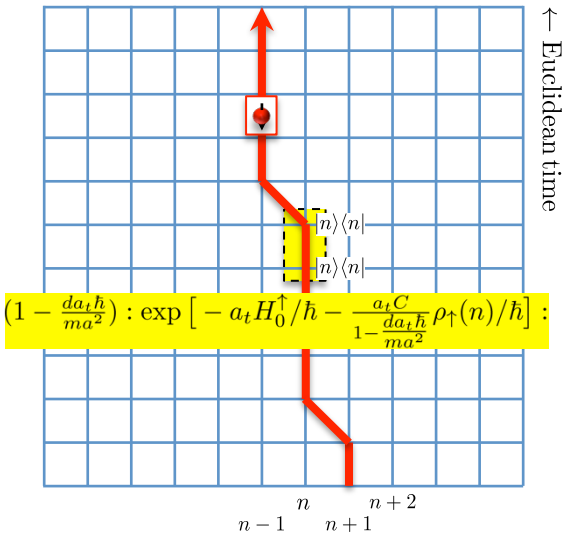
Ab initio lattice results for Fermi polarons in two and three dimensions



Dean Lee (NC State)

Shahin Bour (Bonn)
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WE-Heraeus-Seminar on
Cold Atoms meet Quantum Field Theory

Physikzentrum, Bad Honnef, Germany
July 6-9, 2015

Outline

Attractive Fermi polarons

Impurity lattice Monte Carlo method

Fermion-dimer scattering in 3D zero-range theory

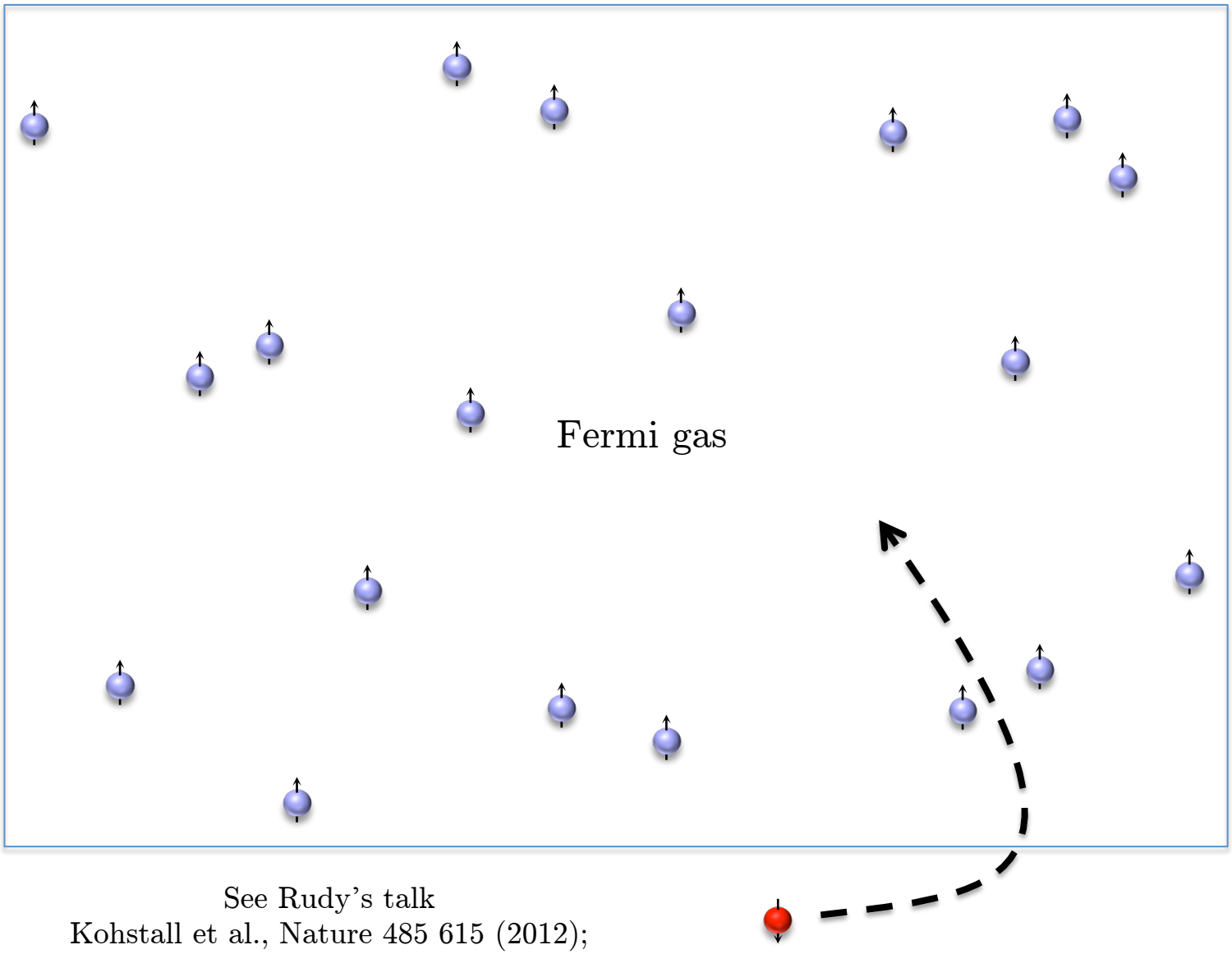
Polarons in 3D at unitarity

Polarons in 2D zero-range theory

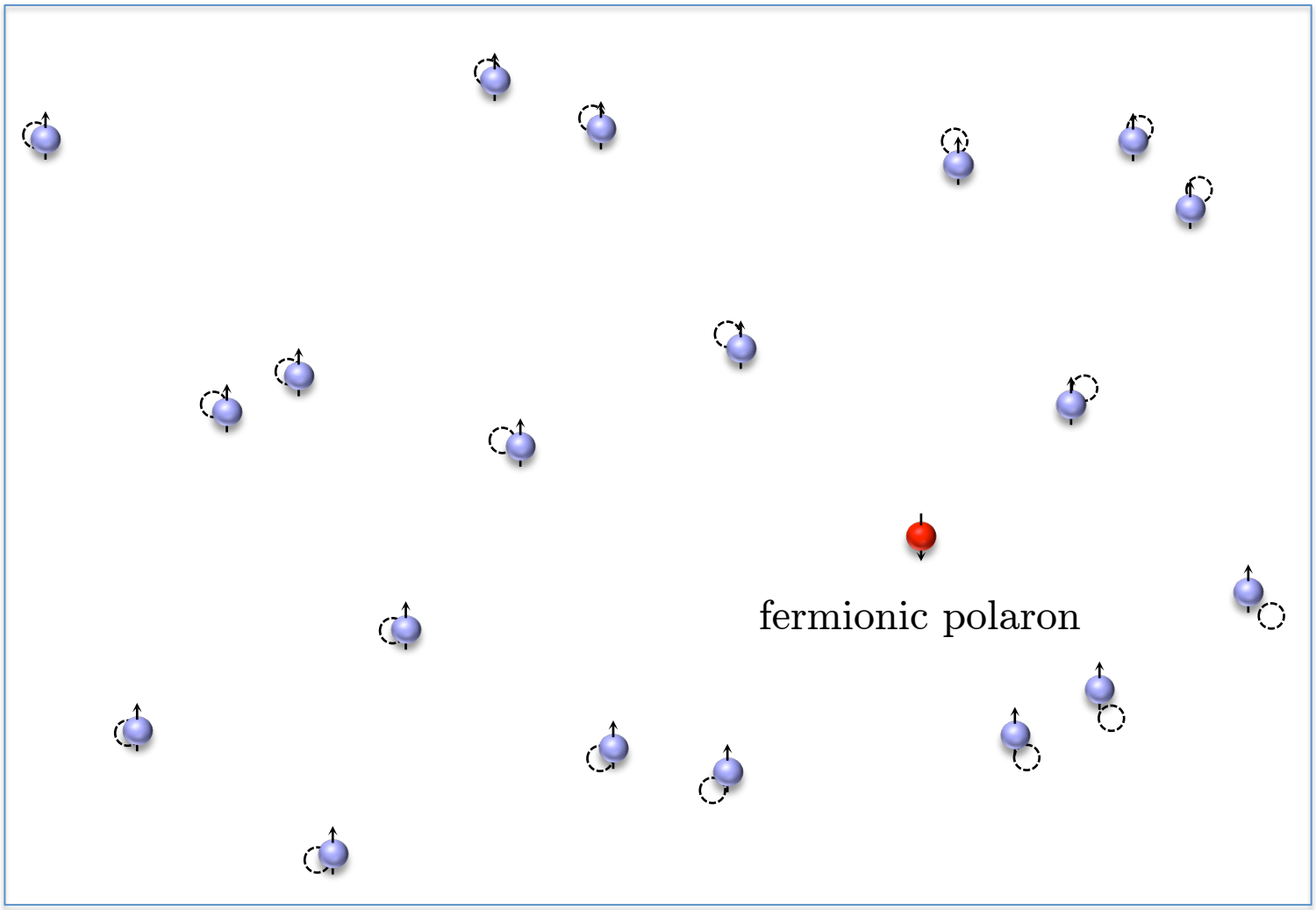
Current work and outlook

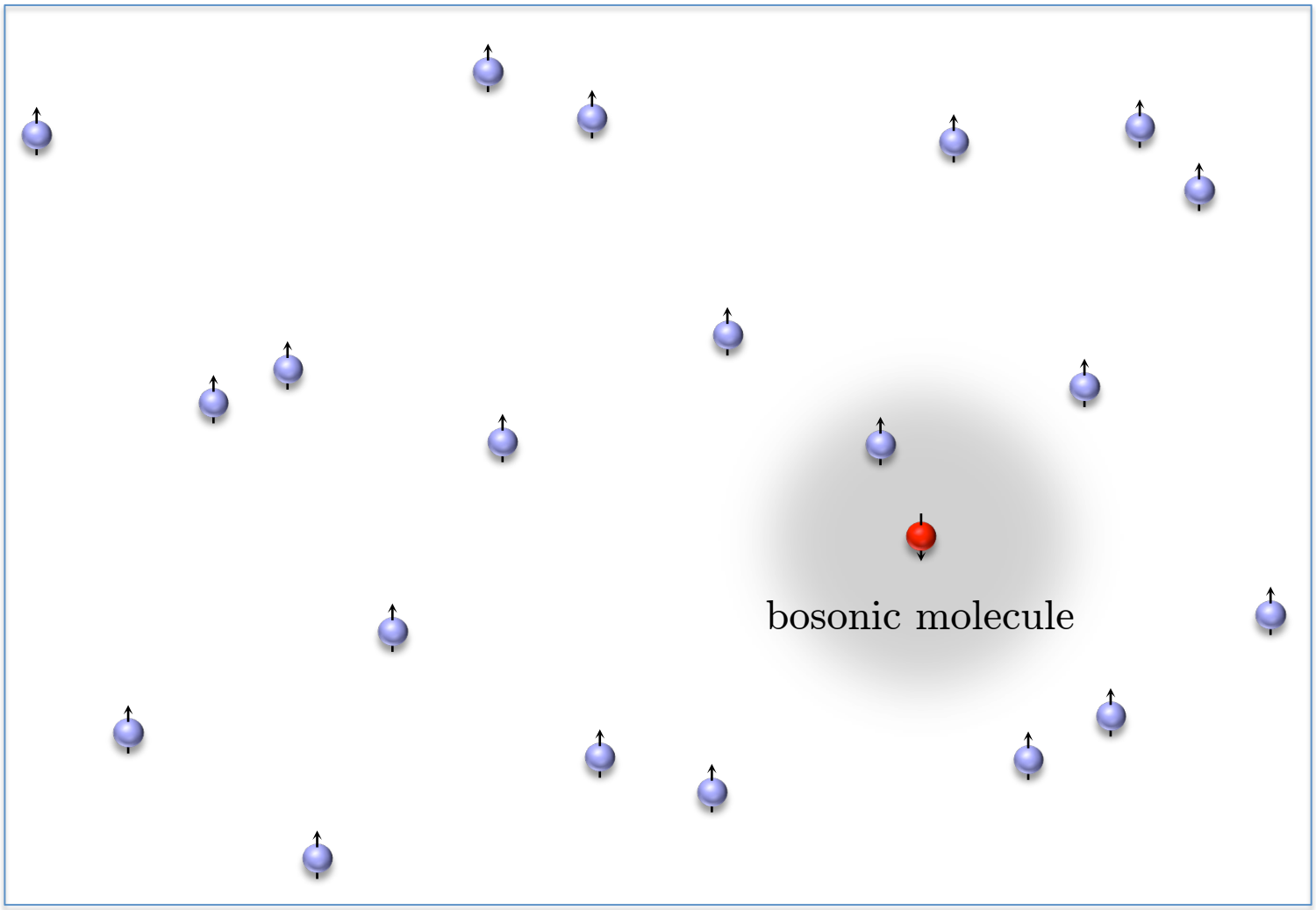
Other developments

Attractive Fermi polarons

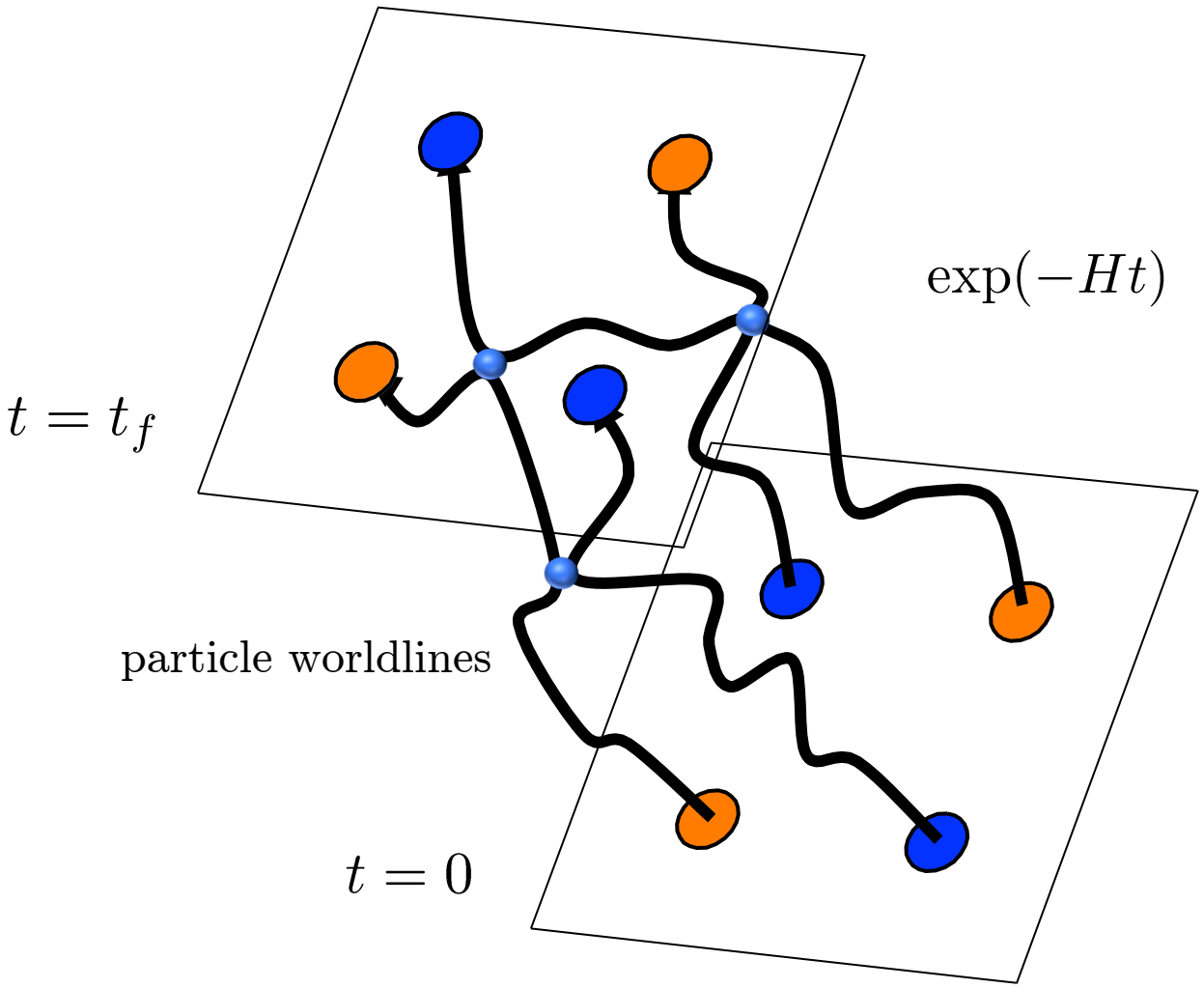


See Rudy's talk
Kohstall et al., Nature 485 615 (2012);
Cetina et al., arXiv:1505.00738


fermionic polaron


bosonic molecule

Diffusion Monte Carlo



Auxiliary field Monte Carlo

We can write exponentials of the interaction using a Gaussian integral identity

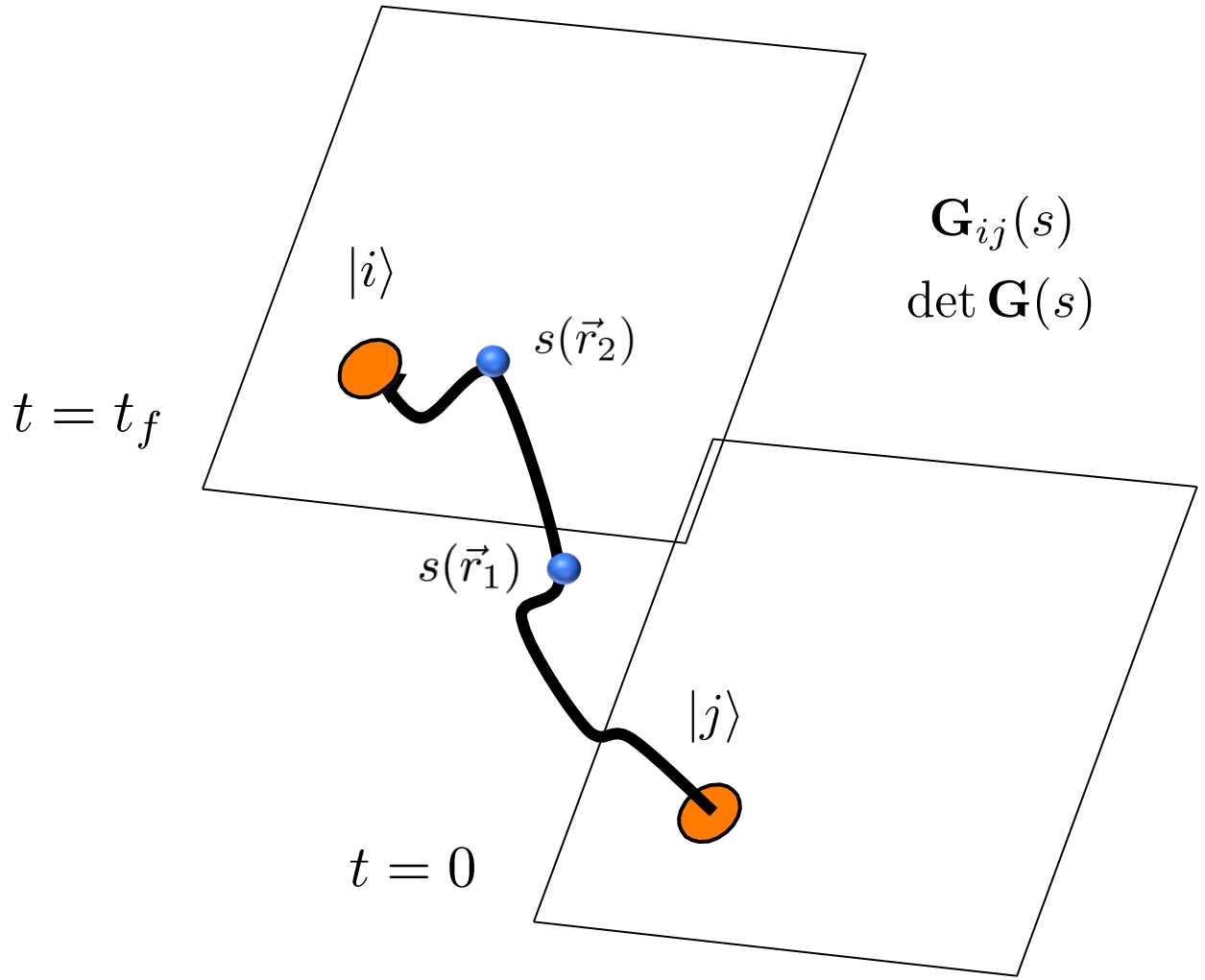
$$\exp\left[-\frac{C}{2}\rho^2\right]$$

$$\rho^2$$

$$= \sqrt{\frac{1}{2\pi}} \int_{-\infty}^{\infty} ds \exp\left[-\frac{1}{2}s^2 + \sqrt{-C}\, s\rho\right]$$

$$s\rho$$

We remove the interaction between particles and replace it with the interactions of each particles with a background field.

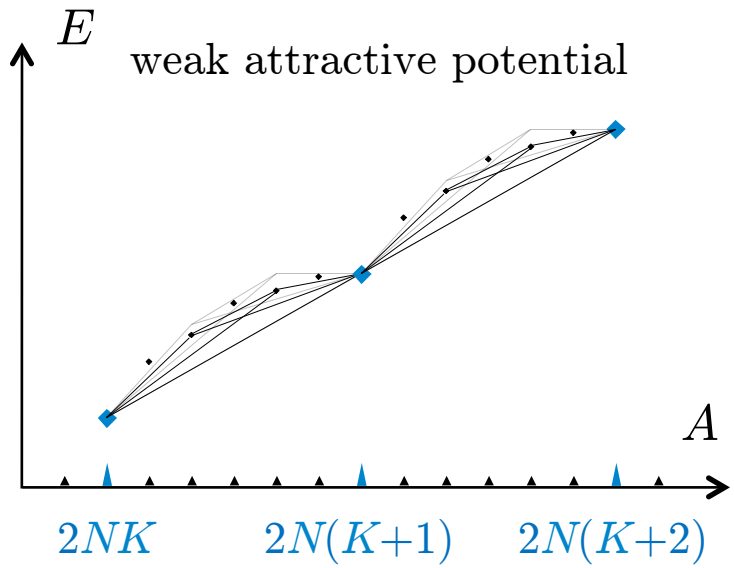


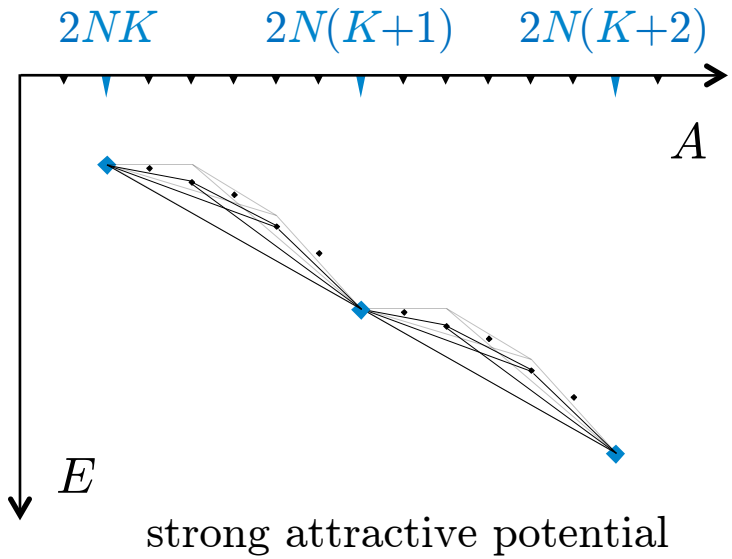
Review: D.L, Prog. Part. Nucl. Phys. 63 117-154 (2009)

Theorem. Any fermionic theory with SU($2N$) symmetry and two-body potential with negative semi-definite Fourier transform obeys SU($2N$) convexity bounds.

Corollary. System can be simulated without sign oscillations

Chen, D.L. Schäfer, PRL 93 (2004) 242302;
D.L., PRL 98 (2007) 182501





Impurity lattice Monte Carlo

Impurity lattice Monte Carlo is a hybrid method which treats the impurity using diffusion Monte Carlo and all other particles using auxiliary field Monte Carlo. We demonstrate using two-component fermions in d spatial dimensions with zero-range interactions. We use lattice units where the lattice spacing $a = 1$.

$$H_{\text{free}} = H_{\text{free}}^{\uparrow} + H_{\text{free}}^{\downarrow} = \frac{-\hbar^2}{2m} \sum_{\mu=1}^{d} \sum_{\vec{n},i=\uparrow,\downarrow} \boxed{b_i^\dagger(\vec{n}) \left[b_i(\vec{n}+\hat{\mu}) - 2b_i(\vec{n}) + b_i(\vec{n}-\hat{\mu}) \right],}$$

$$\rightarrow b_i^\dagger \partial_\mu^2 b_i$$

$$H = H_{\text{free}} + C \sum_{\vec{n}} \rho_\uparrow(\vec{n}) \rho_\downarrow(\vec{n})$$

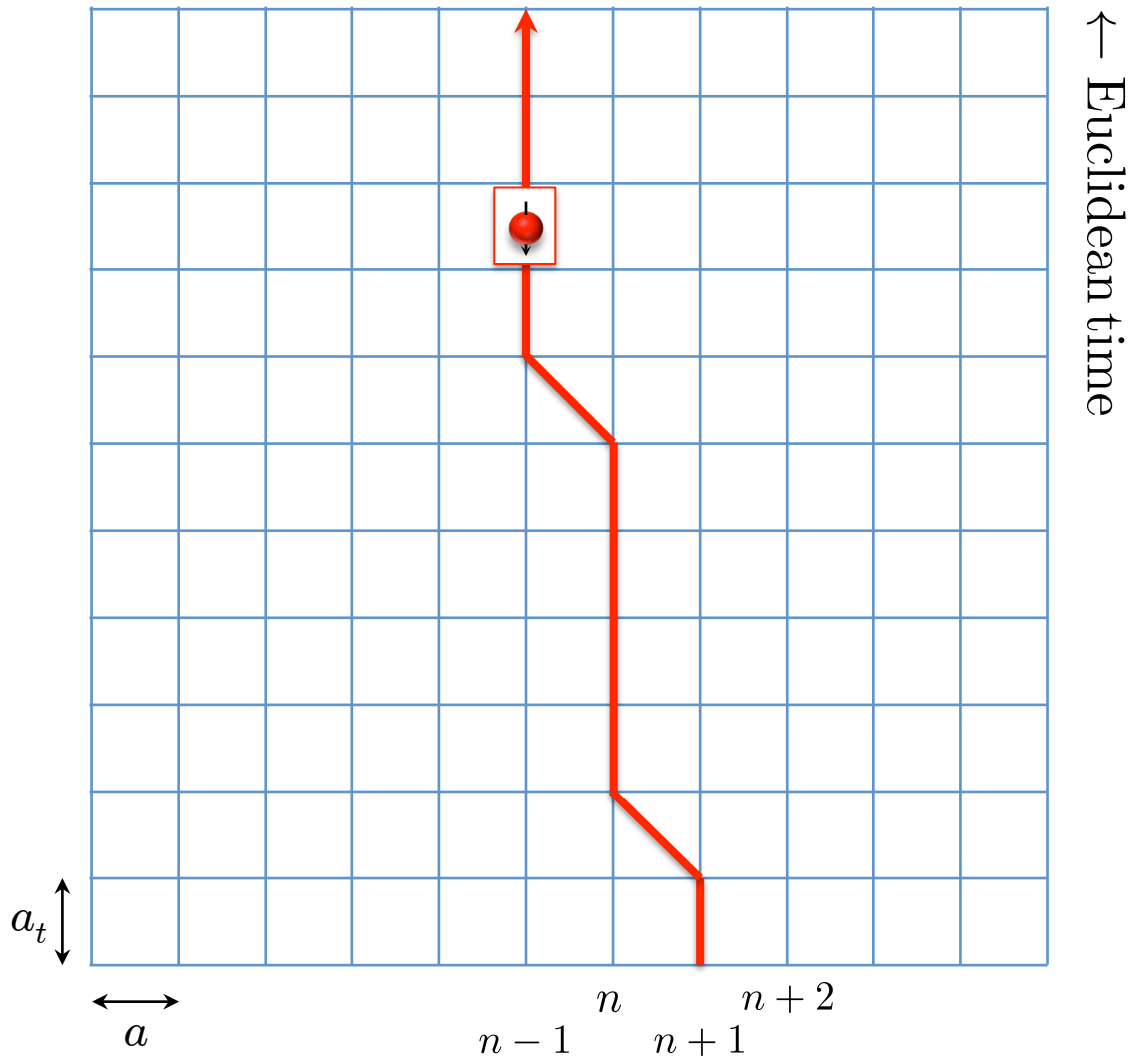
We use the transfer matrix formalism with temporal lattice spacing a_t

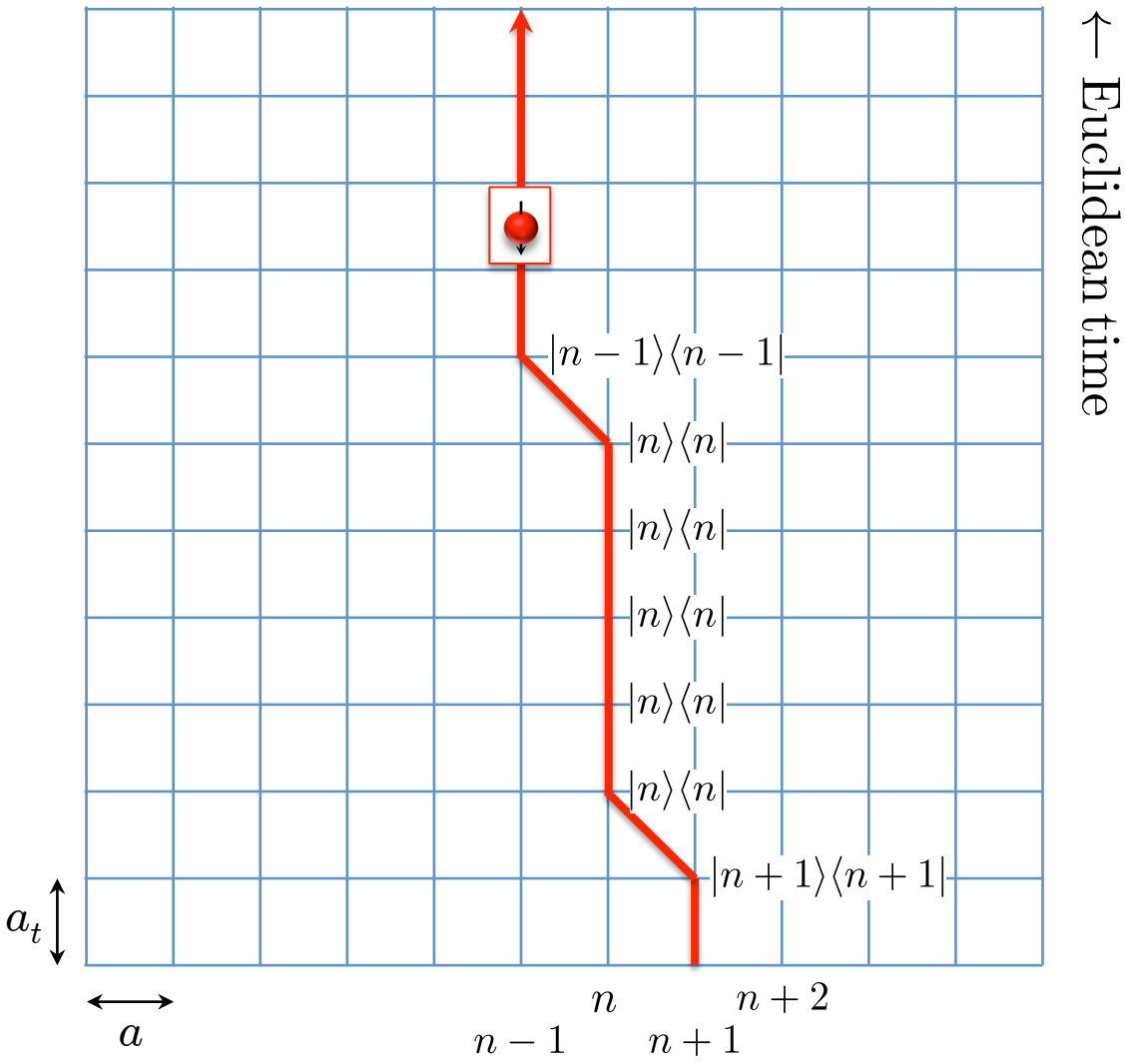
$$M =: e^{-a_t H/\hbar} :$$

The :: symbols indicate normal ordering. Using our lattice Hamiltonian, we get

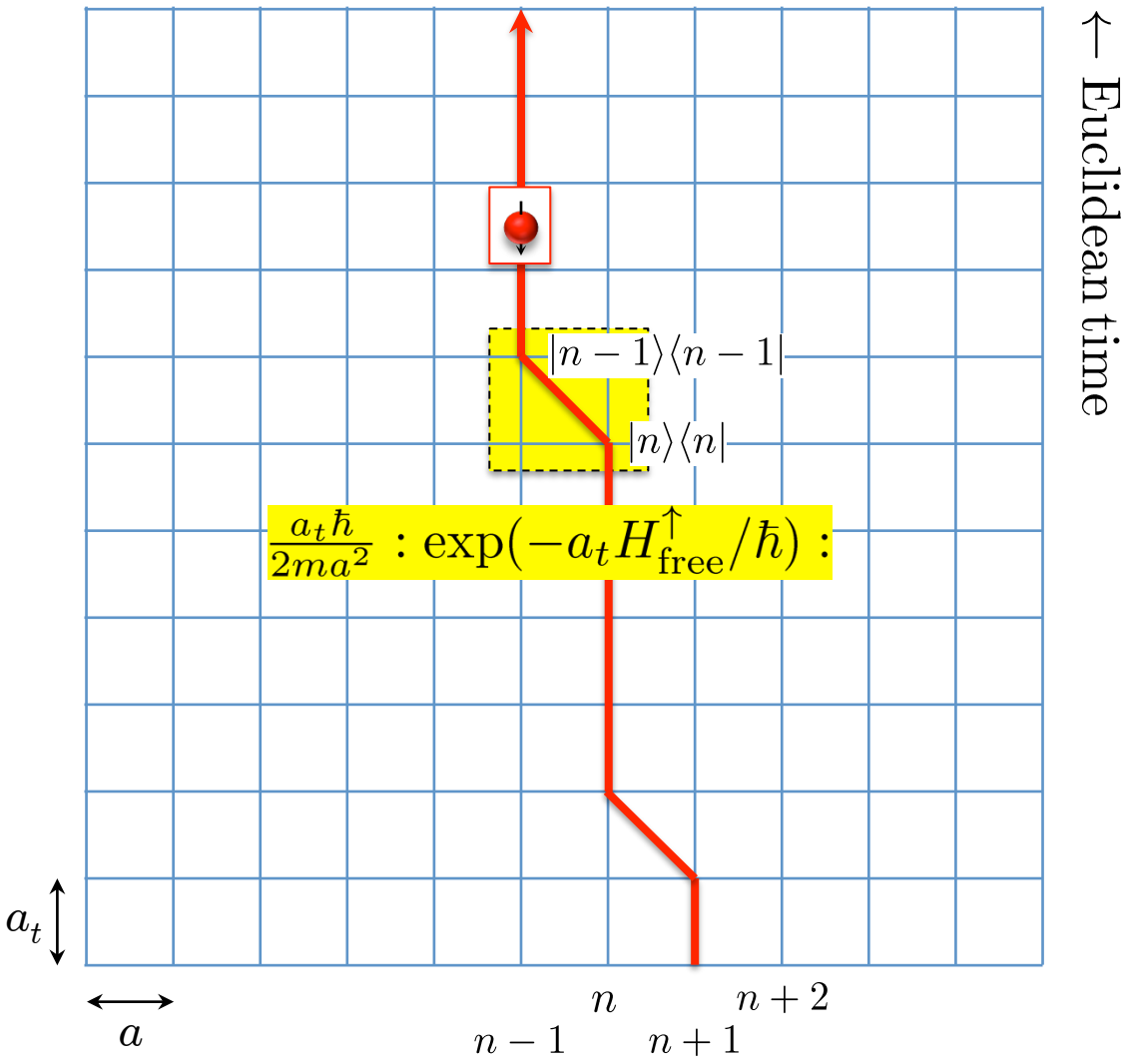
$$M =: e^{-a_t \left[H_{\text{free}} + C \sum_{\vec{n}} \rho_\uparrow(\vec{n}) \rho_\downarrow(\vec{n})\right]/\hbar} :$$

We now consider a system where we have N up-spin particles and just one down-spin particle. We consider any worldline for the down-spin particle. For simplicity we show the case for one spatial dimension.

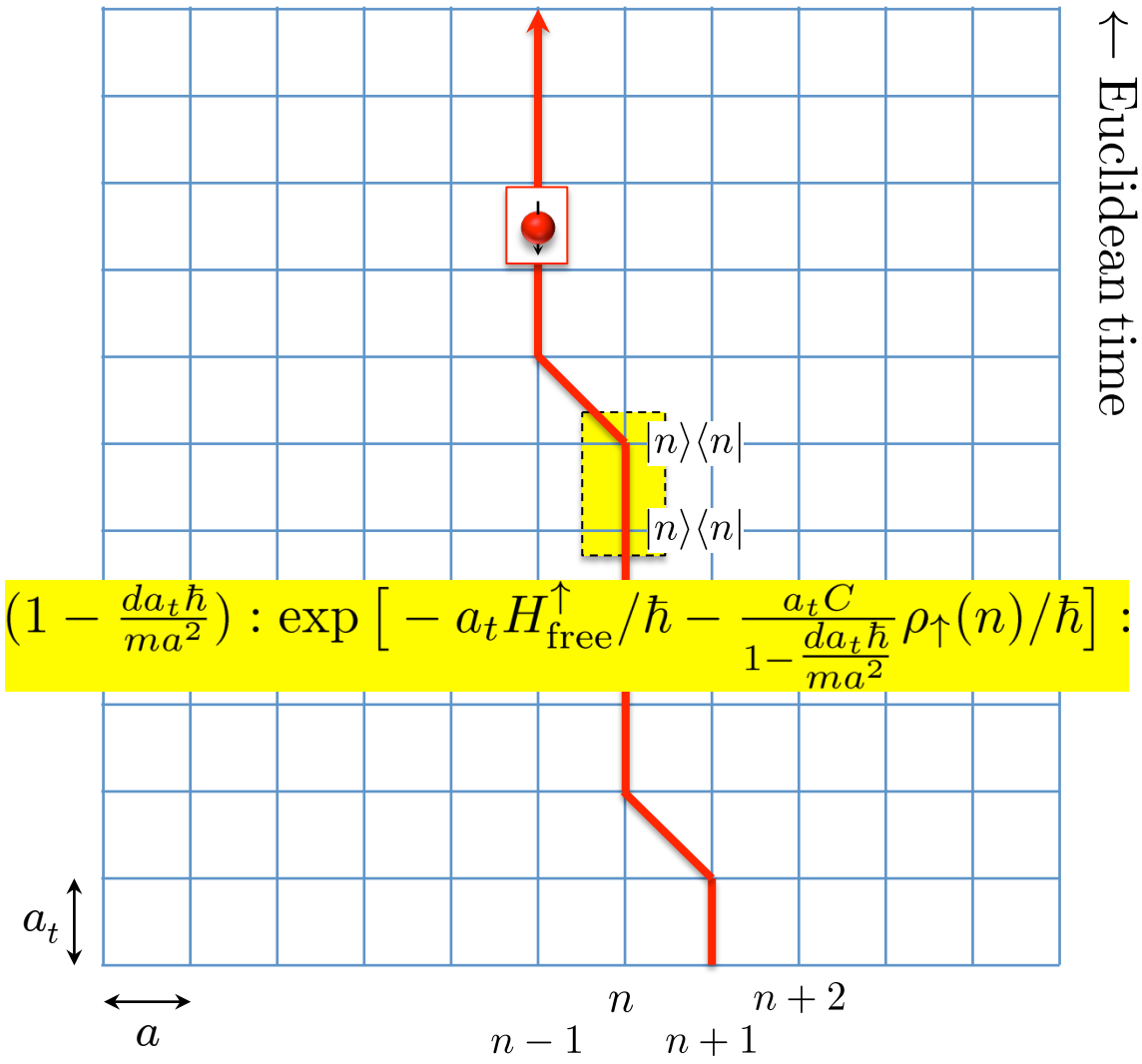

← Euclidean time
a_t
a
$n-1$
n
$n+1$
$n+2$



Elhatisari, D.L., PRC 90 064001 (2014)
Bour, D.L, Hammer, Meißner, arXiv:1412.8175



Elhatisari, D.L., PRC 90 064001 (2014)
Bour, D.L, Hammer, Meißner, arXiv:1412.8175

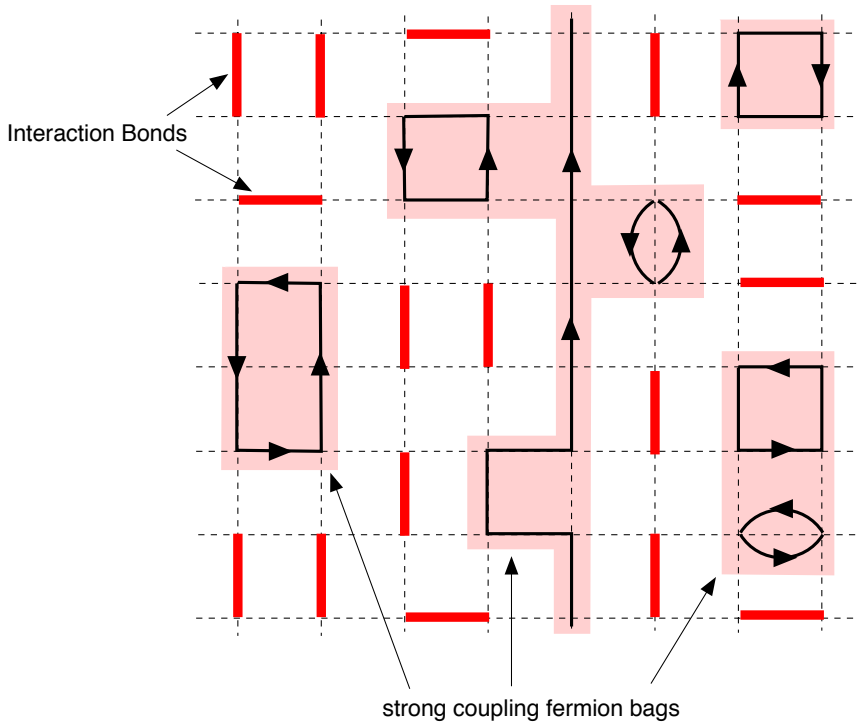


Elhatisari, D.L., PRC 90 064001 (2014)
Bour, D.L, Hammer, Meißner, arXiv:1412.8175

Different but somewhat similar in spirit to the fermion bag approach where certain terms of the lattice action are expanded out and others are computed using determinants on the remaining lattice.

Chandrasekharan, PRD 82 (2010) 025007

Chandrasekharan, Li, PRL 108 (2012) 140404



Fermion-dimer scattering in 3D zero-range theory

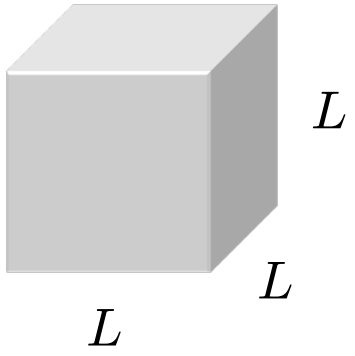
We consider two up-spin particles and one down-spin particle with attractive zero-range interactions in 3D. This few-body system can be calculated exactly using sparse eigenvalue methods. We use the exact calculations to benchmark impurity lattice Monte Carlo calculations.

We use Lüscher's finite volume method to calculate fermion-dimer scattering phase shifts. Two-body energy levels near threshold in a periodic cube are related to the elastic phase shifts

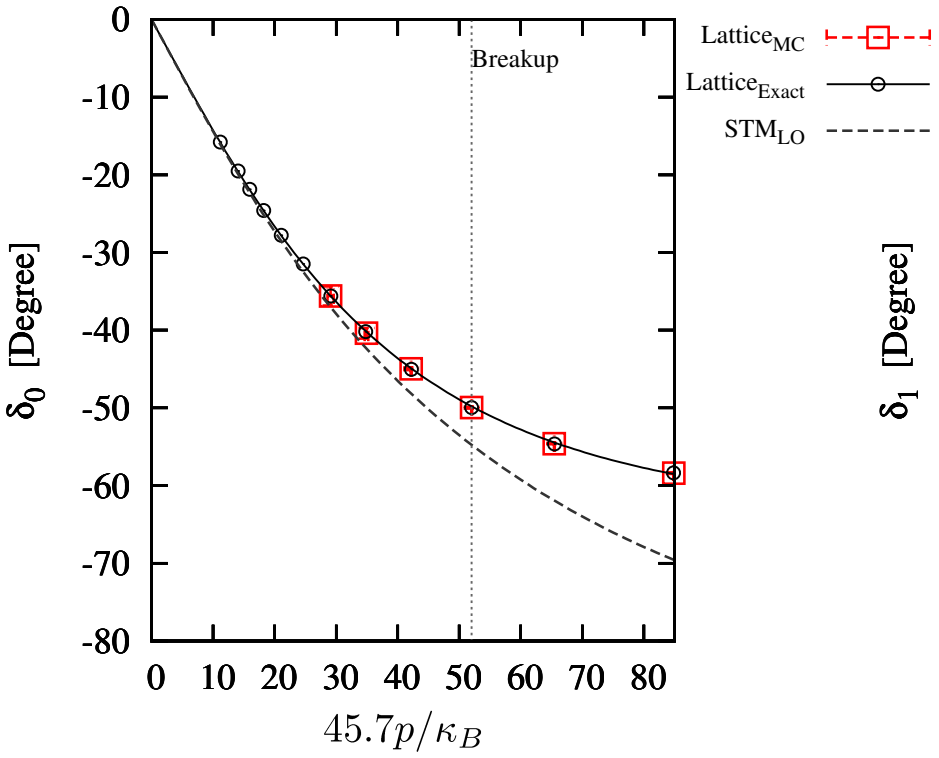
Lüscher, Comm. Math. Phys. 105 (1986) 153; NPB 354 (1991) 531

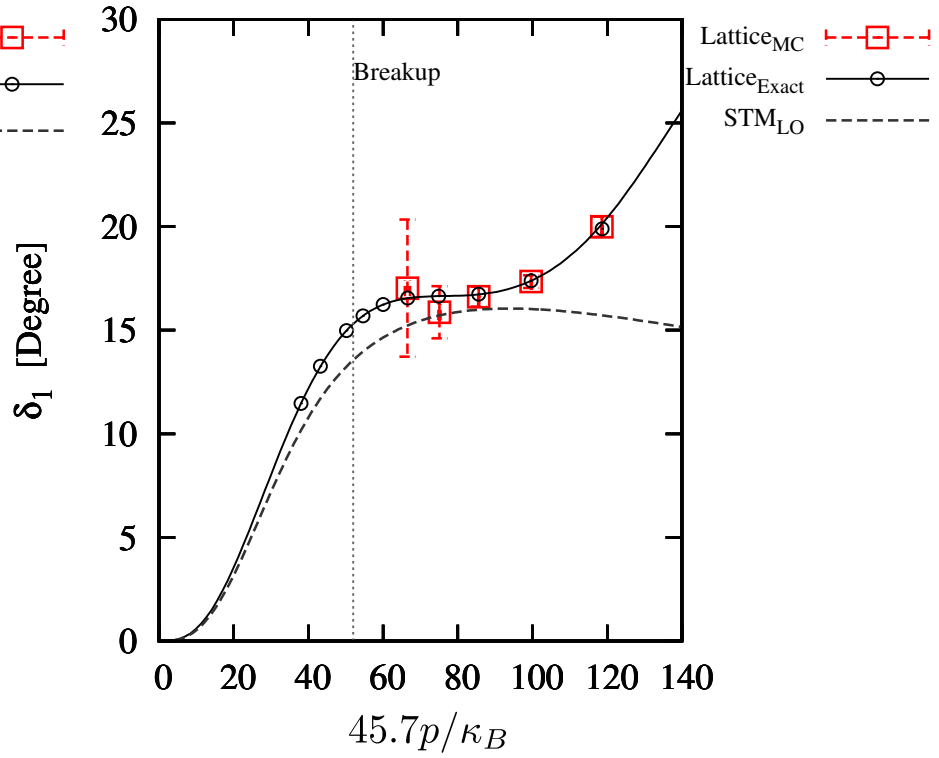
$$p \cot \delta_0(p) = \frac{1}{\pi L} S(\eta), \qquad \eta = \left(\frac{Lp}{2\pi}\right)^2$$

$$S(\eta) = \lim_{\Lambda \to \infty} \left[\sum_{\vec{n}} \frac{\theta(\Lambda^2 - \vec{n}^2)}{\vec{n}^2 - \eta} - 4\pi\Lambda \right]$$



Fermion-dimer scattering phase shifts





Elhatisari, D.L., PRC 90 064001 (2014)

Polarons in 3D at unitarity

We consider N up-spin particles and one down-spin particle with attractive zero-range interactions in 3D tuned to the unitarity limit. We use the results in the literature to benchmark impurity lattice Monte Carlo calculations.

We start with an initial state which is the ground state of the non-interacting $(N, 1)$ system. If we project for a sufficiently large number of time steps, L_t, we get the ground state of the interacting system.

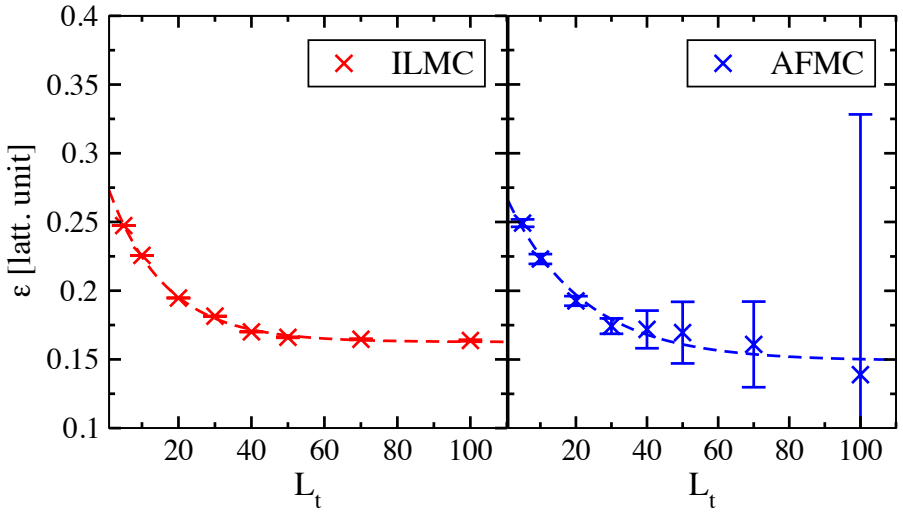
$$M^{L_t}|\Psi_0^{\text{free}}(N,1)\rangle \to e^{i\theta}\sqrt{Z}e^{-E_0 a_t L_t/\hbar}|\Psi_0(N,1)\rangle$$

where

$$Z = |\langle\Psi_0(N,1)|\Psi_0^{\text{free}}(N,1)\rangle|^2$$

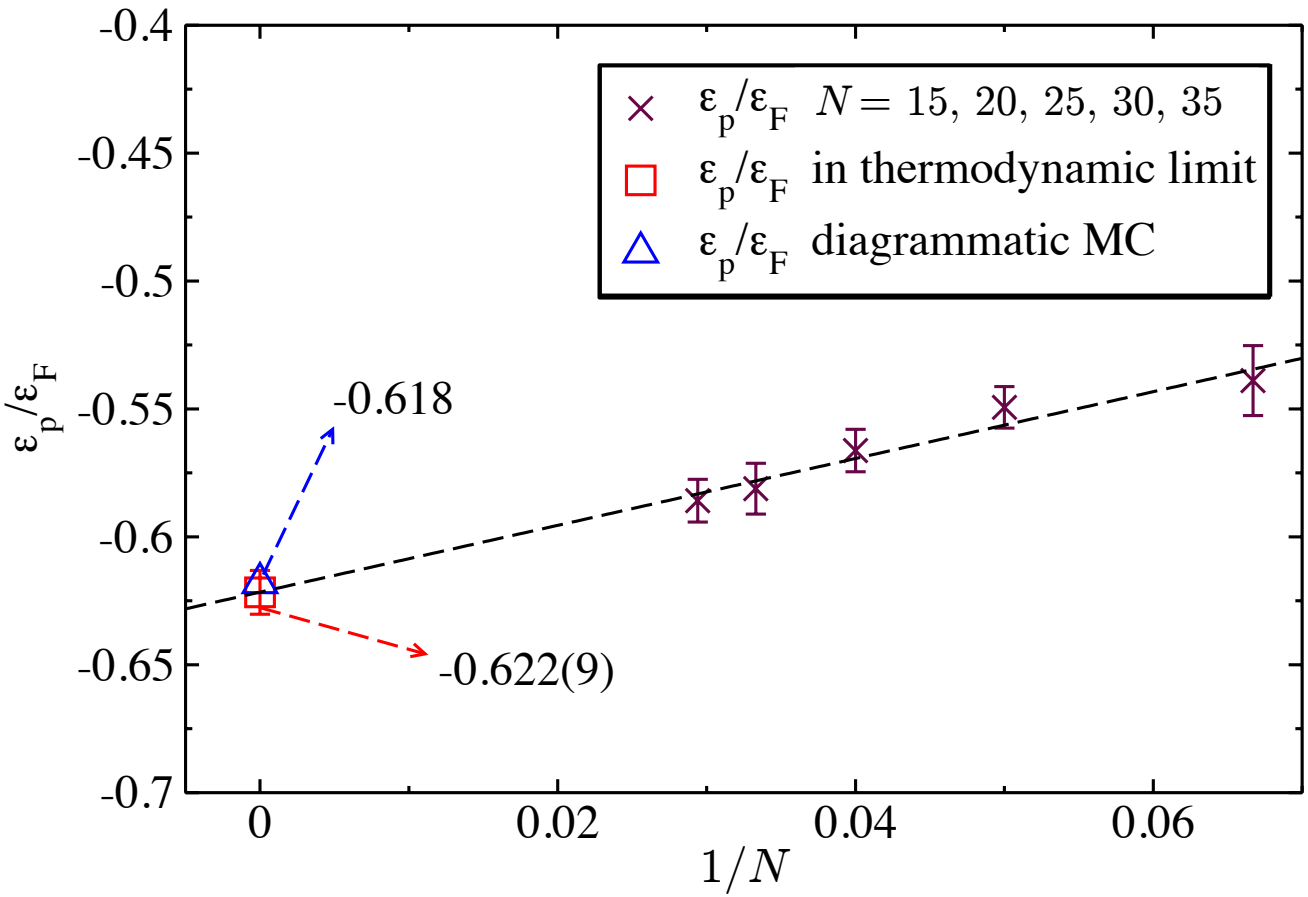
While we don't explicit calculate Z, we can easily find the point where Z approaches zero. This occurs when the non-interacting initial state produces very noisy Monte Carlo results. In such cases we should use a different initial state.

Here is a comparison of impurity lattice Monte Carlo results versus auxiliary-field Monte Carlo results for $N = 10$ and $L^3 = 10^3$.



Bour, D.L, Hammer, Meißner, arXiv:1412.8175

We extrapolate to the continuum limit ($L^3 = 6^3, 7^3, 8^3, 9^3, 10^3$) and thermodynamic limit ($N = 15, 20, 25, 30, 35$). The simulations at unitarity have very little noise starting from the non-interacting initial state, indicating that the value of Z is not small.



Diagrammatic Monte Carlo: −0.618

Prokofev, Svistunov, PRL 81 (1998) 2514

Polaron variational calculation with one particle-hole pair: −0.6066

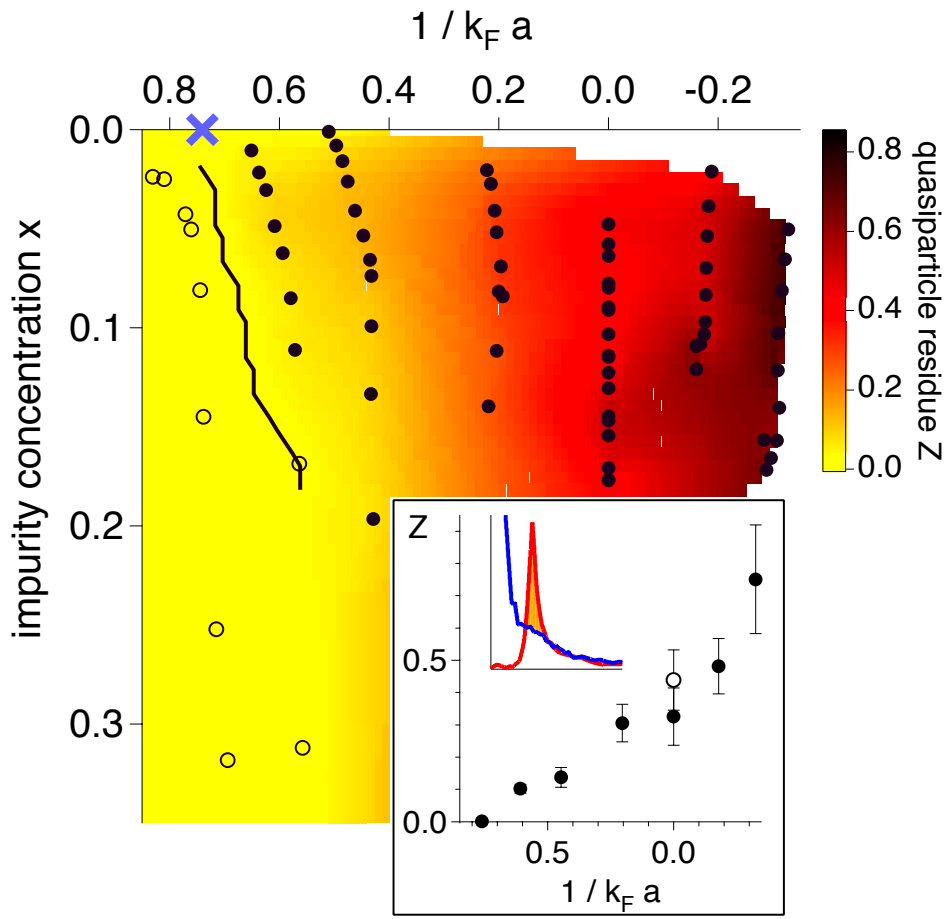
Chevy, PRA 74 (2006) 063628

Polaron variational calculation with two particle-hole pairs: −0.6158

Combescot, Giraud, PRL 101 (2008) 050404

Experimental observations: −0.58(5) Y. Shin, PRA 77 (2008) 041603

−0.64(7) Schirotzek, Wu, Sommer, Zwierlein, PRL 102 (2009) 230402



Schirotzek, Wu, Sommer, Zwierlein, PRL 102 (2009) 230402

Polarons in 2D zero-range theory

We consider one down-spin particle and N up-spin particles with attractive zero-range interactions in 2D tuned to according the two-body binding energy $E_{\rm B}$ or binding momentum $\kappa_{\rm B}$.

We consider two possible sets of initial states.

The first is again an initial state which is the ground state of the non-interacting $(N, 1)$ system,

$$M^{L_t}|\Psi_0^{\rm free}(N,1)\rangle \to e^{i\theta}\sqrt{Z}e^{-E_0 a_t L_t/\hbar}|\Psi_0(N,1)\rangle$$

where

$$Z = |\langle\Psi_0(N,1)|\Psi_0^{\rm free}(N,1)\rangle|^2$$

Bour, Lee, Hammer, Meißner, arXiv:1412.8175

We also consider the molecular initial state

$$|\Psi_\ell^{\rm mol}(N,1)\rangle = \sum_{\vec{n}_1,\vec{n}_2} b_\uparrow^\dagger(\vec{n}_1) b_\downarrow^\dagger(\vec{n}_2) e^{-(\vec{n}_1-\vec{n}_2)^2/\ell^2} |\Psi_0^{\rm free}(N-1,0)\rangle$$

where the pair length ℓ is adjustable. It is convenient to define the quantity

$$\eta = \ln(k_F a_{\rm 2D}) = \ln(k_F/\kappa_B) = \tfrac{1}{2}\ln(2E_F/|E_B|)$$

The free initial state

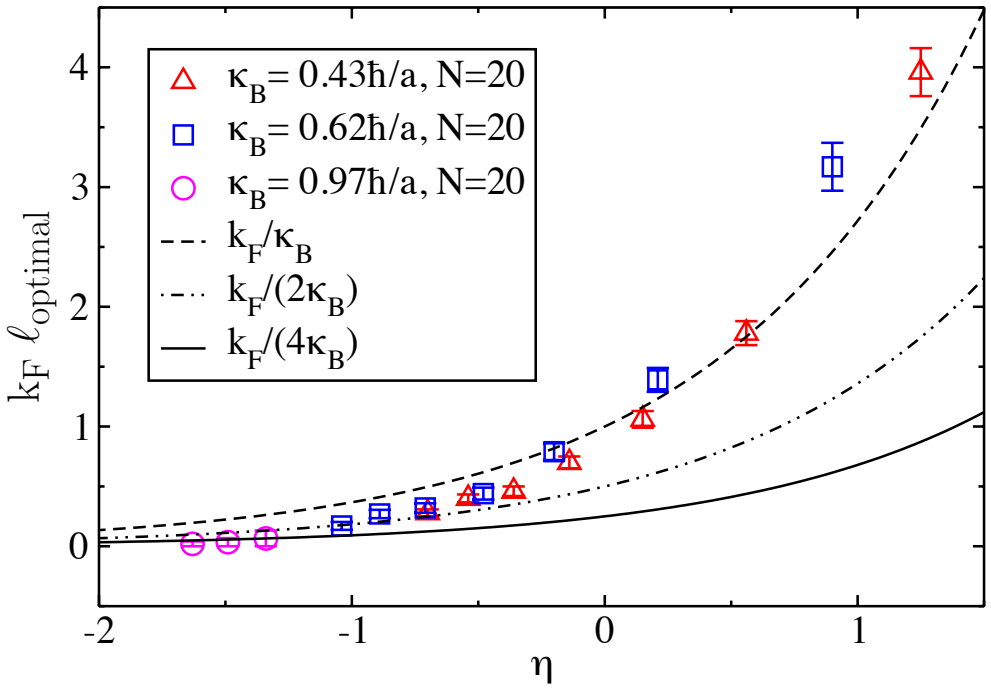
$$|\Psi_0^{\rm free}(N,1)\rangle$$

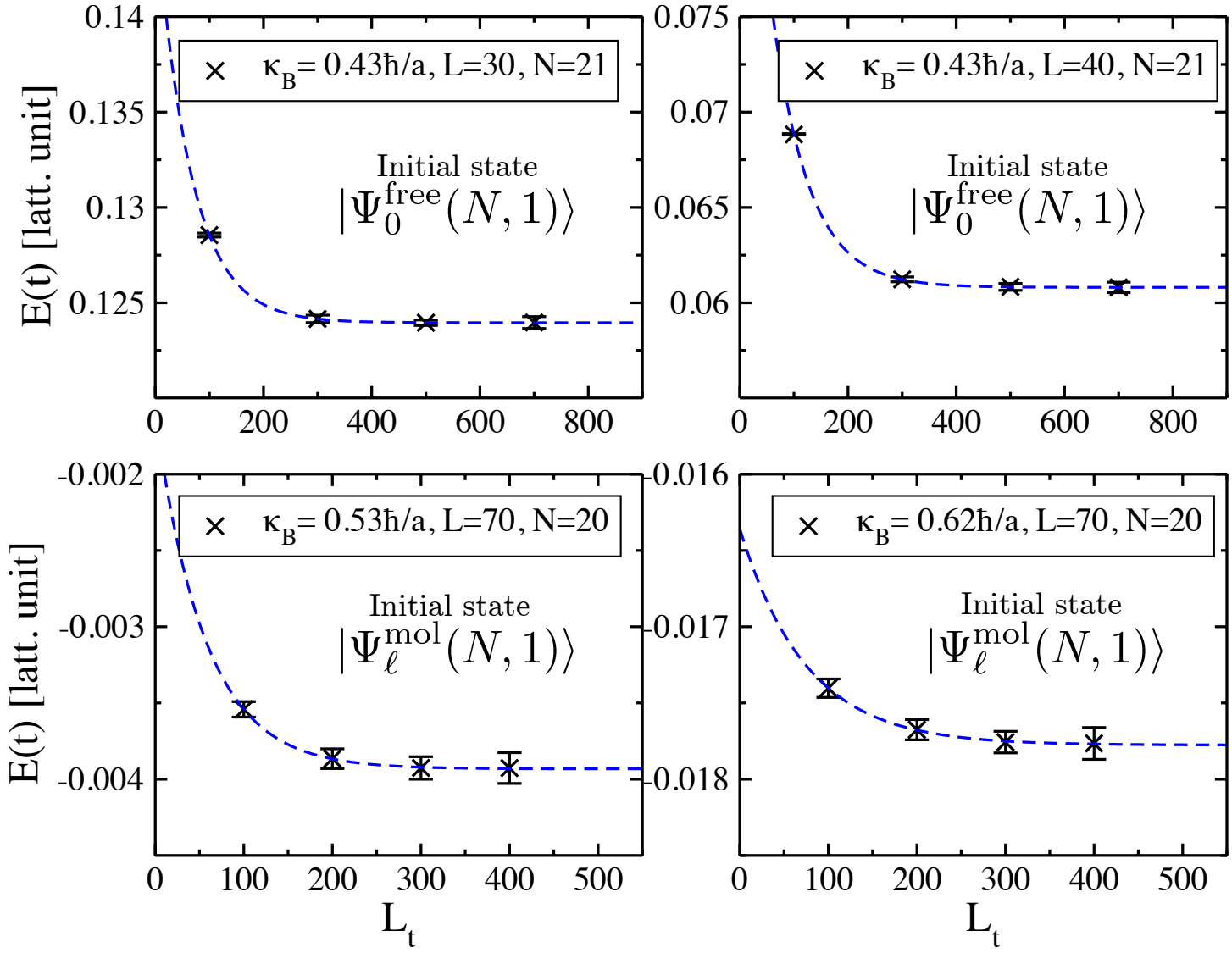
works well for $\eta > -0.8$ but becomes very noisy for lower η. This indicates that Z approaches zero for η below −0.8.

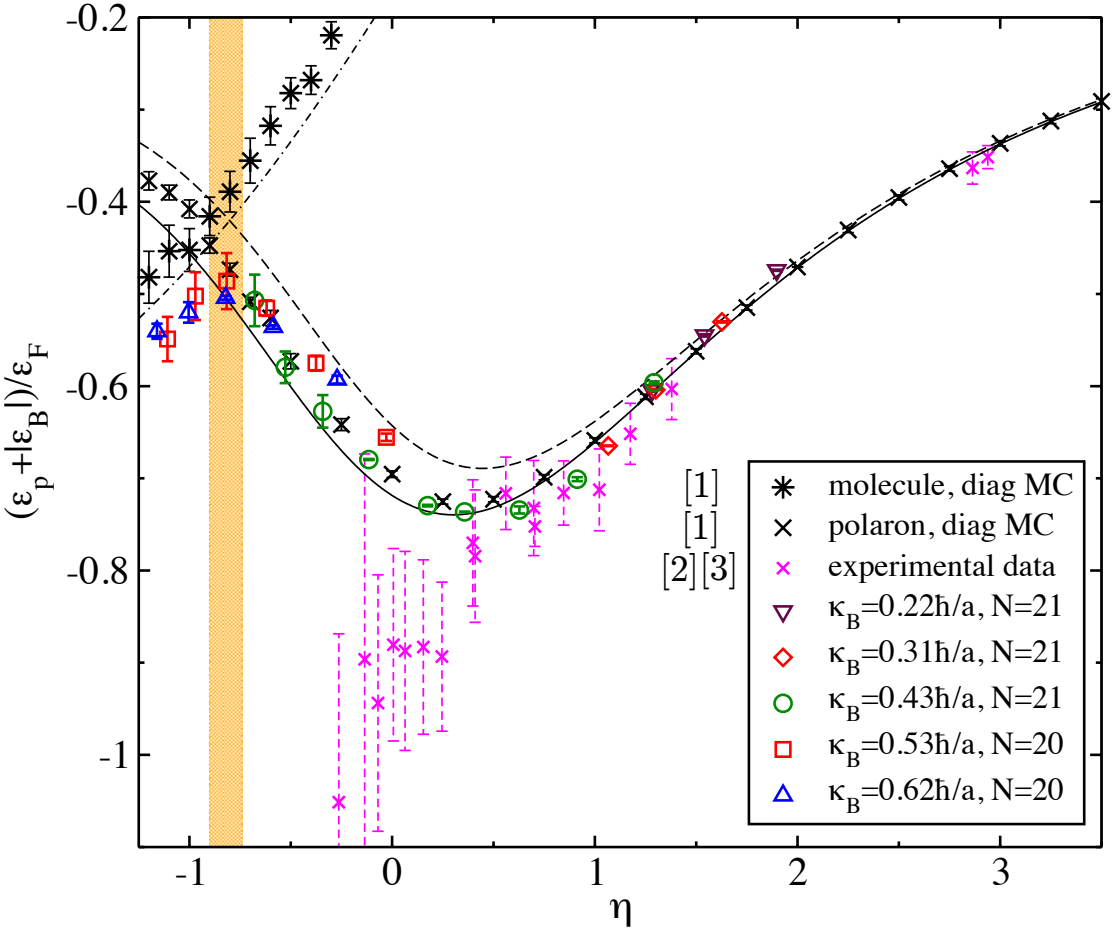
The molecular initial state

$$|\Psi_\ell^{\rm mol}(N,1)\rangle$$

works well for all values of η, but we must adjust the pair length ℓ.




E(t) [latt. unit]
0.14
0.135
0.13
0.125
κB= 0.43ħ/a, L=30, N=21
Initial state
$|\Psi_0^{\rm free}(N,1)\rangle$
0
200
400
600
800
0.075
0.07
0.065
0.06
κB= 0.43ħ/a, L=40, N=21
Initial state
$|\Psi_0^{\rm free}(N,1)\rangle$
0
200
400
600
800
E(t) [latt. unit]
-0.002
-0.003
-0.004
κB= 0.53ħ/a, L=70, N=20
Initial state
$|\Psi_\ell^{\rm mol}(N,1)\rangle$
0
100
200
300
400
500
Lt
-0.016
-0.017
-0.018
κB= 0.62ħ/a, L=70, N=20
Initial state
$|\Psi_\ell^{\rm mol}(N,1)\rangle$
0
100
200
300
400
500
Lt



Dashed: [4] Polaron variational calculation including one particle-hole pair

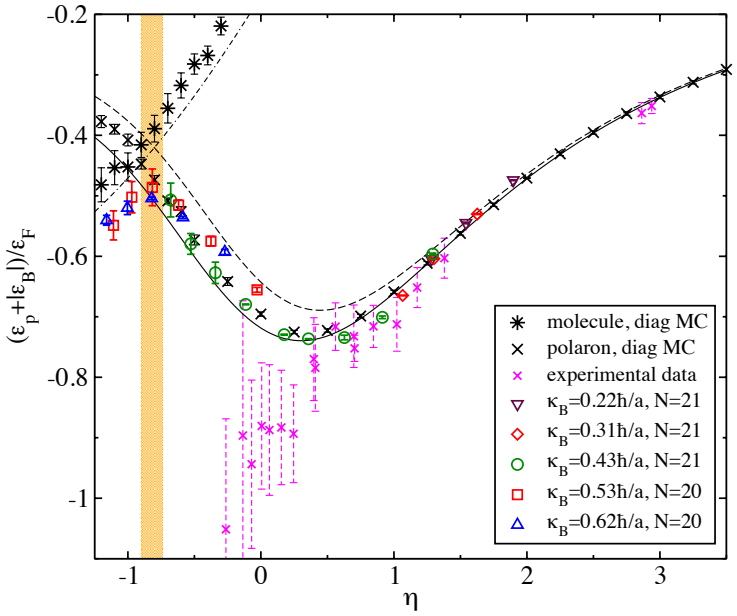
Solid: [5] Polaron variational calculation including two particle-hole pairs

Dot-dashed: [5] Molecule variational calculation including one particle-hole pairs

Calculations done on Jülich supercomputer JUQUEEN

1. Vlietinck, Ryckebusch, Van Houcke, PRB 89 (2014) 085119
2. Koschorreck, et al., Nature 485, 619 (2012); M. Köhl talk at APS 2012
3. Levinsen, Baur, PRA 86 (2012) 041602 – discusses correction from quasi-2D to pure 2D
4. Parish, PRA 83 (2011) 051603; see also Zhang et al., PRL 108 (2012) 235302
5. Parish, Levinsen, PRA 87 (2013) 033616

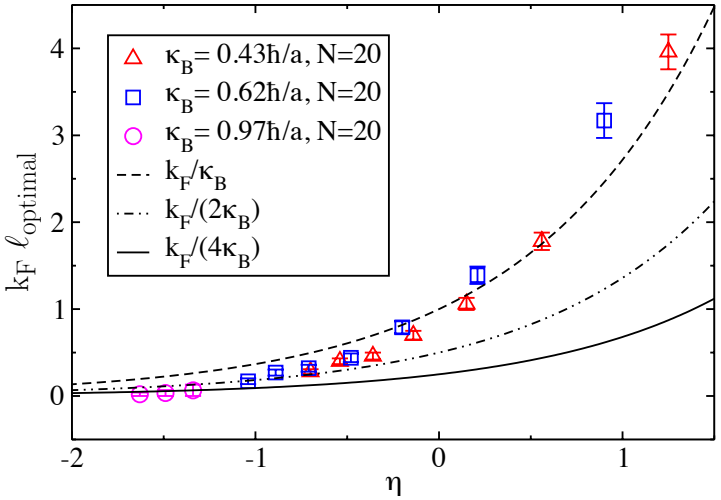
Fermionic polaron versus bosonic molecule

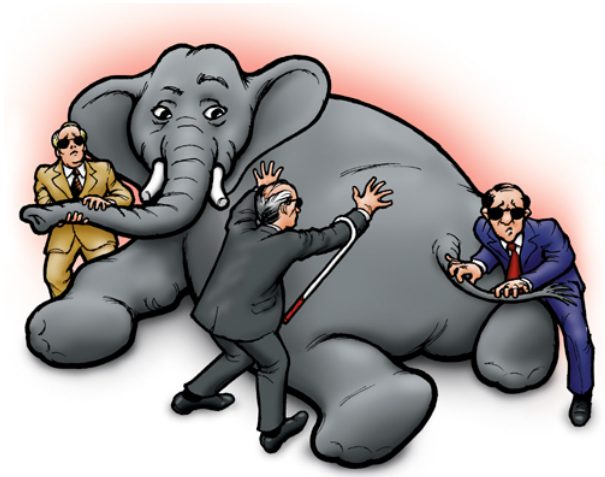


$Z \approx 0$ for $\eta < -0.8$

Smooth crossover transition at

$\eta \approx -0.8$





Bour, Lee, Hammer, Meißner, arXiv:1412.8175

Diagrammatic Monte Carlo calculations find a transition at

$$\eta = -0.95 \pm 0.15$$

Vlietinck, Ryckebusch, Van Houcke,
PRB 89 (2014) 085119

$$\eta = -1.1 \pm 0.2$$

Kroiss, Pollet,
PRB 90 (2014) 104510

Analysis of experimental data with conversion from quasi 2D to pure 2D gives a transition at

$$-0.97 < \eta < -0.80$$

Koschorreck, et al., Nature 485, 619 (2012);
M. Köhl talk at APS 2012;
Levinsen, Baur, PRA 86 (2012) 041602

For discussion of polarons and density profiles in 2D spin-imbalanced systems see

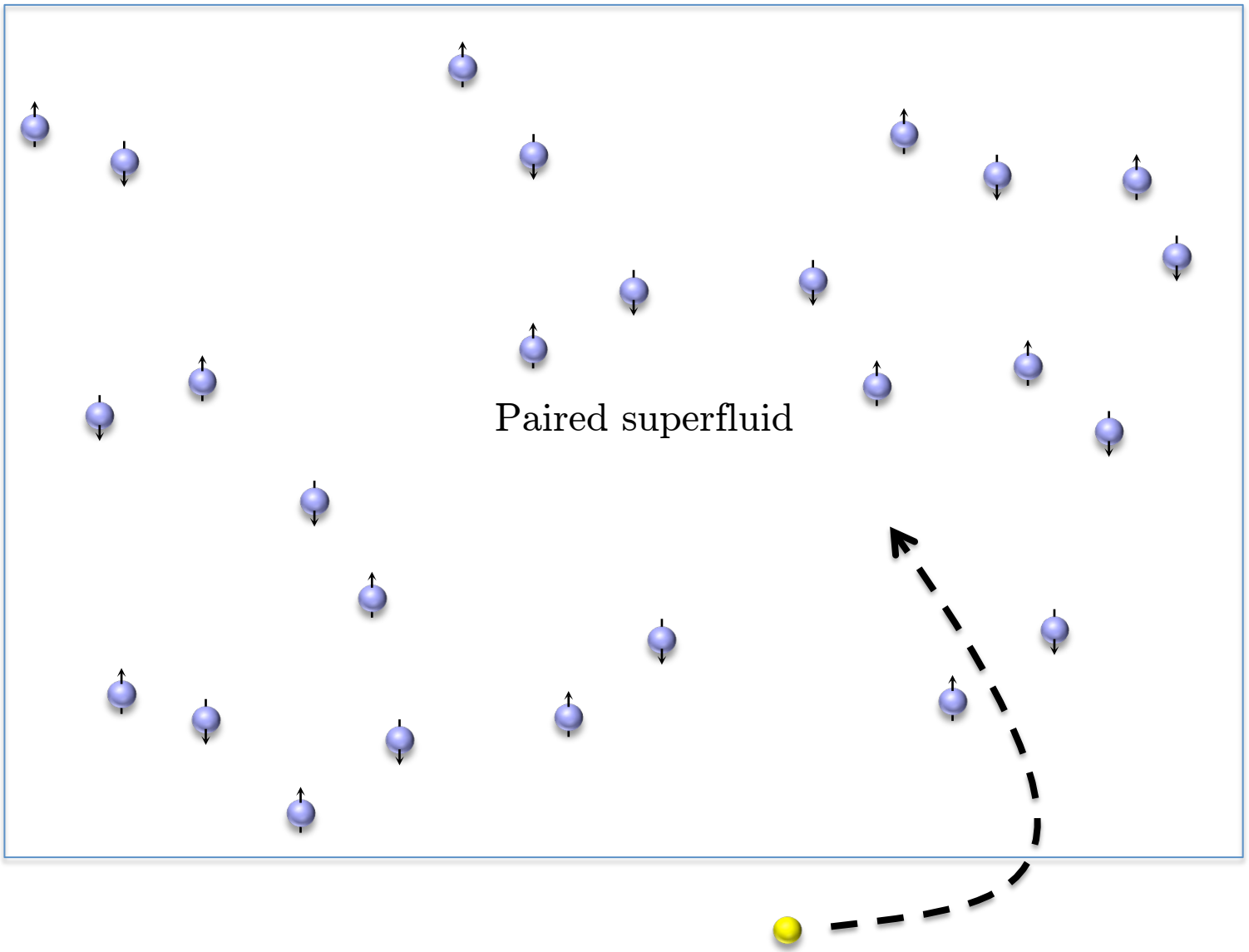
Ong, Cheng, Arakelyan, Thomas, PRL 114 (2015) 110403

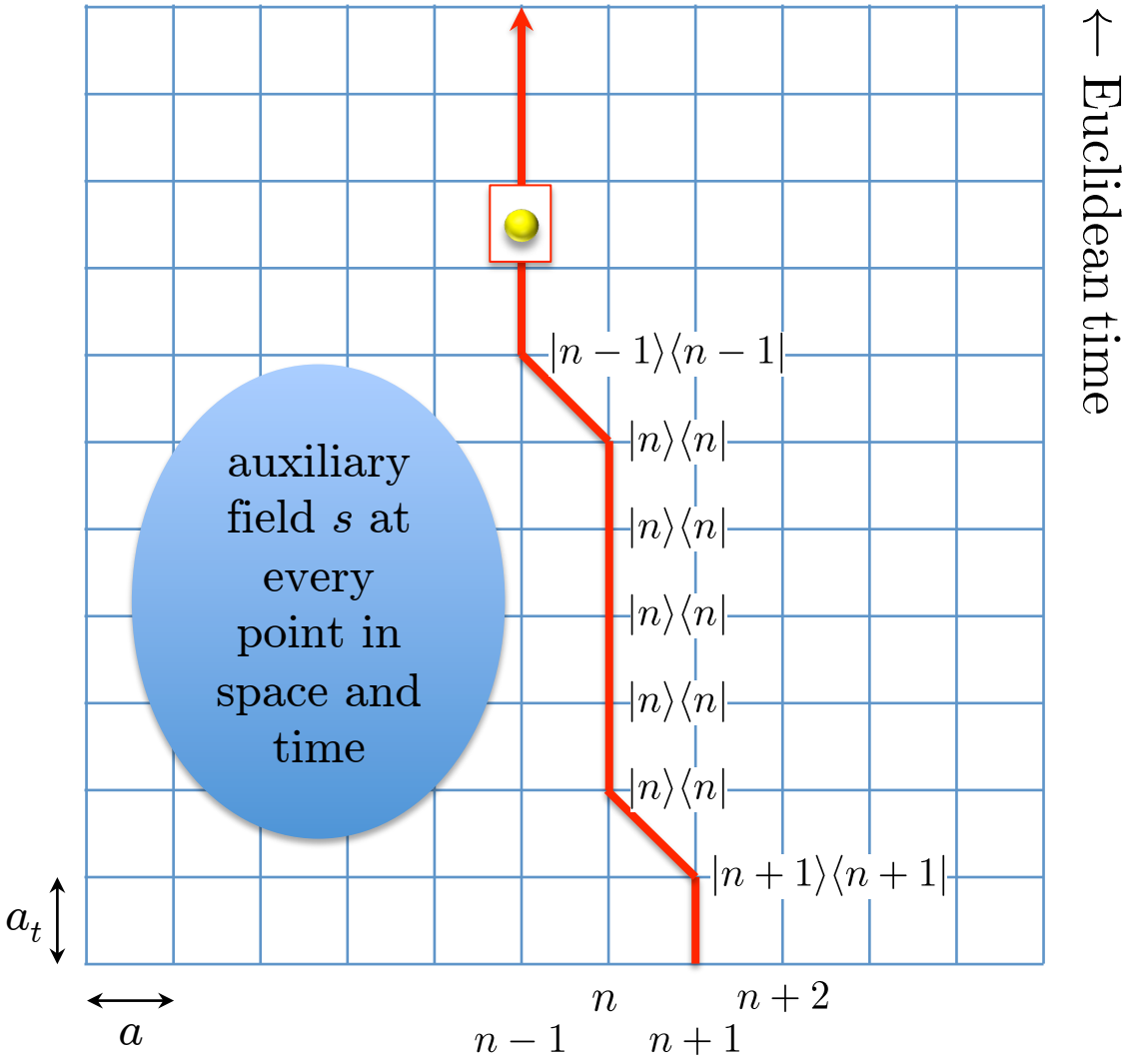
Current work and outlook

We are continuing with 2D polaron system using impurity lattice Monte Carlo calculations to measure pair density correlations, Z factor, and the effective mass.

We also starting calculations which apply impurity lattice Monte Carlo to impurities in a paired superfluid.

These simulations should have numerous applications to cold atomic systems as well as alpha particles in a superfluid neutron gas.


Paired superfluid


$|n-1\rangle\langle n-1|$
$|n\rangle\langle n|$
$|n\rangle\langle n|$
$|n\rangle\langle n|$
$|n\rangle\langle n|$
$|n\rangle\langle n|$
$|n+1\rangle\langle n+1|$
auxiliary field s at every point in space and time
a_t
a
$n-1$
n
$n+1$
$n+2$
← Euclidean time

Other developments

Adiabatic projection method

A new *ab initio* method for scattering and reactions of multi-particle bound states.

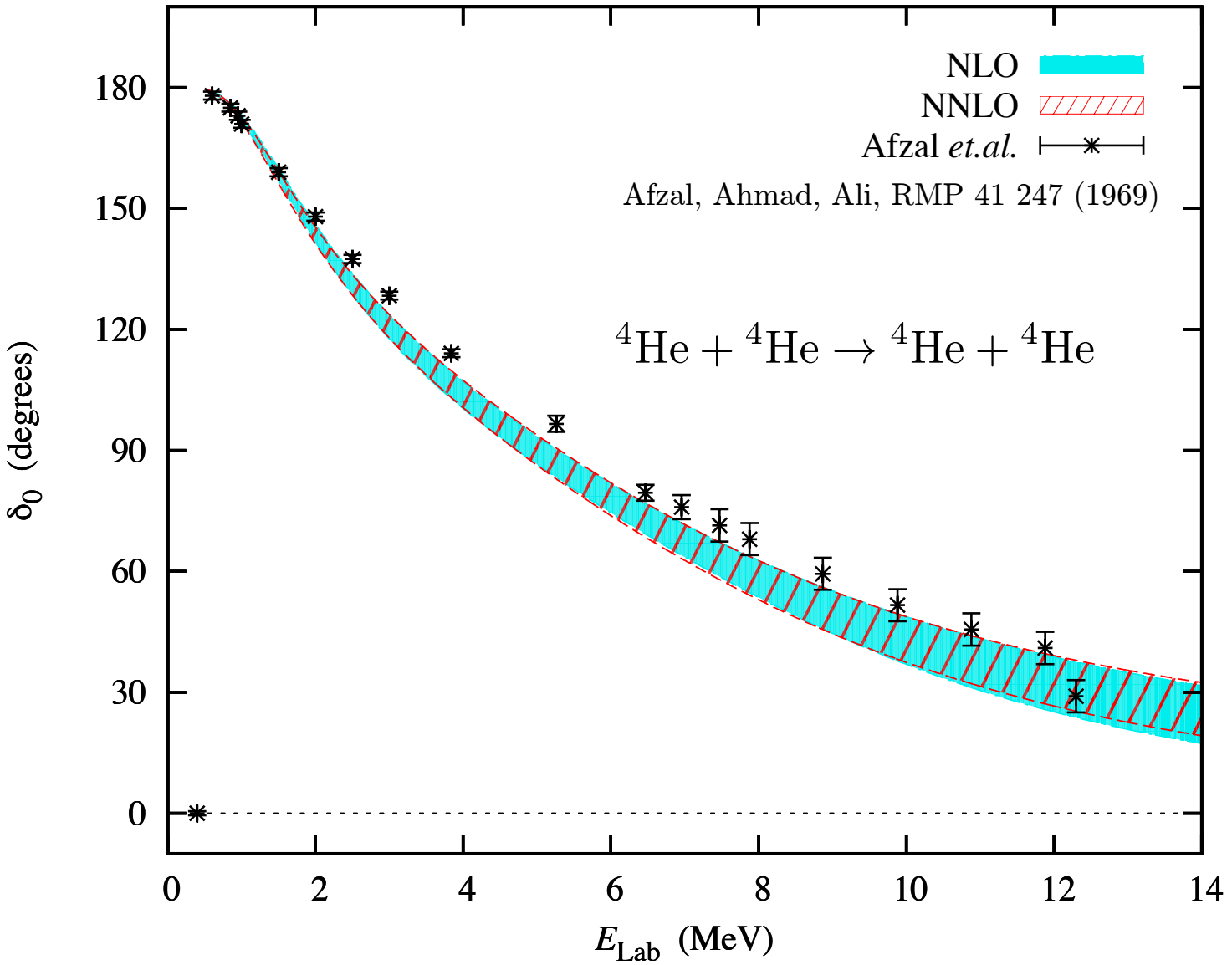
Rupak, D.L., PRL 111 032502 (2013)

Rokash, Pine, Elhatisari, D.L., Epelbaum, Krebs, arXiv:1505.02967

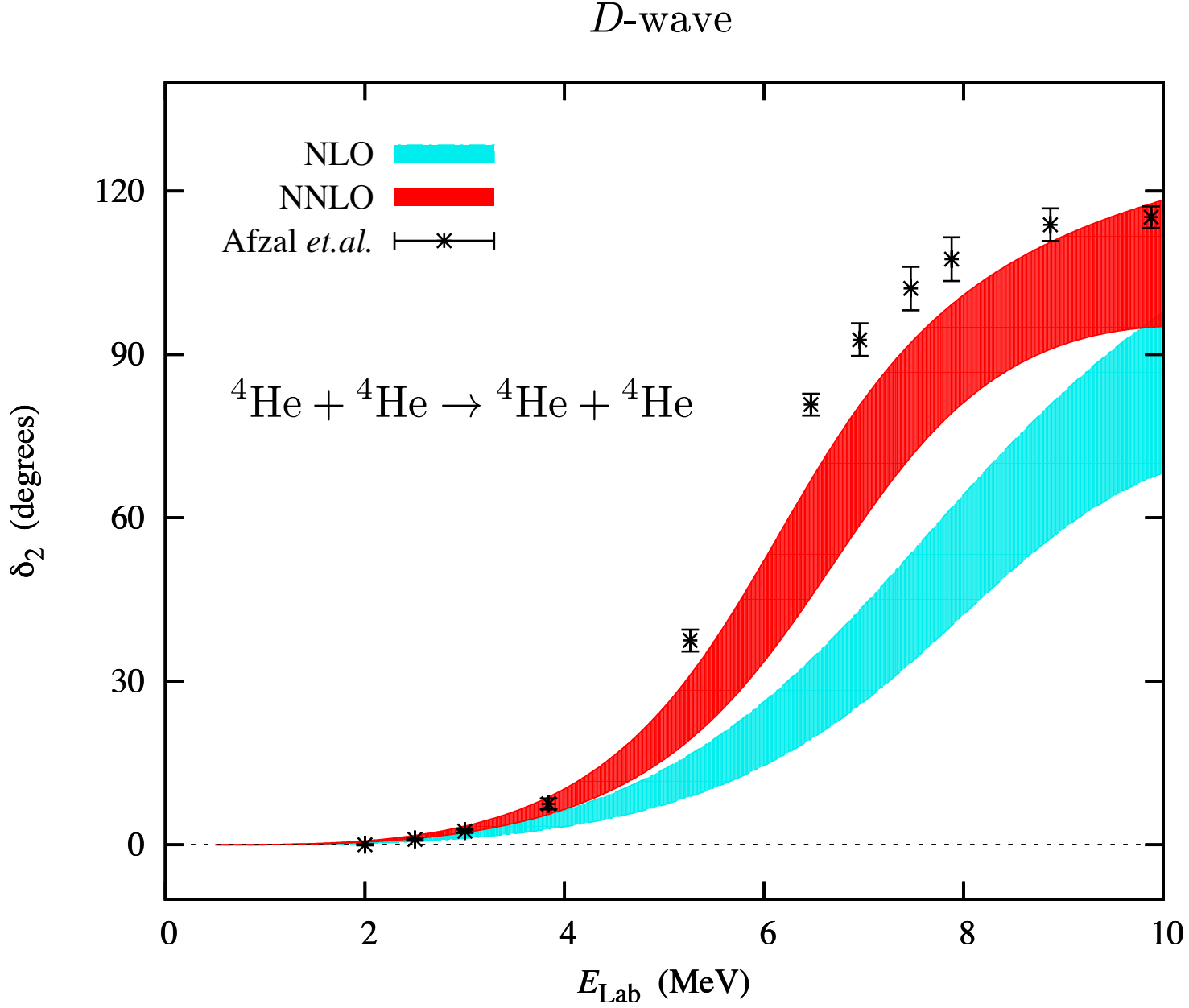
Elhatisari, Epelbaum, Krebs, Lähde, Lee, Luu, Meißner, Rupak, arXiv:1506.03513

Strategy is to divide the problem into two parts. In the first part, we use Euclidean time projection and lattice Monte Carlo to derive an *ab initio* low-energy cluster Hamiltonian, called the adiabatic Hamiltonian (adiabatic transfer matrix for nonzero temporal lattice spacing).

In the second part, we use the adiabatic Hamiltonian to compute scattering phase shifts or reaction amplitudes.



Elhatisari, Epelbaum, Krebs, Lähde, Lee, Luu, Meißner, Rupak, arXiv:1506.03513



Elhatisari, Epelbaum, Krebs, Lähde, Lee, Luu, Meißner, Rupak, arXiv:1506.03513

In addition to multi-particle bound state scattering and reactions, the adiabatic projection method can be used to probe the scattering and reactions of quasiparticles in medium. And when combined with impurity lattice Monte Carlo, this could be used to probe the scattering of impurities.

In summary, there are new and robust computational methods available now which hold promise for describing the properties of impurities, quasiparticles, and bound states from first principles. Hopefully this can lead to new and deeper insights.

End.