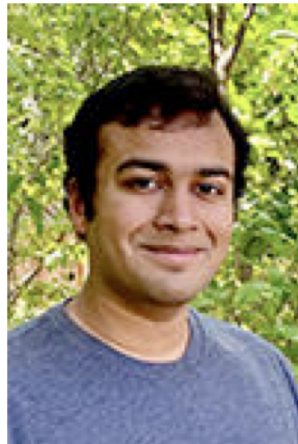


Exploring the Fermi polaron problem with canonical-ensemble auxiliary-field quantum Monte Carlo

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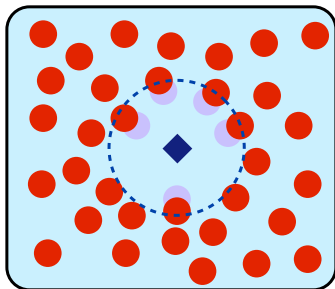
Exploring the Fermi polaron problem with canonical-ensemble auxiliary-field quantum Monte Carlo

- Introduction: the Fermi polaron problem
- Canonical-ensemble auxiliary-field Monte Carlo (AFMC) methods
- Monte Carlo sign problem
- The contact
- The free energy gap
- Conclusion and outlook

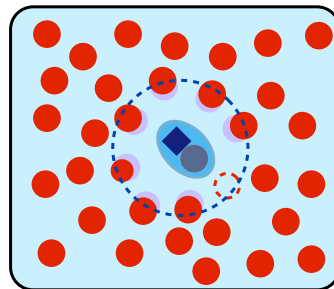
Introduction: the Fermi polaron problem

A mobile impurity interacting with a spin-polarized medium (Fermi sea)
- a fundamental many-body problem, first described by Landau and Pekar (1948)

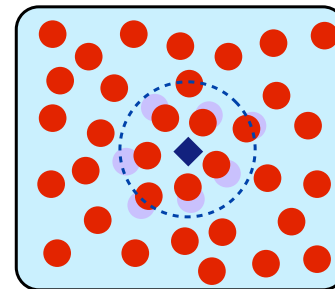
- Realized in cold atom experiments of two-components (i.e., spin-1/2) Fermi gas interacting with a short-range interaction.
- This system has several quasi-particle excitations:
attractive polaron, dressed dimer (molecule), repulsive polaron



repulsive polaron



dressed dimer + hole

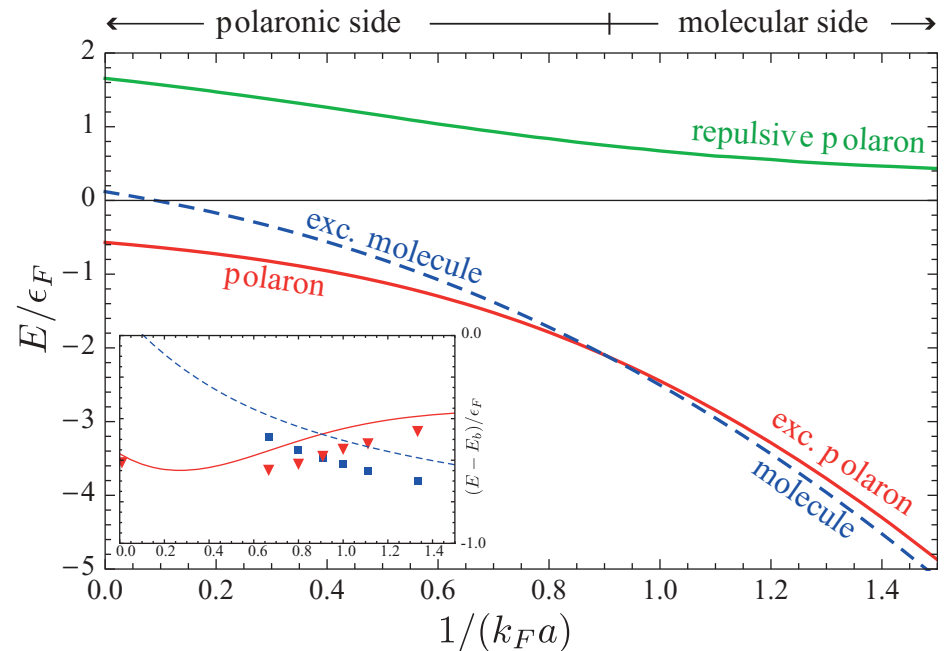


attractive polaron

Consider a two-component (spin up/down) fermionic atoms with $N_{\uparrow} = N$ and $N_{\downarrow} = 1$ interacting with a short-range interaction $V_0 \delta(\mathbf{r} - \mathbf{r}')$ characterized by a scattering length a .

- In the unitary limit $a \rightarrow \infty$, there is a crossover from a Fermi polaron at low temperatures to a classical Boltzmann gas at higher temperatures.

- At zero temperature, there is phase transition from a polaron to a dressed dimer (molecule) as a function of $1/(k_F a)$



Ground-state ($T=0$) properties were studied by several methods: diffusion Monte Carlo, diagrammatic Monte Carlo, functional renormalization group, ...

At finite temperature, variational one particle-hole approximations were used but there have been no controlled calculations.

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

We carried out the first controlled calculations of the polaron problem at finite temperature using AFMC

AFMC is based on the Hubbard-Stratonovich transformation, which describes the Gibbs ensemble $e^{-\beta H}$ at inverse temperature $\beta=1/T$ as a path integral over time-dependent auxiliary fields $\sigma(\tau)$

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

G_σ is a Gaussian weight and U_σ is a propagator of *non-interacting* particles moving in external auxiliary fields $\sigma(\tau)$

- The integrand reduces to matrix algebra in the single-particle space.

The high-dimensional integration over σ is evaluated by importance sampling.

We implemented the canonical ensemble by exact particle-number projection.

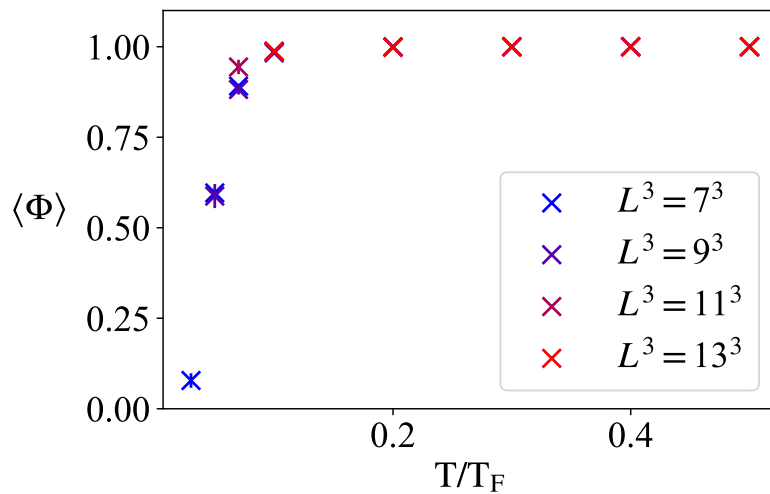
Recent review of AFMC: [Y. Alhassid](#), in *Emergent Phenomena in Atomic Nuclei from Large-Scale Modeling*, ed. [K.D. Launey](#) (World Scientific 2017)

Monte Carlo sign

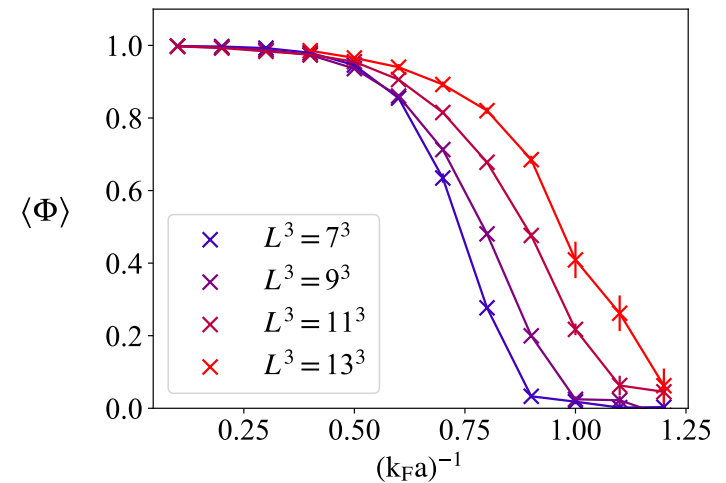
In the spin-balanced case, the Monte Carlo sign is positive for all samples.

However, for a spin-imbalanced system (e.g., the polaron), the sign can be negative for some samples and the average sign $\langle \Phi \rangle < 1$

Sign vs temperature at unitarity



Sign vs coupling at $T = 0.2 T_F$



- At unitarity, the sign problem is moderate for temperatures $T > 0.1 T_F$
- At low temperatures, the sign problem is moderate up to a coupling of $1/(k_F a) < 0.7$

A lattice approach

S. Jensen, C.N. Gilbreth, and Y. Alhassid, Phys. Rev. Lett. **124** (2020)

We use a discrete spatial lattice with spacing δx

Lattice Hamiltonian:
$$H = \sum_{\mathbf{k}\sigma} \frac{\hbar^2 k^2}{2m} a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma} + \frac{V_0}{2(\delta x)^3} \sum_{\mathbf{x}_i\sigma} \psi_{\mathbf{x}_i\sigma}^\dagger \psi_{\mathbf{x}_i\sigma}^\dagger \psi_{\mathbf{x}_i\sigma'} \psi_{\mathbf{x}_i\sigma}$$

\mathbf{k}, σ is a single-particle state with momentum \mathbf{k} and spin σ
 $\psi_{\mathbf{x}_i\sigma}^\dagger$ is a creation operator at site \mathbf{x}_i and spin σ .

- Two important limits must be taken:

(i) **Continuum limit** $\delta x \rightarrow 0$ or filling factor $\nu \rightarrow 0$ at a fixed particle number N

(ii) **Thermodynamic limit** of large particle number $N \rightarrow \infty$

The contact C

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

- The contact C describes the short-range pair correlation at distance r

$$\langle n_{\uparrow}(r)n_{\downarrow}(0) \rangle \sim \frac{C}{4\pi r^2}$$

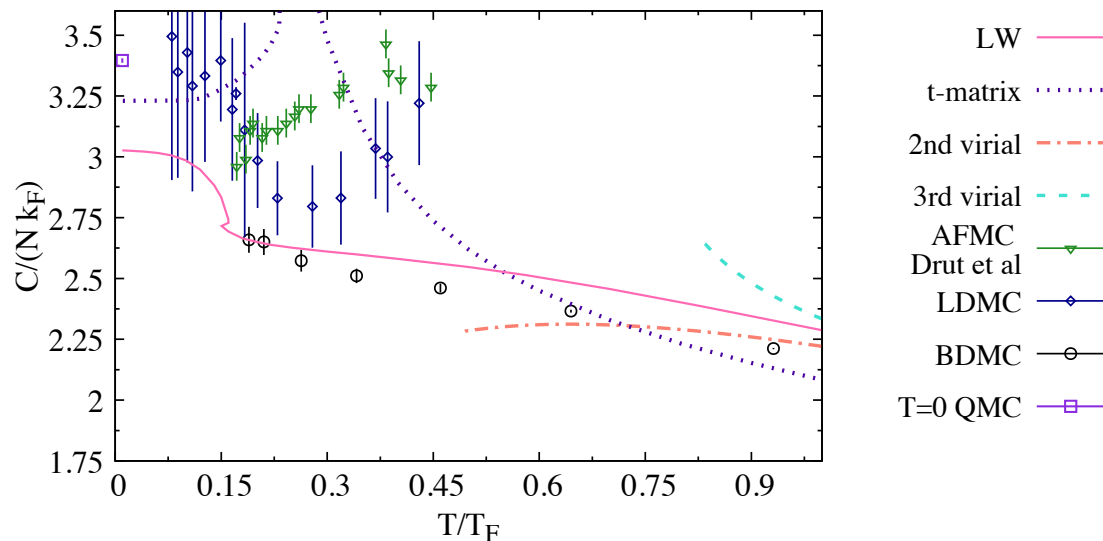
- Characterizes the tail of the momentum distribution $n_{\sigma}(k) \sim \frac{C}{k^4}$
- Characterizes the high-frequency tail of the shear viscosity spectral function
- Can be expressed as the adiabatic derivative of the energy with respect to the inverse scattering length

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

...

Contact in the unitary Fermi gas (spin-balanced case)

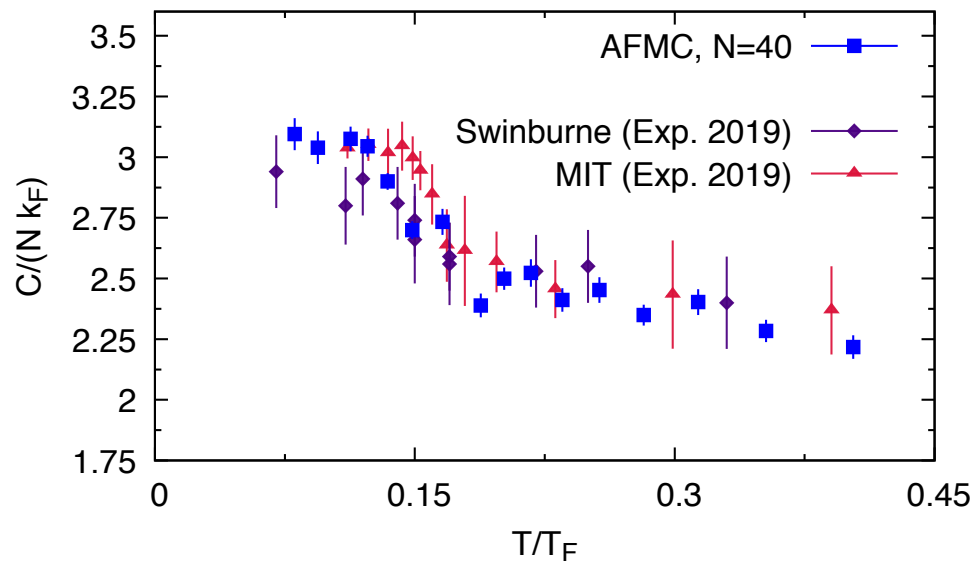
Theoretical calculations differ widely, even on a qualitative level.



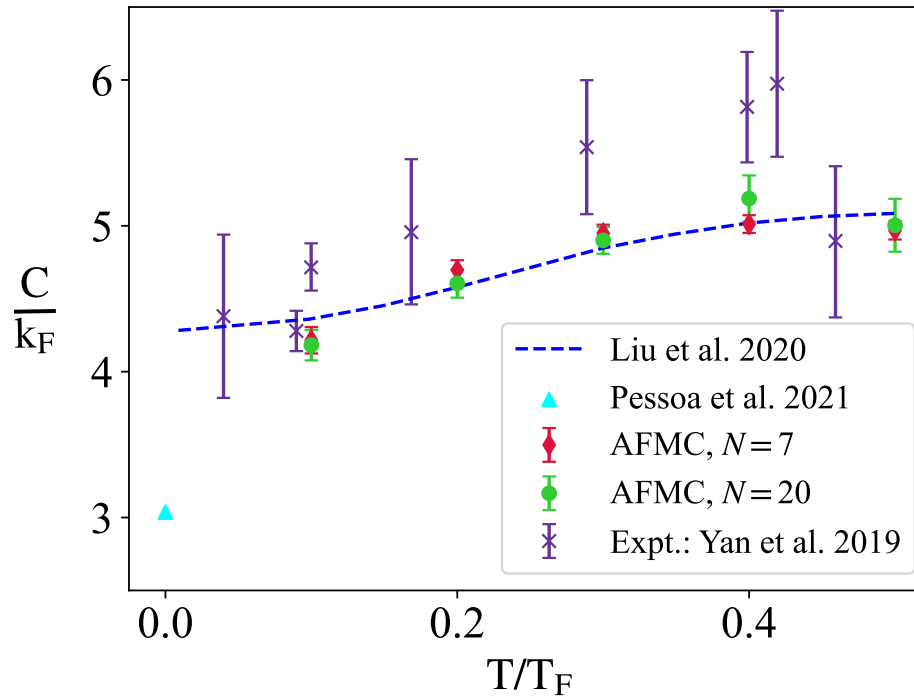
--Many of the strong coupling theories are based on uncontrolled approximations

Our continuum limit AFMC results provide the best quantitative agreement with the recent precision experiments.

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

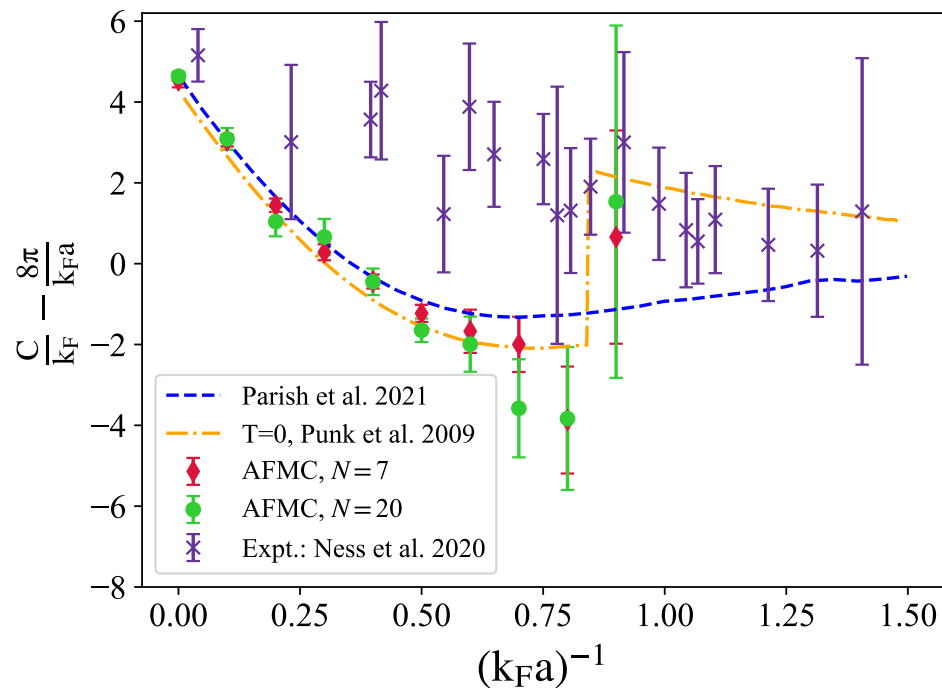
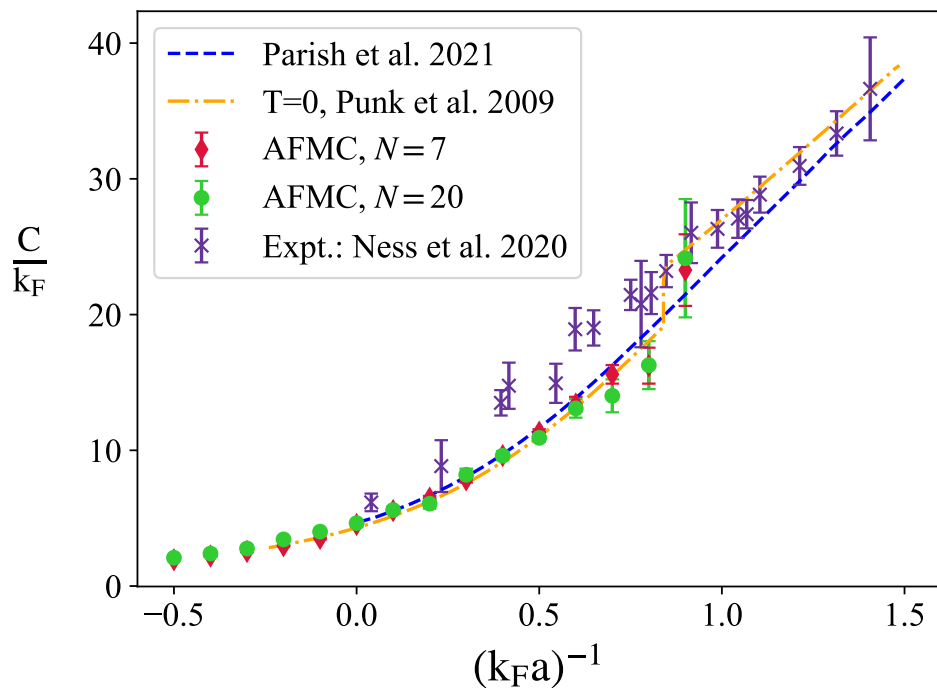


Contact vs temperature at unitarity for the polaron problem



- Good agreement with the variational particle-hole results (Liu et al 2020)
- In overall agreement with the experimental data by the MIT group (2019)
- The monotonic increase with T reflects the increased population of the excited molecular state (in which the pair correlation is larger)

Contact versus coupling $1/(k_F a)$ at $T=0.2T_F$



- The leading order contribution $\frac{8\pi}{k_F a}$ arises from the two-particle binding energy
- Our results are close to the variational one particle-hole results
- Deviations from experiment for $0.2 < 1/(k_F a) < 0.7$

Free energy gap ΔF

$\Delta F = F - F_0$ where F_0 is the non-interacting free energy

ΔF relates the injection and ejection spectral functions through detailed balance

$$A_{ej}(k, \omega) = e^{\beta \Delta F} e^{\beta \omega} e^{-\beta \epsilon_k} A_{inj}(k, -\omega)$$

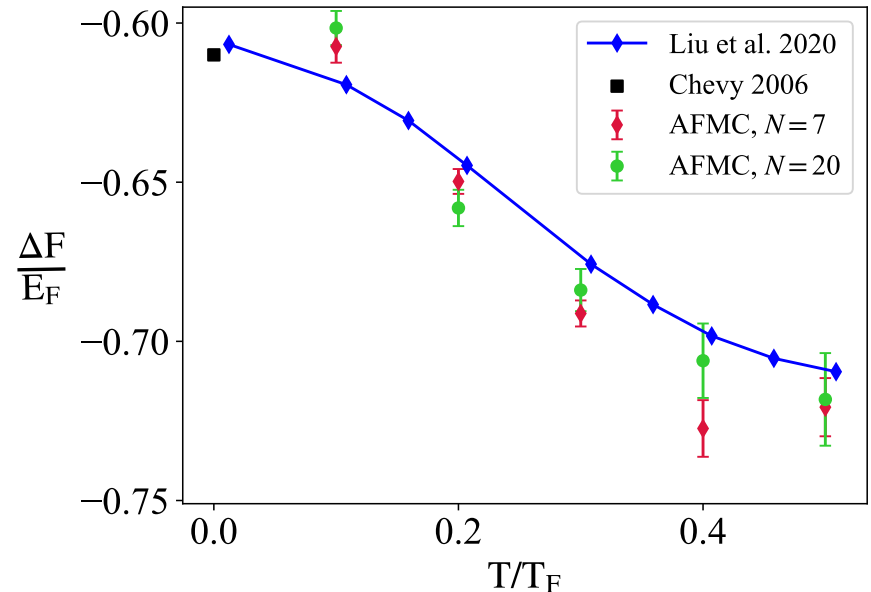
A formula to calculate ΔF in AFMC without the need for numerical analytic continuation:

$$e^{\beta \Delta F} = \frac{Z_{imp} Z_{med}}{Z_{int}} = Z_{imp} \frac{\langle \frac{1}{\text{tr} U_{\sigma}^{\downarrow}} \Phi_{\sigma} \rangle_W}{\langle \Phi_{\sigma} \rangle_W}$$

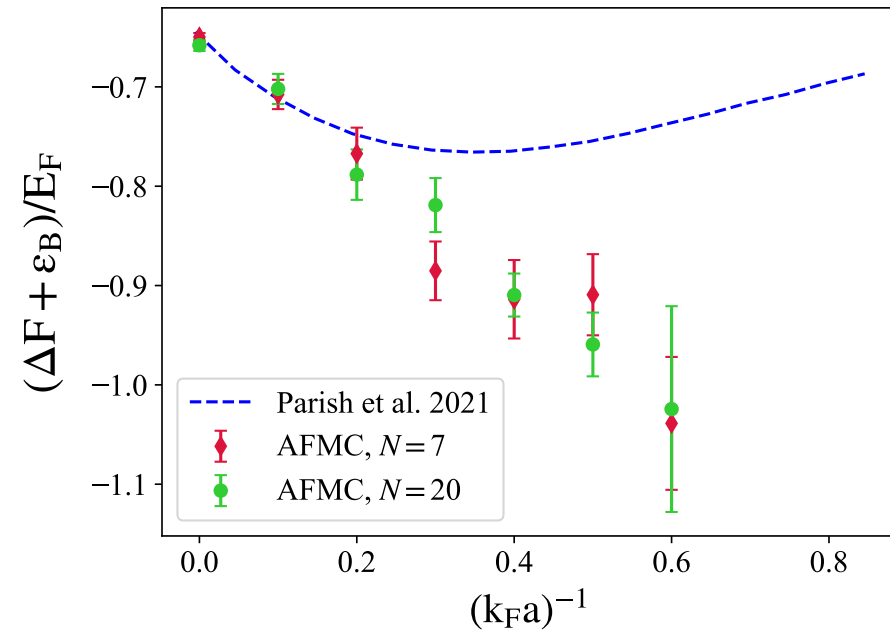
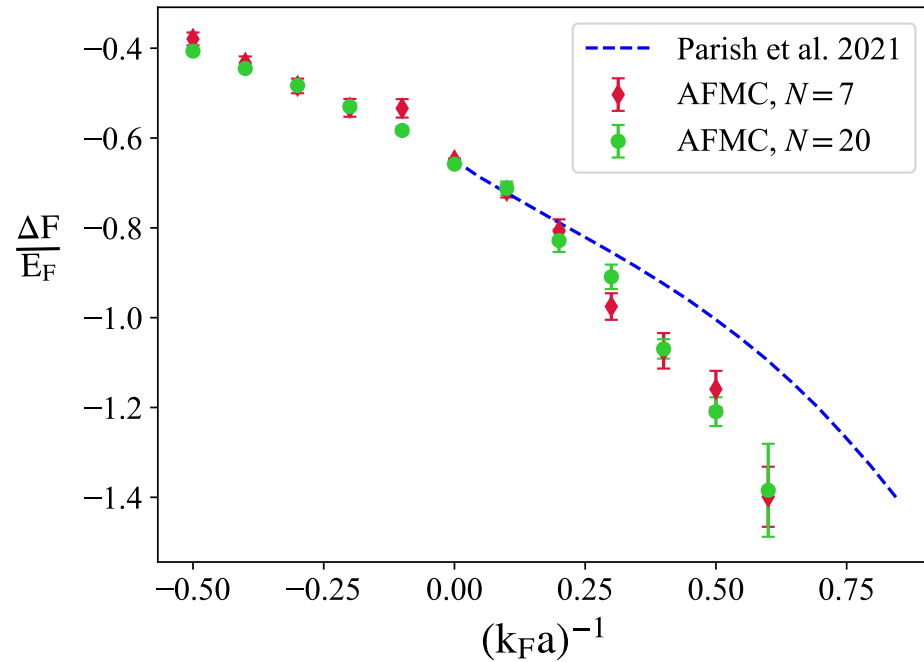
ΔF decreases with T more steeply than the one particle-hole approximation

\Rightarrow molecular state is occupied more rapidly than previously thought

Free energy gap vs temperature



Free energy gap vs coupling $1/(k_F a)$



Large deviations from the variational one particle-hole approximation beyond $1/(k_F a) \sim 0.5$

⇒ Higher-order contributions to the spectrum beyond the one particle-hole approximation become more significant.

Conclusion

- Canonical-ensemble AFMC methods are particularly suitable for the Fermi polaron problem
- We employed AFMC methods on discrete lattices and eliminated systematic errors associated with the finite lattice spacing by taking a continuum extrapolation.
- First controlled calculations of the Fermi polaron at finite temperature
- Our AFMC results for the contact are in overall agreement with the variational one particle-hole method.
- The free energy gap exhibits significant deviations from the variational one particle-hole method.

Outlook

- Calculate the spectral weight of the impurity to determine the quasi-particle excitations of the system