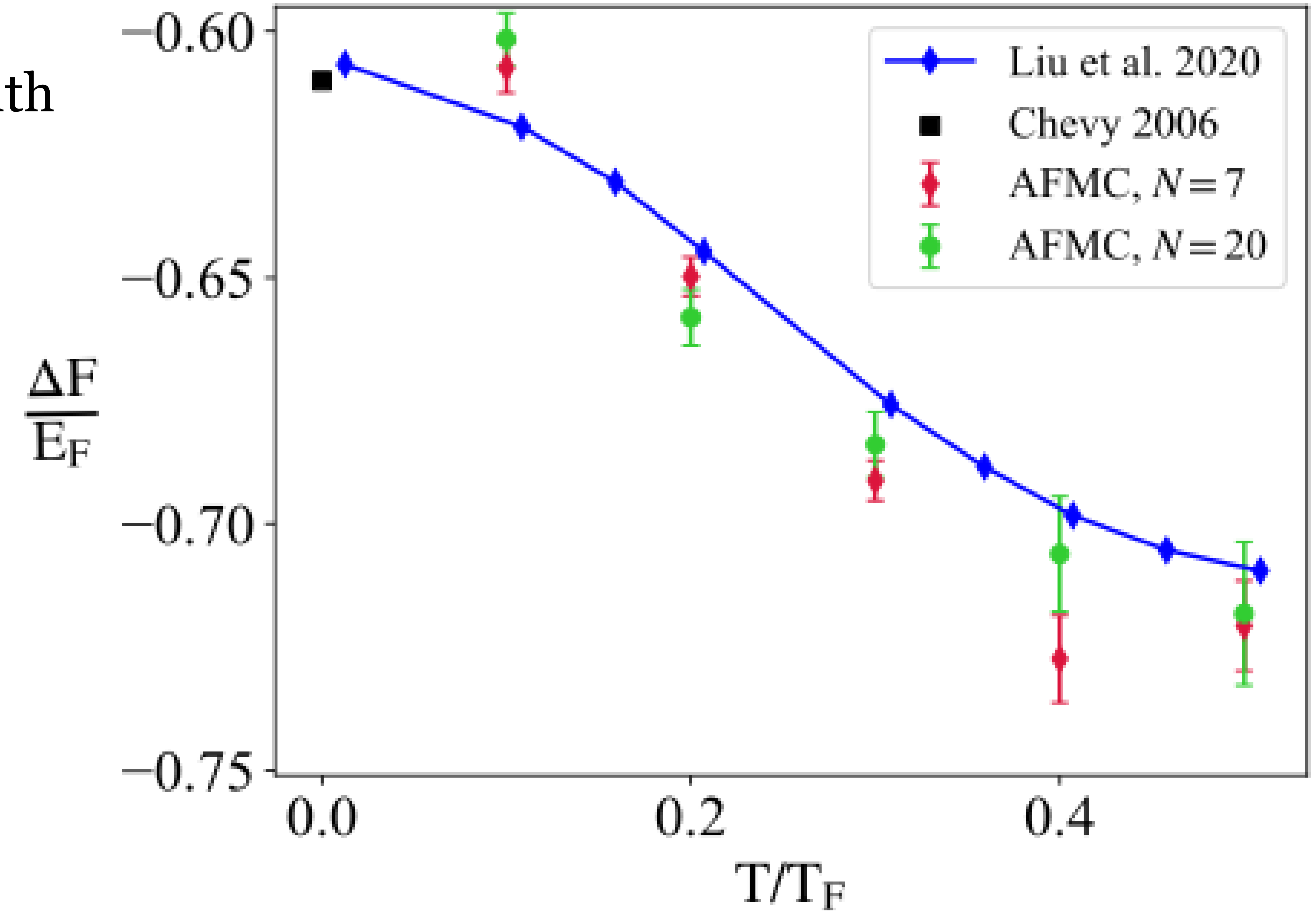
The free energy can not be calculated directly with AFMC; instead, we calculate the ratio

$$\left\langle \frac{Z_{\text{med}}}{Z_{\text{int}}} \right\rangle_\sigma = \frac{\text{Tr}\left[\hat{a}^\dagger_{\mathbf{k},\downarrow} \hat{U}_\sigma \hat{a}_{\mathbf{k},\downarrow}\right]}{\text{Tr}\left[\hat{U}_\sigma\right]} = 1/\text{Tr}[\mathbf{U}_\sigma]$$

and take

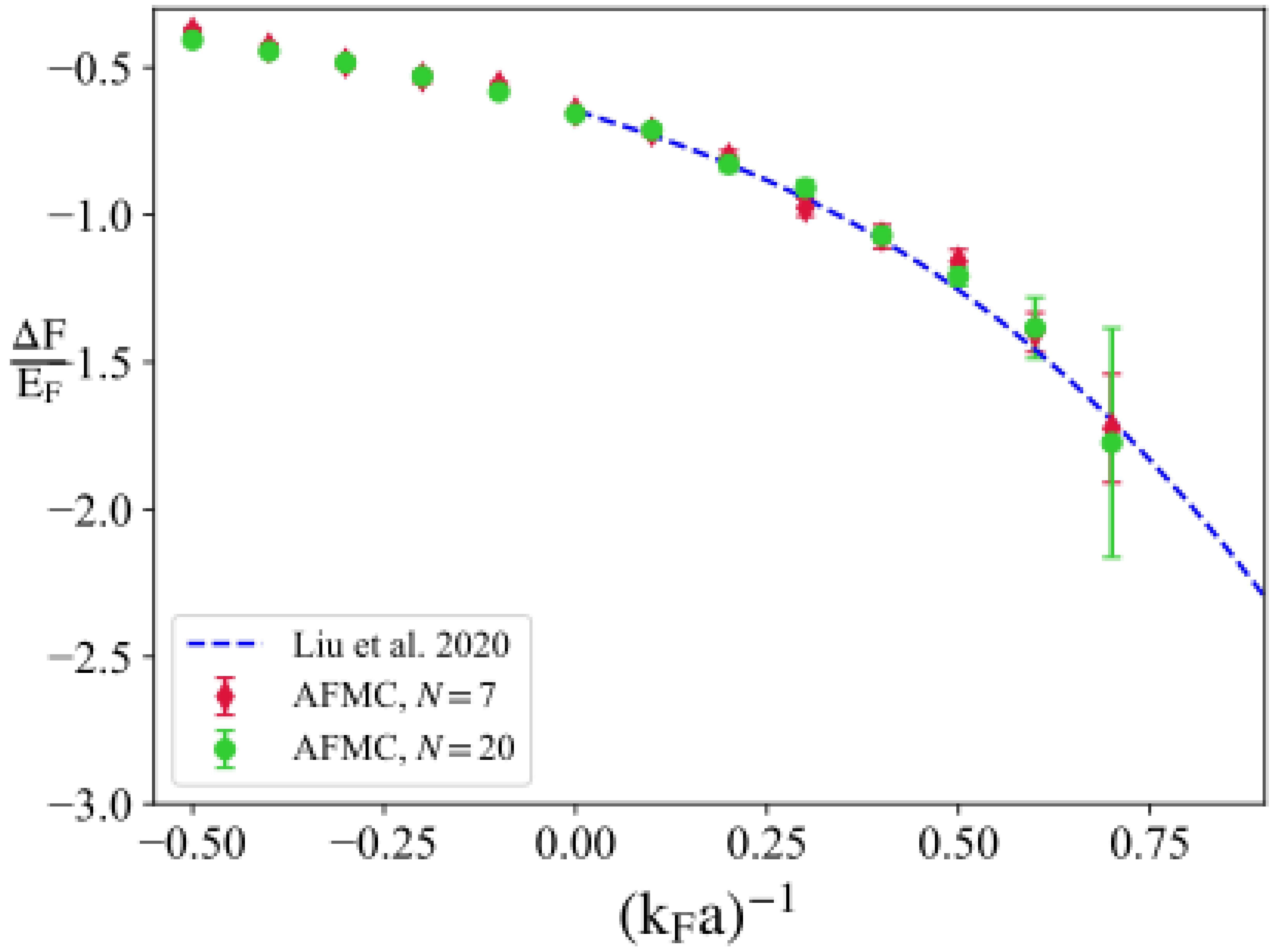
$$e^{\beta \Delta F} = \frac{Z_{\text{imp}} Z_{\text{med}}}{Z_{\text{int}}}$$

We find overall agreement with the variational results of Liu et al



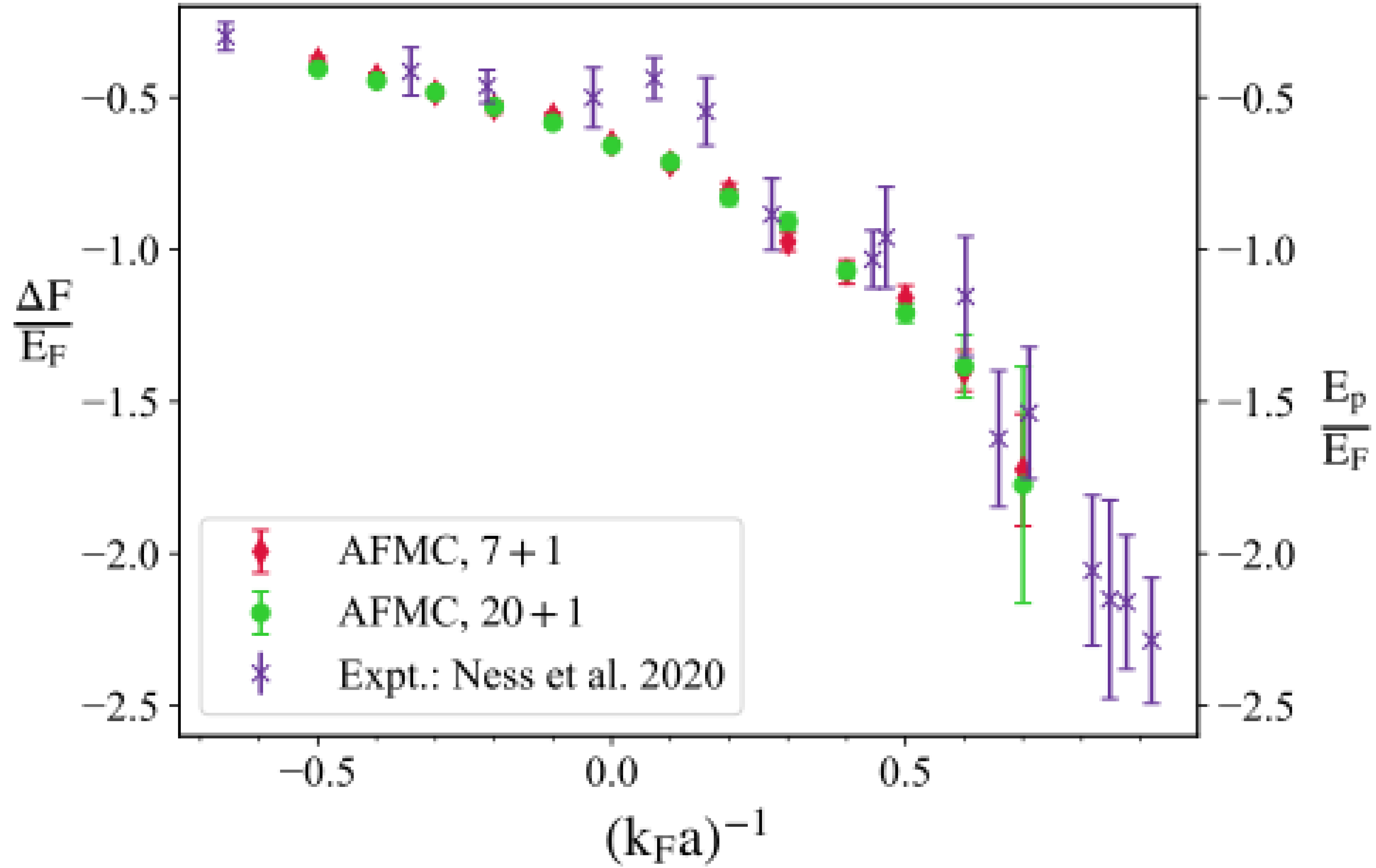
$$A_{\text{ej}}(\mathbf{p}, \omega) = e^{\beta \Delta F} e^{\beta \omega} n_B(\mathbf{p}) A_{\text{inj}}(\mathbf{p}, -\omega)$$

Impurity free energy vs. $\frac{1}{k_F a}$ at $T = 0.2\ T_F$



Our results are in overall agreement with the variational results of Liu et. al.

Free energy and polaron energy at $T = 0.2\ T_F$



At low temperatures $\Delta F \sim E_p$

We find good agreement of ΔF with experimental results for the attractive polaron energy E_p

Conclusion

- Canonical-ensemble AFMC simulations are particularly suitable for the polaron
- First controlled calculation for the polaron at finite temperature
- Our results for the contact agree overall with the variational method, but deviate from experiment in the regime $\frac{1}{k_F a} \sim 0.2 - 0.7$
- Our results for the impurity free energy approximate the experimental polaron energy well

Outlook

- Polaron-Molecule transition: investigate the system near the critical interaction strength
- Calculate the spectral function of the impurity to determine the quasiparticle excitations of the system
- Compare our results to DiagMC and T-Matrix results
- Study the strongly driven polaron: steady-state response of the polaron driven by Rabi oscillations