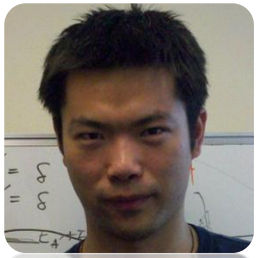
Benchmark calculations at unitarity

arXiv: 1104.2102 [cond-mat-quant-gas]



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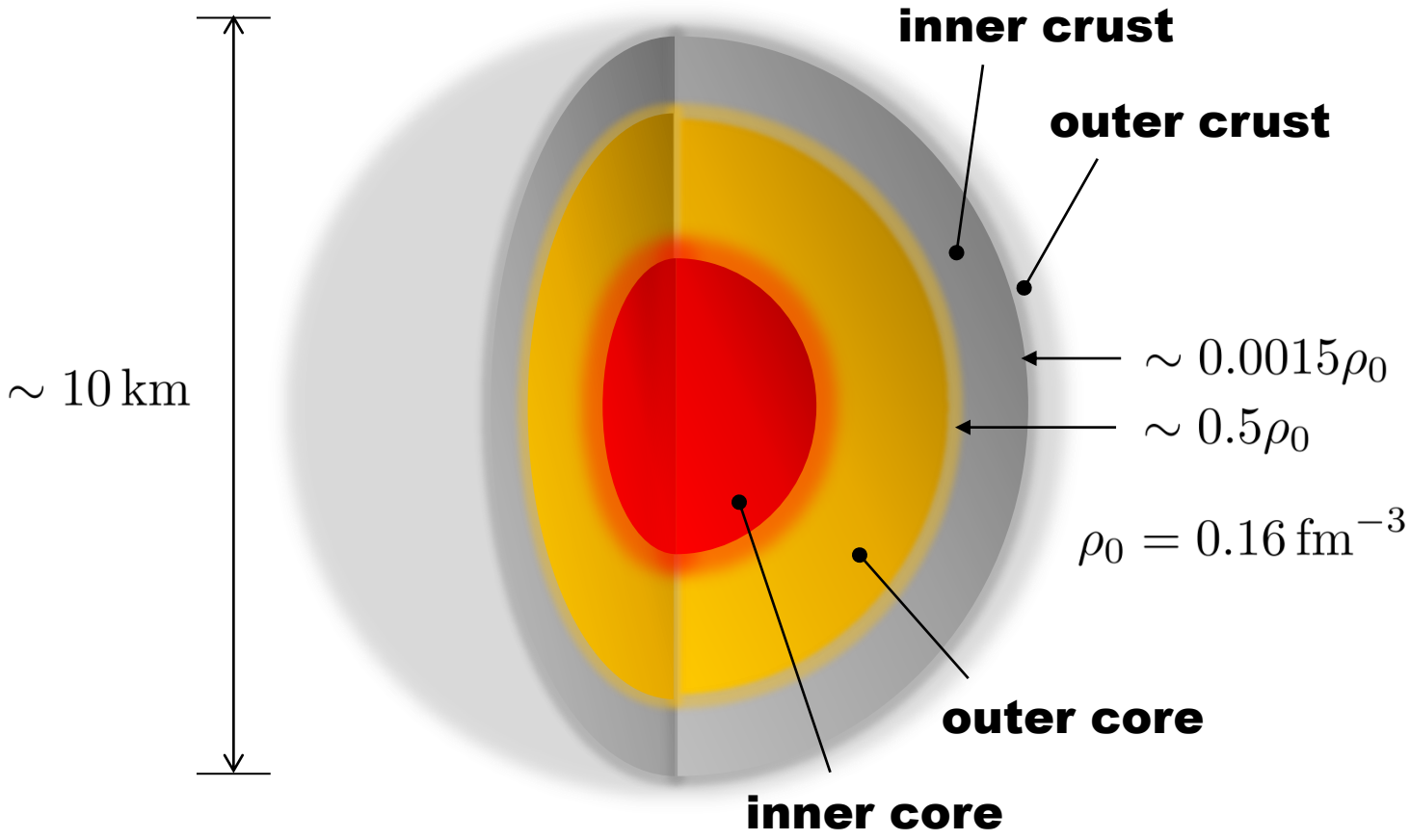
Fermions from Cold Atoms to Neutron Stars:
Benchmarking the Many-Body Problem
INT, Seattle, May 9, 2011

Outline

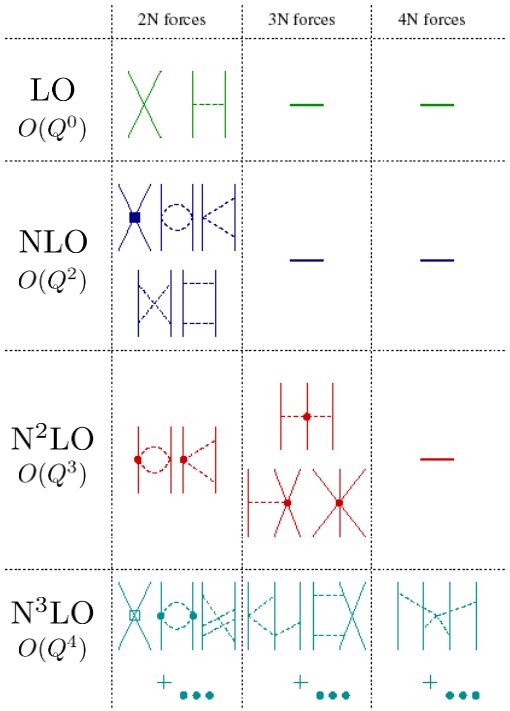
1. Unitarity limit
2. Results in the literature
3. Hamiltonian lattice calculation
4. Euclidean lattice calculation
5. Diffusion Monte Carlo calculation
6. Summary

Neutron star

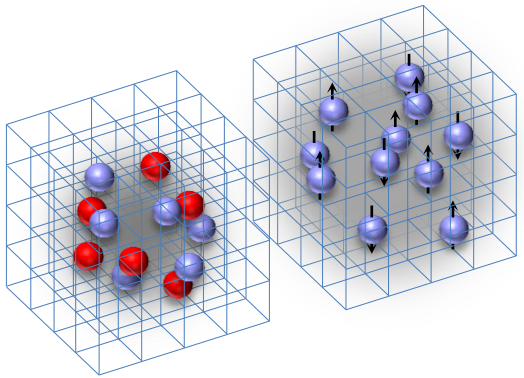


Lattice Effective Field Theory

From effective field theory

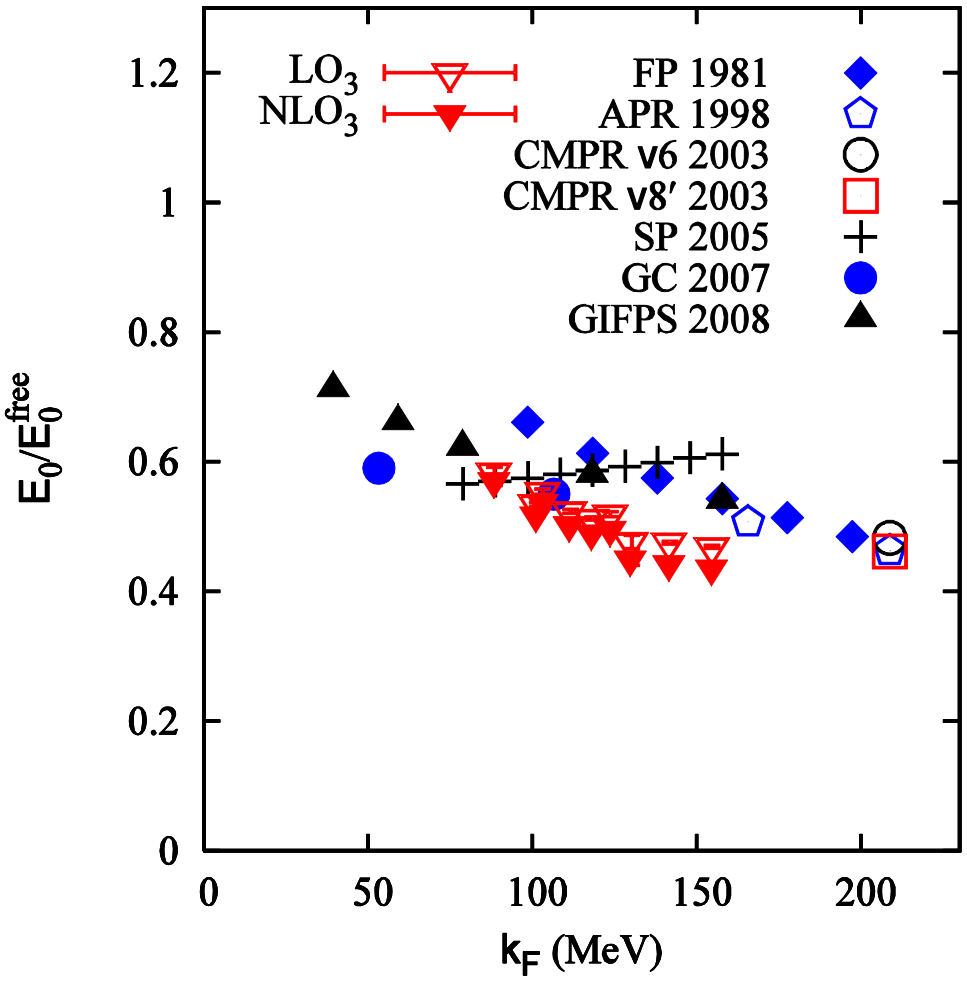


to first principles calculations



$N = 8, 12, 16$ neutrons at $L^3 = 4^3, 5^3, 6^3, 7^3$

$a = 1.97$ fm $\quad a_t = 1.32$ fm



Epelbaum, Krebs, D.L, Meißner, EPJA 40 (2009) 199

Unitarity limit

S-wave scattering amplitude:

$$f_0(k) = \frac{1}{k\cot\delta_0(k) - ik} \qquad k\cot\delta_0(k) \approx -a_0^{-1} + \frac{1}{2}r_0k^2 + \cdots$$

Unitarity limit: $\qquad k\cot\delta_0(k) \approx 0 \qquad f_0(k) \to \frac{i}{k}$

Free Fermi gas ground state

$$\frac{E_0^{\text{free}}}{A} = \frac{3}{5}E_F$$

$$E_F = \frac{k_F^2}{2m}$$

Unitarity limit ground state

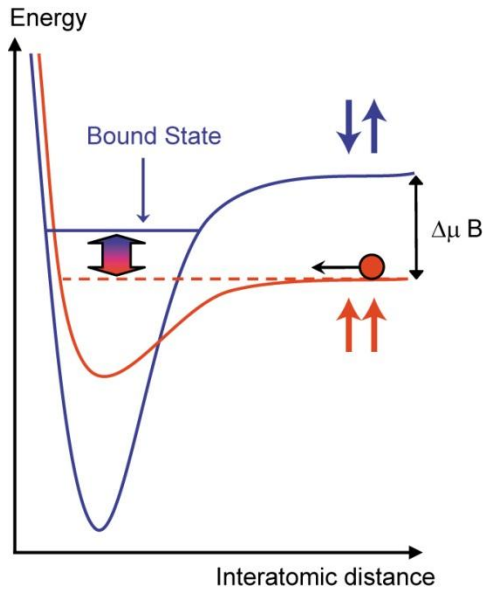
$$\frac{E_0}{A} = \xi \cdot \frac{E_0^{\text{free}}}{A} = \xi \cdot \frac{3}{5}E_F$$

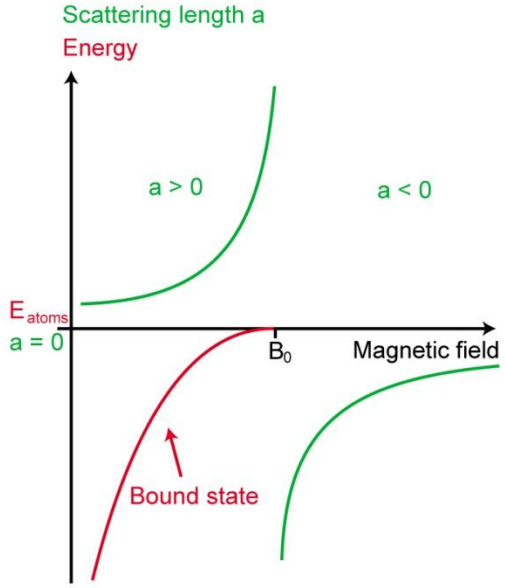
ξ is a dimensionless number (Bertsch parameter)

Neutron matter close to unitarity limit for $\quad k_F \sim 80\ \text{MeV}$

Cold atomic Fermi gases

Experiments done with cold ^{6}Li and ^{40}K atoms. Different hyperfine states. Open two-atom channel and closed diatomic molecule channel.





Zeeman tune energy of the diatomic molecule with external magnetic field to produce Feshbach resonance near threshold. [*O'Hara et. al., Science 298 (2002) 2179; Regal, Jin, PRL (2003) 230404; etc.]*

Cold atom experimental values for ξ

$0.32(+13)(-10)$ [9]
$0.36(15)$ [10]
$0.51(4)$ [11]
$0.46(5)$ [12]
$0.46(+05)(-12)$ [13]
$0.435(15)$ [14]
$0.41(15)$ [15]
$0.41(2)$ [16]
$0.39(2)$ [16]
$0.36(1)$ [17]

references in *arXiv: 1104.2102 [cond-mat-quant-gas]*

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Analytical values for ξ

Saddle point and variational approximations [18, 19]
Pade approximations and truncated series methods [20–22]
Mean field theory with pairing [23, 24]
Density functional theory extrapolated from small systems [25]
Renormalization group flow [26]
Dimensional expansions [27–33]
Large-N expansions [34]
Other methods [35]

The values for ξ range from 0.2 to 0.6, with most predictions in the range from 0.3 to 0.4.

references in *arXiv: 1104.2102 [cond-mat-quant-gas]*

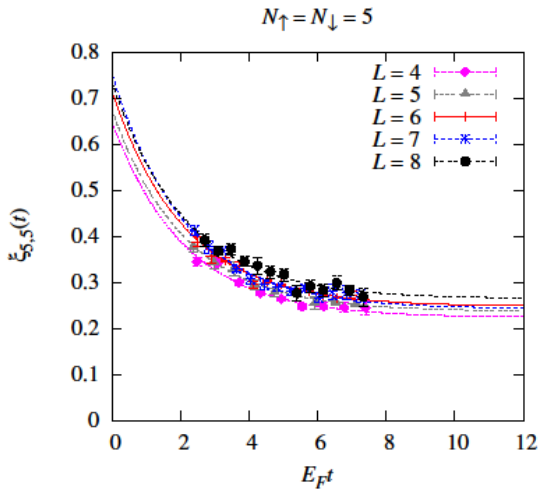
Fixed-node diffusion Monte Carlo values for ξ

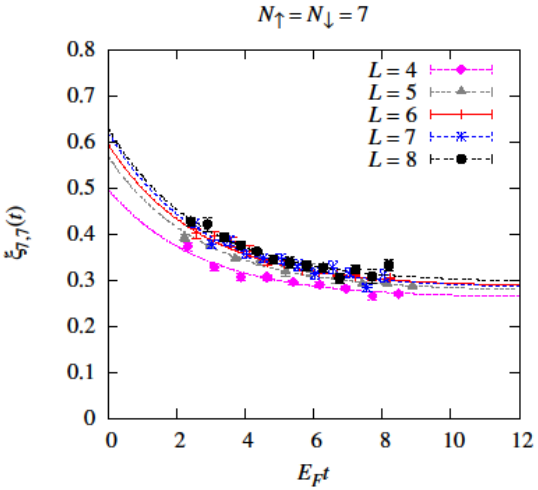
$$\xi = 0.44(1), 0.42(1), 0.383(1)$$

[Carlson, Chang, Pandharipande, Schmidt, PRL 91 (2003) 50401
Astrakharchik, Boronat, Casulleras, Giorgini, PRL 93 (2004) 200404
Forbes, Gandolfi, Gezerlis, arXiv:1011.2197]

Other diffusion Monte Carlo calculations referenced in
arXiv: 1104.2102 [cond-mat-quant-gas]

Monte Carlo lattice calculations



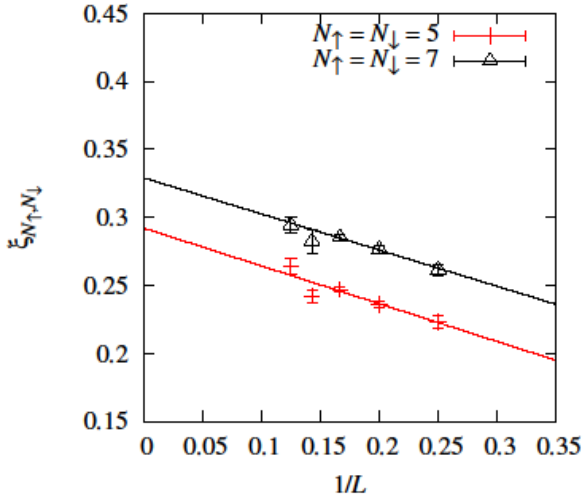


$$\xi_{N_\uparrow,N_\downarrow} = E^0_{N_\uparrow,N_\downarrow} / E^{0,\mathrm{free}}_{N_\uparrow,N_\downarrow}$$

$$\xi_{5,5} = 0.292(12)$$

$$\xi_{7,7} = 0.329(5)$$

D.L., PRC 78 (2008) 024001



Other lattice calculations referenced in
arXiv: 1104.2102 [cond-mat-quant-gas]

Ground state energy ratio

There are at least two different definitions for the ground state energy ratio. We use a "few-body" definition, which is an energy ratio for the interacting and non-interacting systems with the same numbers of particles and volume,

$$\xi_{N_\uparrow,N_\downarrow} = E^0_{N_\uparrow,N_\downarrow} / E^{0,\mathrm{free}}_{N_\uparrow,N_\downarrow}$$

Others prefer a "thermodynamical" definition where the non-interacting energy is replaced by a thermodynamic limit value based on particle density

$$k_{F,\uparrow} = \left(6\pi^2 \frac{N_\uparrow}{L^3}\right)^{1/3}, \quad k_{F,\downarrow} = \left(6\pi^2 \frac{N_\downarrow}{L^3}\right)^{1/3}$$

$$E_{F,\uparrow} = \frac{k^2_{F,\uparrow}}{2m}, \quad E_{F,\downarrow} = \frac{k^2_{F,\downarrow}}{2m}$$

$$\xi^{\mathrm{thermo}}_{N_\uparrow,N_\downarrow} = \frac{E^0_{N_\uparrow,N_\downarrow}}{\frac{3}{5}N_\uparrow E_{F,\uparrow} + \frac{3}{5}N_\downarrow E_{F,\downarrow}}$$

Table of conversion factors between the two energy ratio definitions

$N_\uparrow = N_\downarrow$	$\xi_{N_\uparrow,N_\downarrow}/\xi^{\text{thermo}}_{N_\uparrow,N_\downarrow}$
2	0.7331
3	0.7204
4	0.7758
5	0.8439
6	0.9149
7	0.9858

$N_\uparrow = N_\downarrow$	$\xi_{N_\uparrow,N_\downarrow}/\xi^{\text{thermo}}_{N_\uparrow,N_\downarrow}$
8	0.9236
9	0.8991
10	0.8931
16	0.9774
24	1.0246
32	1.0064

Physical scattering data → Unknown operator coefficients

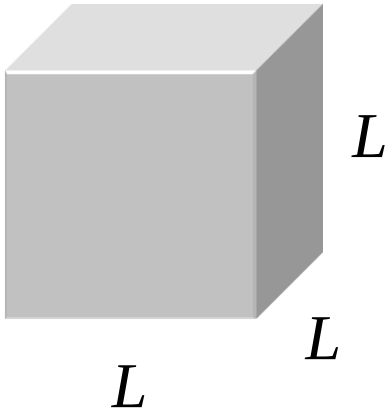
Lüscher's finite-volume formula

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

Two-particle energy levels near threshold in a periodic cube related to phase shifts

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

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



Hamiltonian lattice calculation of $\xi_{2,2}$

Start with a lattice Hamiltonian for the non-interacting system

$$H_{\rm free} = \frac{3}{m} \sum_{\vec{n},i=\uparrow,\downarrow} a_i^\dagger(\vec{n}) a_i(\vec{n}) - \frac{1}{2m} \sum_{l=1,2,3} \sum_{\vec{n},i=\uparrow,\downarrow} \left[a_i^\dagger(\vec{n}) a_i(\vec{n}+\hat{l}) + a_i^\dagger(\vec{n}) a_i(\vec{n}-\hat{l}) \right]$$

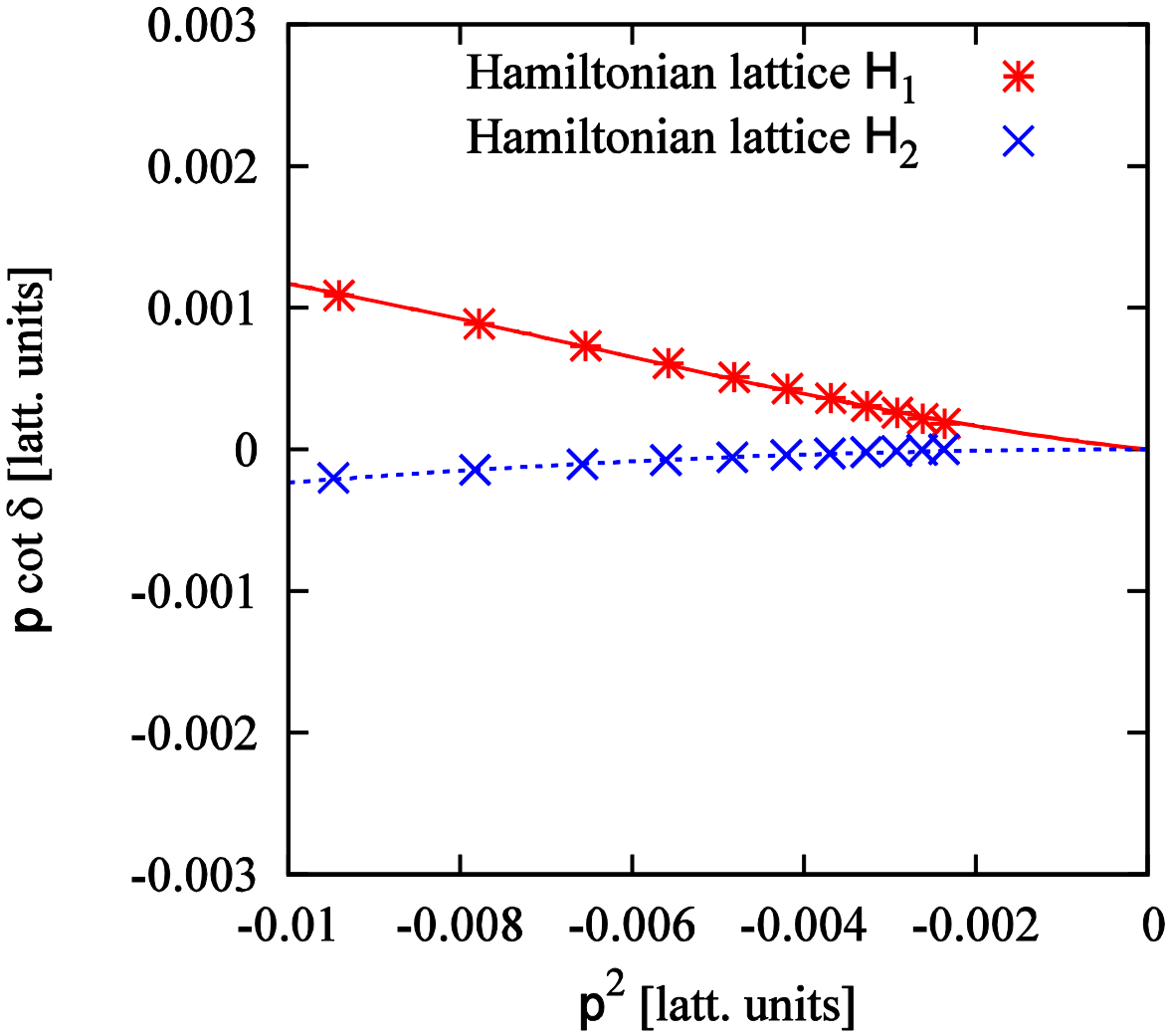
We consider two different lattice Hamiltonians, both of which give the unitarity limit in the limit of large lattice volume in lattice units. H_1 has infinite scattering length. H_2 has infinite scattering length and zero effective range.

$$H_1 = H_{\rm free} + C_1 \sum_{\vec{n}} \rho_\uparrow(\vec{n}) \rho_\downarrow(\vec{n}).$$

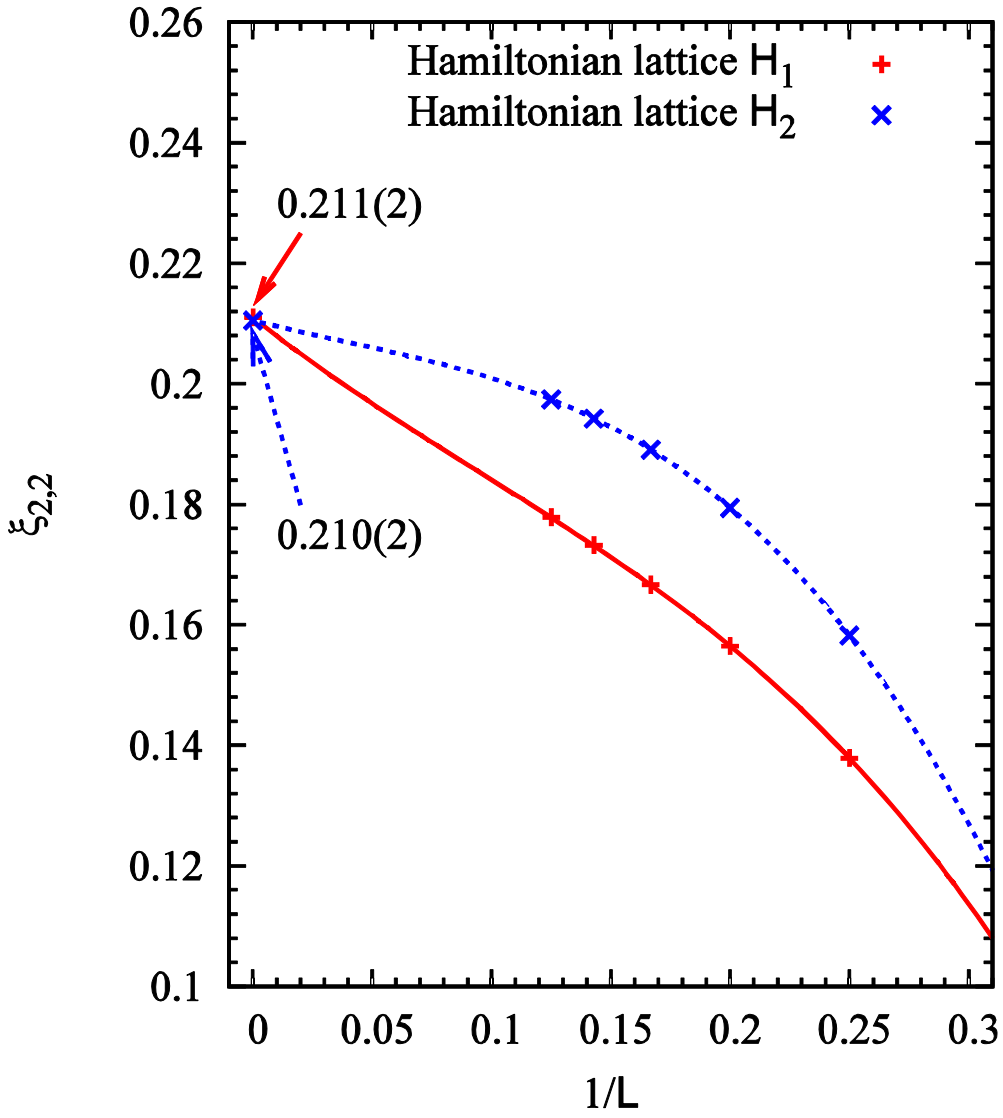
$$H_2 = H_{\rm free} + C_2 \sum_{\vec{n}} \rho_\uparrow(\vec{n}) \rho_\downarrow(\vec{n}) + C_2' \sum_{l=1,2,3} \sum_{\vec{n}} \left[\rho_\uparrow(\vec{n}) \rho_\downarrow(\vec{n}+\hat{l}) + \rho_\uparrow(\vec{n}+\hat{l}) \rho_\downarrow(\vec{n}) \right]$$

$$\rho_\uparrow(\vec{n}) = a_\uparrow^\dagger(\vec{n}) a_\uparrow(\vec{n}), \qquad \rho_\downarrow(\vec{n}) = a_\downarrow^\dagger(\vec{n}) a_\downarrow(\vec{n}).$$

From Lüscher's formula



Results using Lanczos eigenvector iteration



Euclidean lattice calculation of $\xi_{2,2}$

We use a normal-ordered Euclidean lattice transfer matrix formalism

$$M = :\exp\left[-H_{\rm free}\alpha_t - C\alpha_t\sum_{\vec{n}}\rho_\uparrow(\vec{n})\rho_\downarrow(\vec{n})\right]:,$$

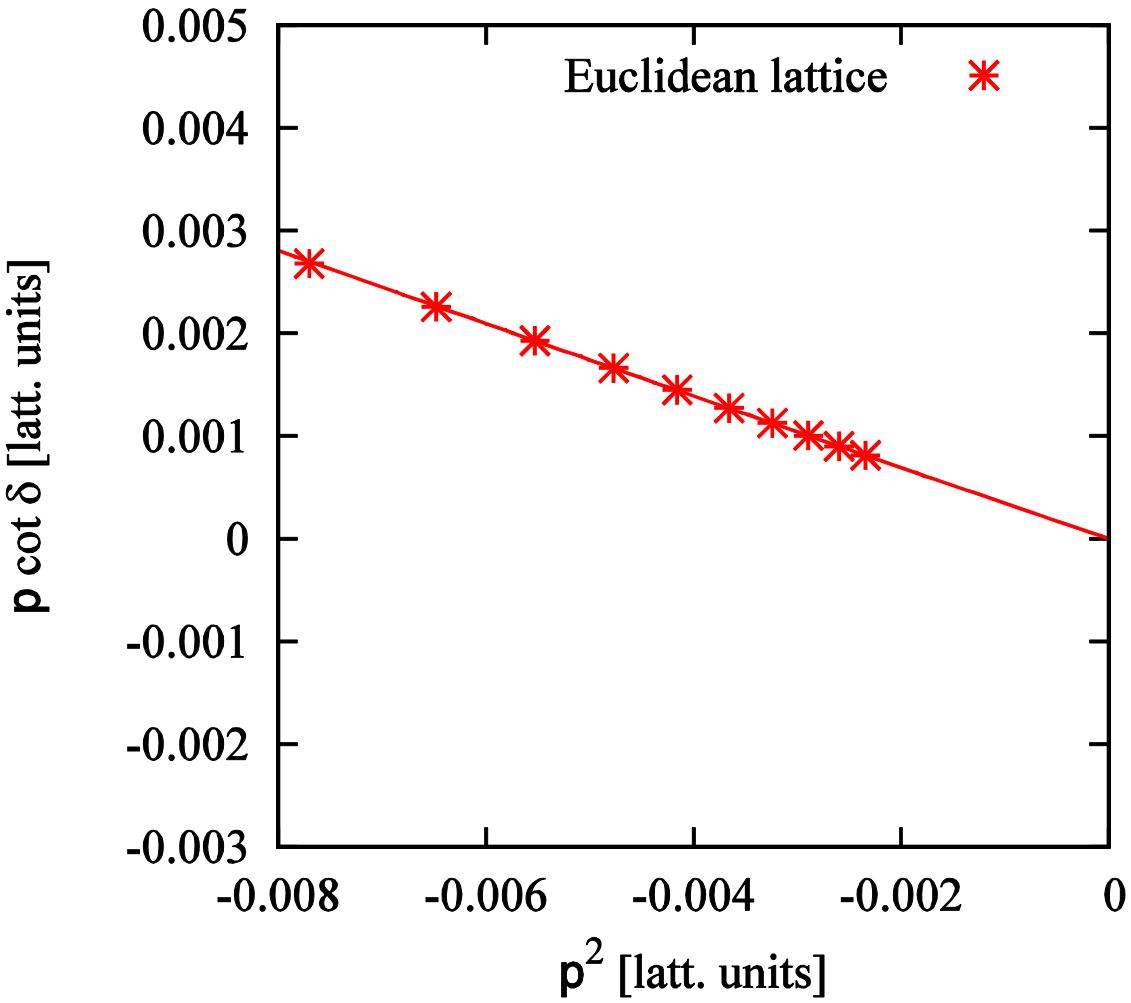
$$\alpha_t = a_t/a$$

$$H_{\rm free} = \frac{3}{m}\sum_{\vec{n},i=\uparrow,\downarrow} a_i^\dagger(\vec{n})a_i(\vec{n}) - \frac{1}{2m}\sum_{l=1,2,3}\sum_{\vec{n},i=\uparrow,\downarrow}\left[a_i^\dagger(\vec{n})a_i(\vec{n}+\hat{l}) + a_i^\dagger(\vec{n})a_i(\vec{n}-\hat{l})\right]$$

$$\rho_\uparrow(\vec{n}) = a_\uparrow^\dagger(\vec{n})a_\uparrow(\vec{n}), \qquad \rho_\downarrow(\vec{n}) = a_\downarrow^\dagger(\vec{n})a_\downarrow(\vec{n}).$$

The coefficient *C* is tuned using Lüscher's formula

From Lüscher's formula



For the Monte Carlo simulation we use a bounded continuous auxiliary field formalism.

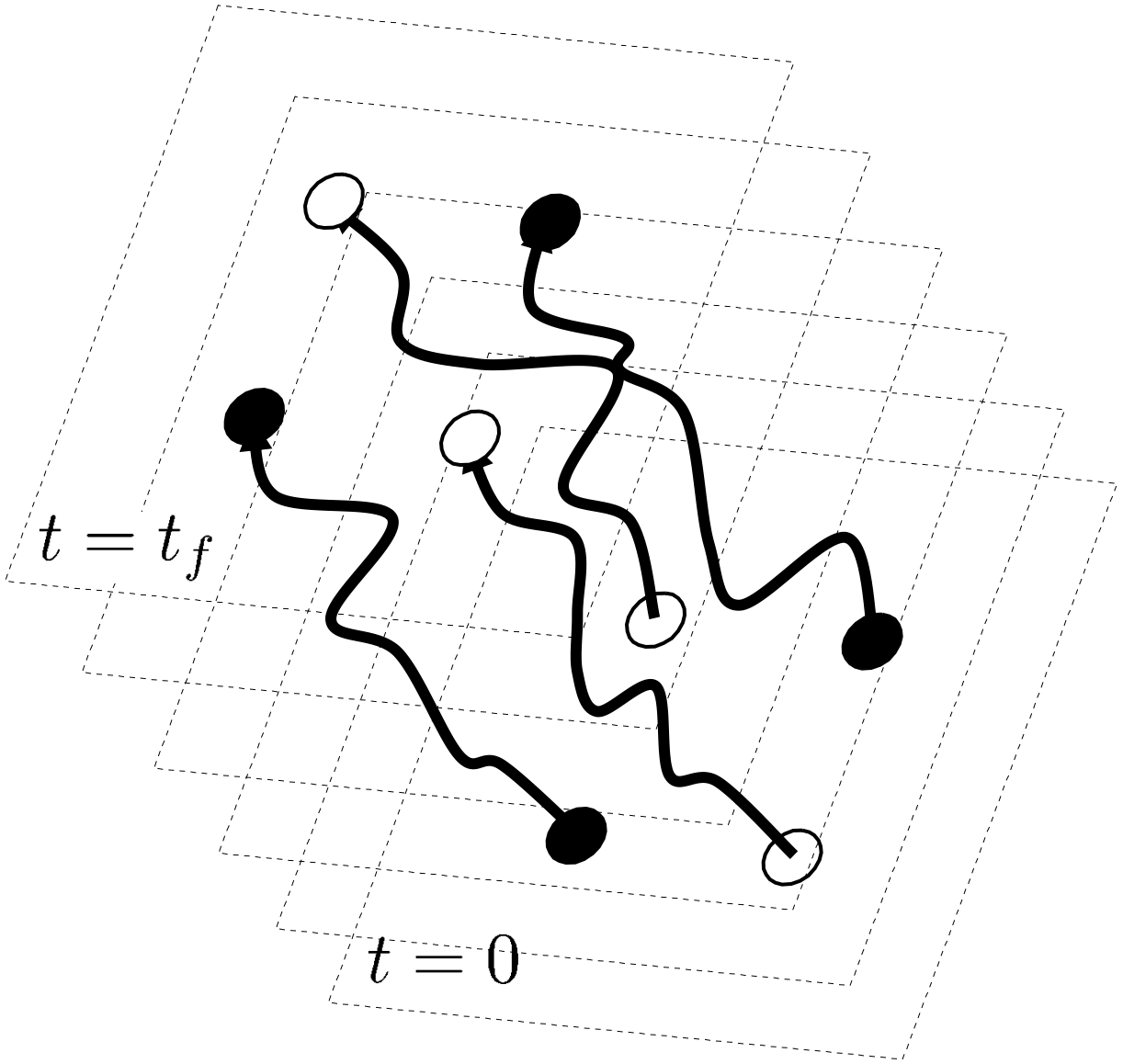
D.L., PRC 78 (2008) 024001

$$M = \prod_{\vec{n}} \left[\frac{1}{2\pi} \int_{-\pi}^{+\pi} ds(\vec{n}, n_t) \right] M(s, n_t)$$

$$M(s, n_t) =: \exp \left\{ -H_{\rm free} \alpha_t + \sum_{\vec{n}} \sqrt{-2C\alpha_t} \sin \left[s(\vec{n}, n_t) \right] \cdot \left[\rho_\uparrow(\vec{n}) + \rho_\downarrow(\vec{n}) \right] \right\} : .$$

$$Z_{2,2}(t) \equiv \prod_{\vec{n}, n_t} \left[\frac{1}{2\pi} \int_{-\pi}^{+\pi} ds(\vec{n}, n_t) \right] \left\langle \Psi_{2,2}^{\rm init} \right| M(s, L_t - 1) \cdot \cdots \cdot M(s, 0) \left| \Psi_{2,2}^{\rm init} \right\rangle ,$$

$$E_{2,2}(t) = \frac{1}{\alpha_t} \ln \frac{Z_{2,2}(t - \alpha_t)}{Z_{2,2}(t)} \qquad\qquad E_{2,2}^0 = \lim_{t \to \infty} E_{2,2}(t)$$



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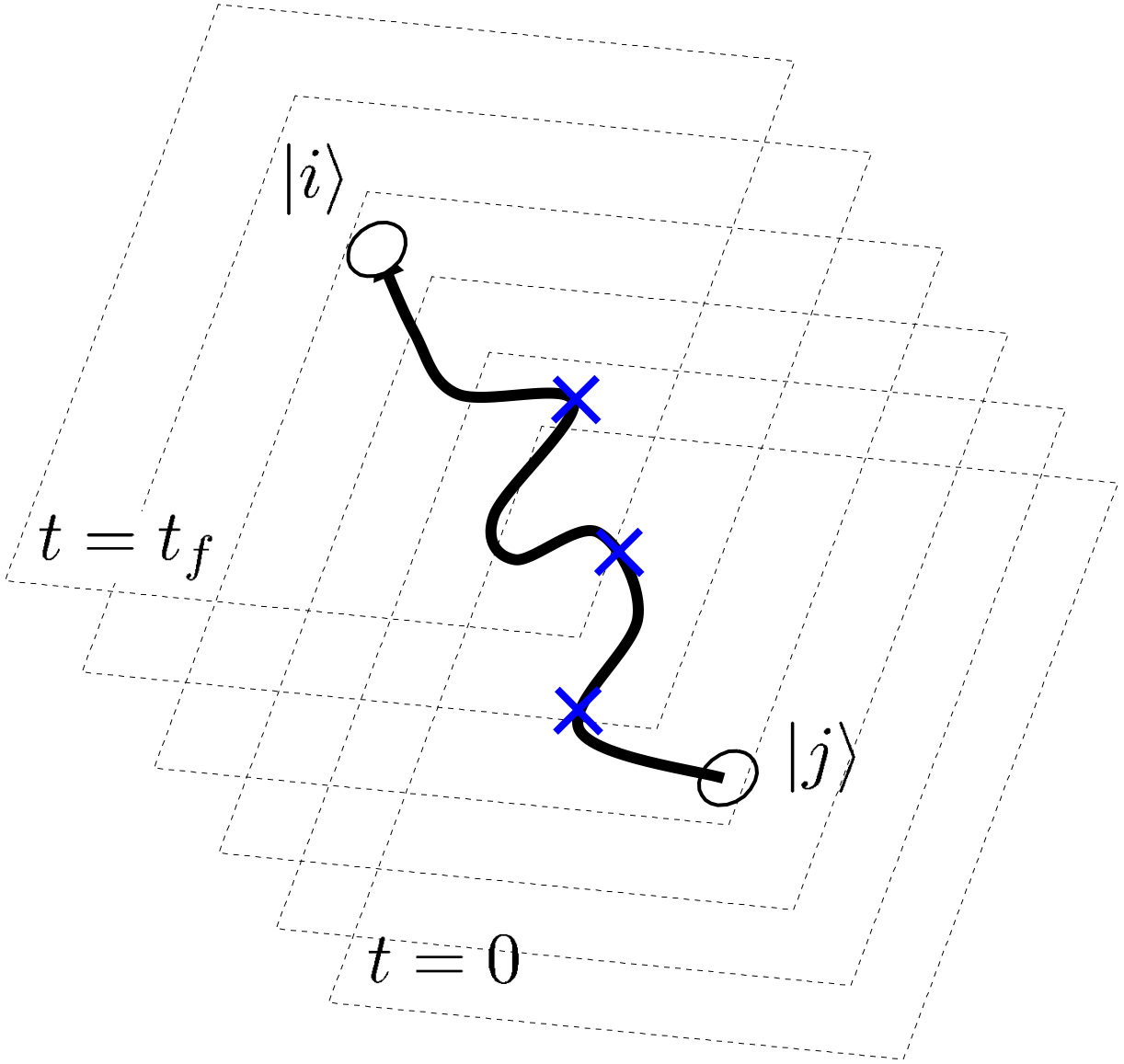

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$$\left|\Psi_{2,2}^{\rm init}\right\rangle = |\psi_1\rangle \wedge |\psi_2\rangle \wedge |\psi_3\rangle \wedge |\psi_4\rangle \,.$$

$$\left\langle\Psi_{2,2}^{\rm init}\right| M(s, L_t-1) \cdot \cdots \cdot M(s,0) \left|\Psi_{2,2}^{\rm init}\right\rangle = \left[\det \mathbf{M}(s,t)\right]^2 ,$$

$$\left[\mathbf{M}(s,t)\right]_{k'k} = \langle\psi_{k'}| M(s, L_t-1) \cdot \cdots \cdot M(s,0) |\psi_k\rangle \,,$$

$$k, k' = 1, 2, 3, 4$$

We use the following initial state:

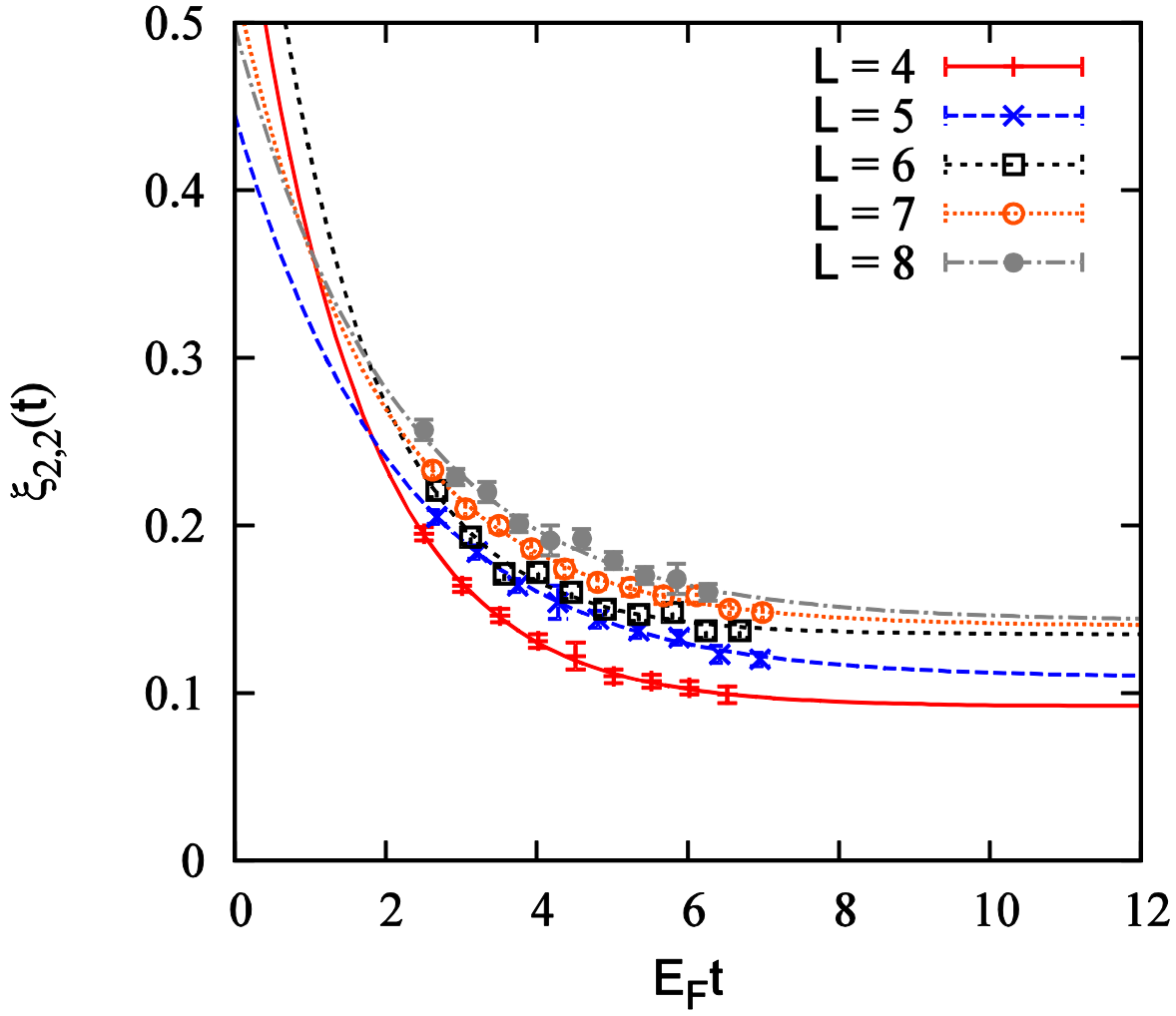
$$|\psi_1\rangle = \sqrt{\frac{1}{L^3}} \sum_{\vec{n}} a_\uparrow^\dagger(\vec{n}) |0\rangle \,, \quad |\psi_2\rangle = \sqrt{\frac{2}{L^3}} \sum_{\vec{n}} \cos(2\pi n_3/L) a_\uparrow^\dagger(\vec{n}) |0\rangle \,,$$

$$|\psi_3\rangle = \sqrt{\frac{1}{L^3}} \sum_{\vec{n}} a_\downarrow^\dagger(\vec{n}) |0\rangle \,, \quad |\psi_4\rangle = \sqrt{\frac{2}{L^3}} \sum_{\vec{n}} \cos(2\pi n_3/L) a_\downarrow^\dagger(\vec{n}) |0\rangle \,.$$

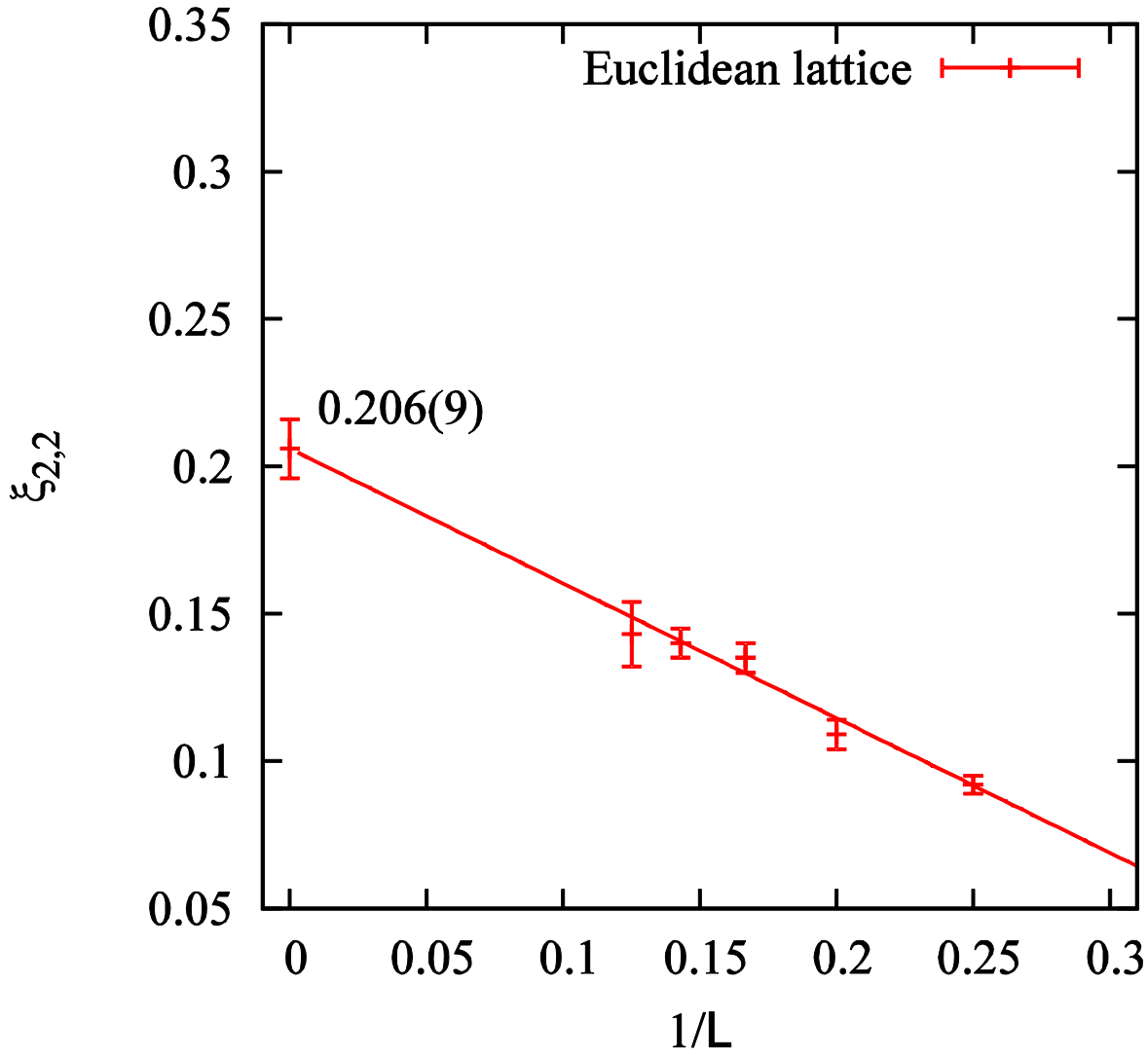
We calculate using the following lattice volumes:

L^3	4^3	5^3	6^3	7^3	8^3
L_t	30	50	72	96	120
	36	60	84	112	140
	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
	78	130	180	256	300

Results using Euclidean lattice Monte Carlo



Results using Euclidean lattice Monte Carlo



Diffusion Monte Carlo calculation of $\xi_{2,2}$

We work with continuous variables. The interaction will be written as a Pöschl-Teller potential tuned to infinite S-wave scattering length,

$$V(r) = -\frac{2}{m}\frac{\mu^2}{\cosh^2(\mu r)}$$

We take the zero-range limit,

$$\mu \to \infty$$

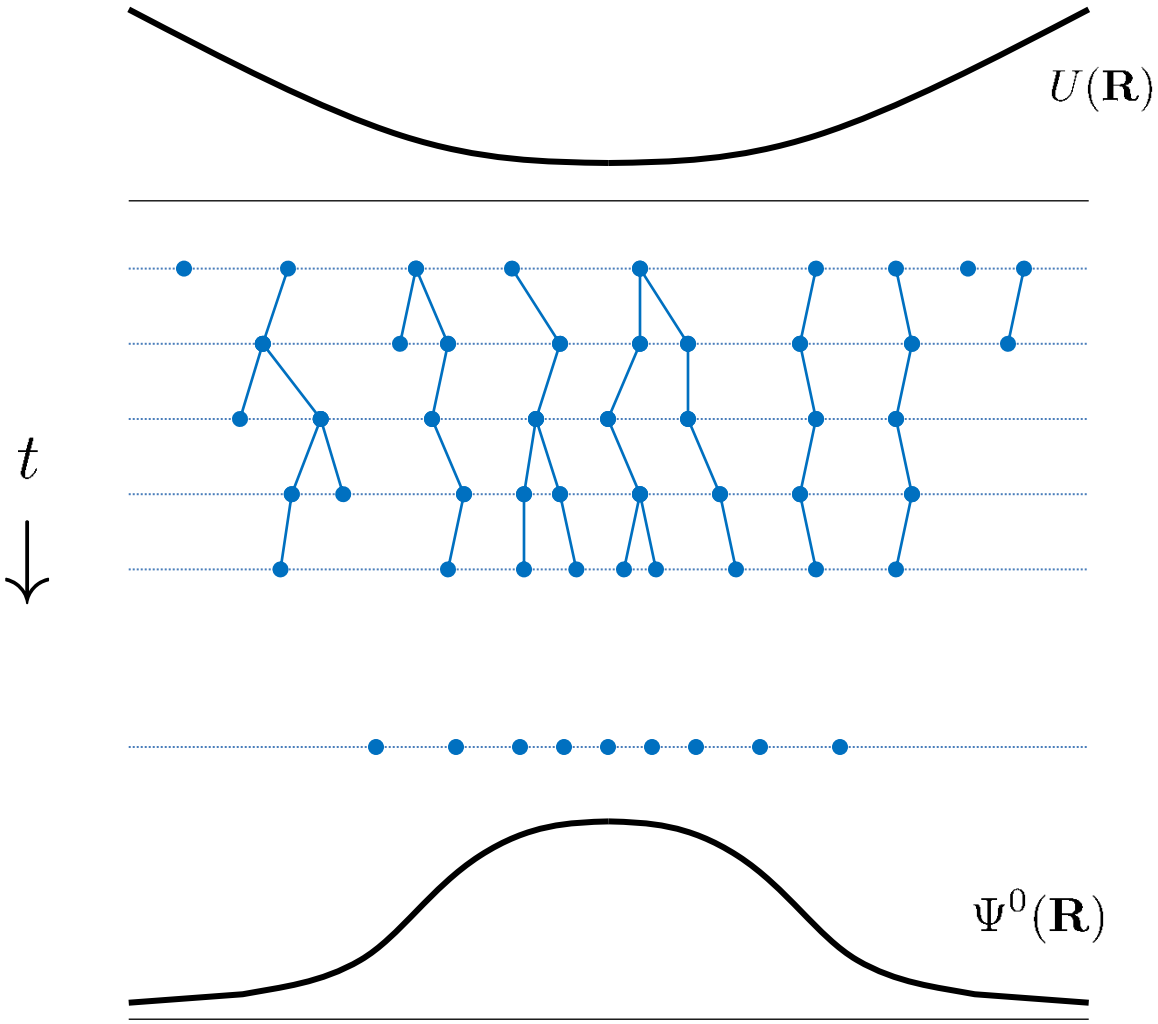
The effective range parameter is given by the relation

$$r_0 = 2\mu^{-1}$$

The four-particle wavefunction will be written as

$$\Psi(\mathbf{R}),\ \mathbf{R} = \left\{\vec{r}_{1_\uparrow}, \vec{r}_{1_\downarrow}, \vec{r}_{2_\uparrow}, \vec{r}_{2_\downarrow}\right\}$$

Diffusion Monte Carlo (no importance sampling)



Fixed-node diffusion Monte Carlo

For simple bosonic diffusion Monte Carlo without importance sampling the density of walkers is given by the wavefunction

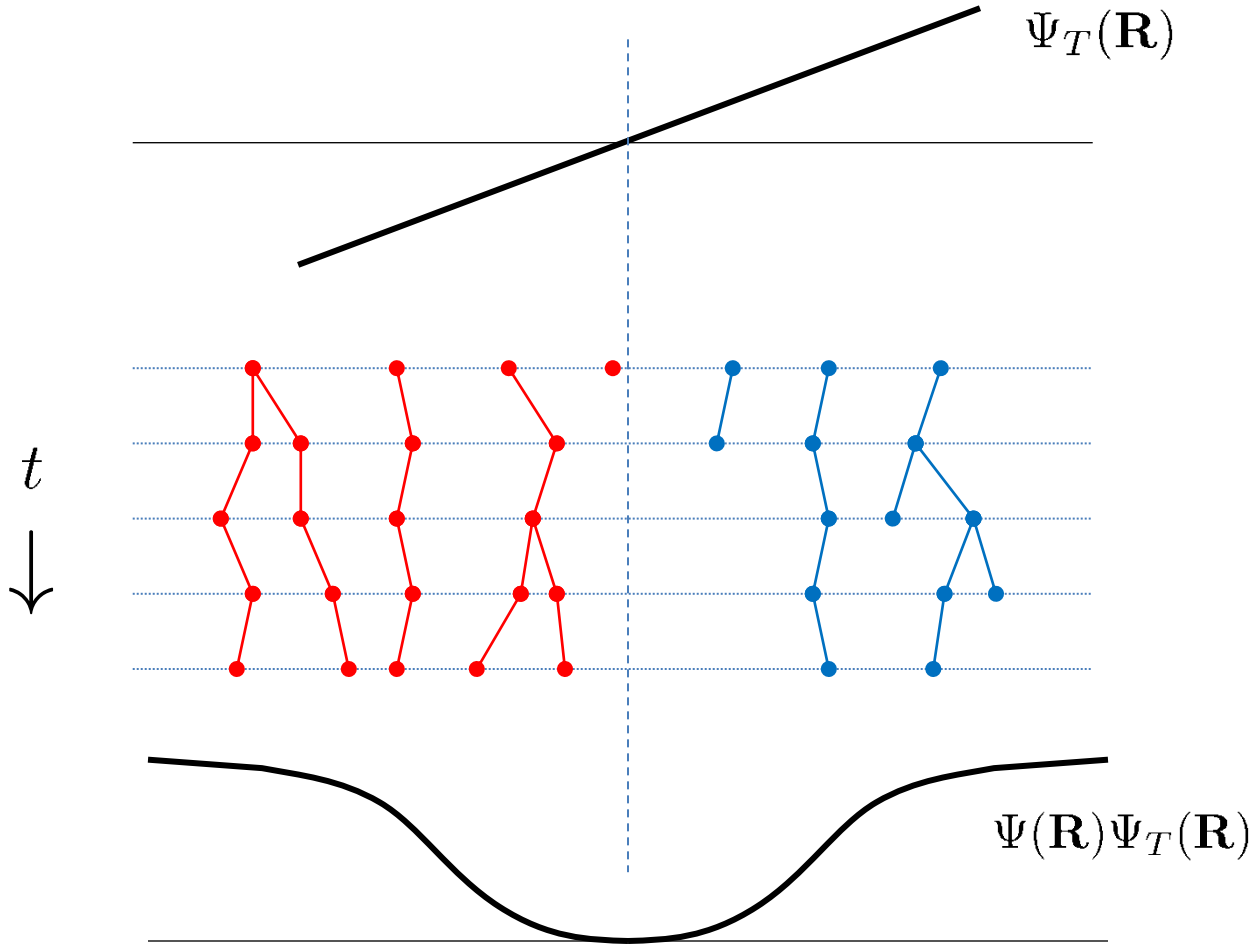
$$\Psi(\mathbf{R})$$

For fixed-node diffusion Monte Carlo, we importance sample using a trial wavefunction

$$\Psi(\mathbf{R})\Psi_T(\mathbf{R})$$

Walkers are not able to cross the nodal surfaces of the trial wavefunction. Hence there are positive-side walkers and negative-side walkers.

Fixed-node diffusion Monte Carlo



We use a trial wavefunction of the form

$$\Psi_T(\mathbf{R}) = \Psi_{\rm BCS}(\mathbf{R}) \exp\left[J(\mathbf{R})\right]$$

$$\Psi_{\rm BCS}(\mathbf{R}) = \det \begin{bmatrix} \phi(\vec{r}_{1_\uparrow} - \vec{r}_{1_\downarrow}) & \phi(\vec{r}_{1_\uparrow} - \vec{r}_{2_\downarrow}) \\ \phi(\vec{r}_{2_\uparrow} - \vec{r}_{1_\downarrow}) & \phi(\vec{r}_{2_\uparrow} - \vec{r}_{2_\downarrow}) \end{bmatrix}$$

Orbitals are Gaussians with nearest periodic copies

$$\phi(\vec{r}) = \sum_k d_k \sum_{s_x,s_y,s_z=-1}^{1} e^{-\frac{\alpha_k}{2}(x+s_x L)^2} e^{-\frac{\alpha_k}{2}(y+s_y L)^2} e^{-\frac{\alpha_k}{2}(z+s_z L)^2}$$

Jastrow factors are also Gaussians with nearest periodic copies. All parameters are optimized using variational Monte Carlo.

Released-node diffusion Monte Carlo

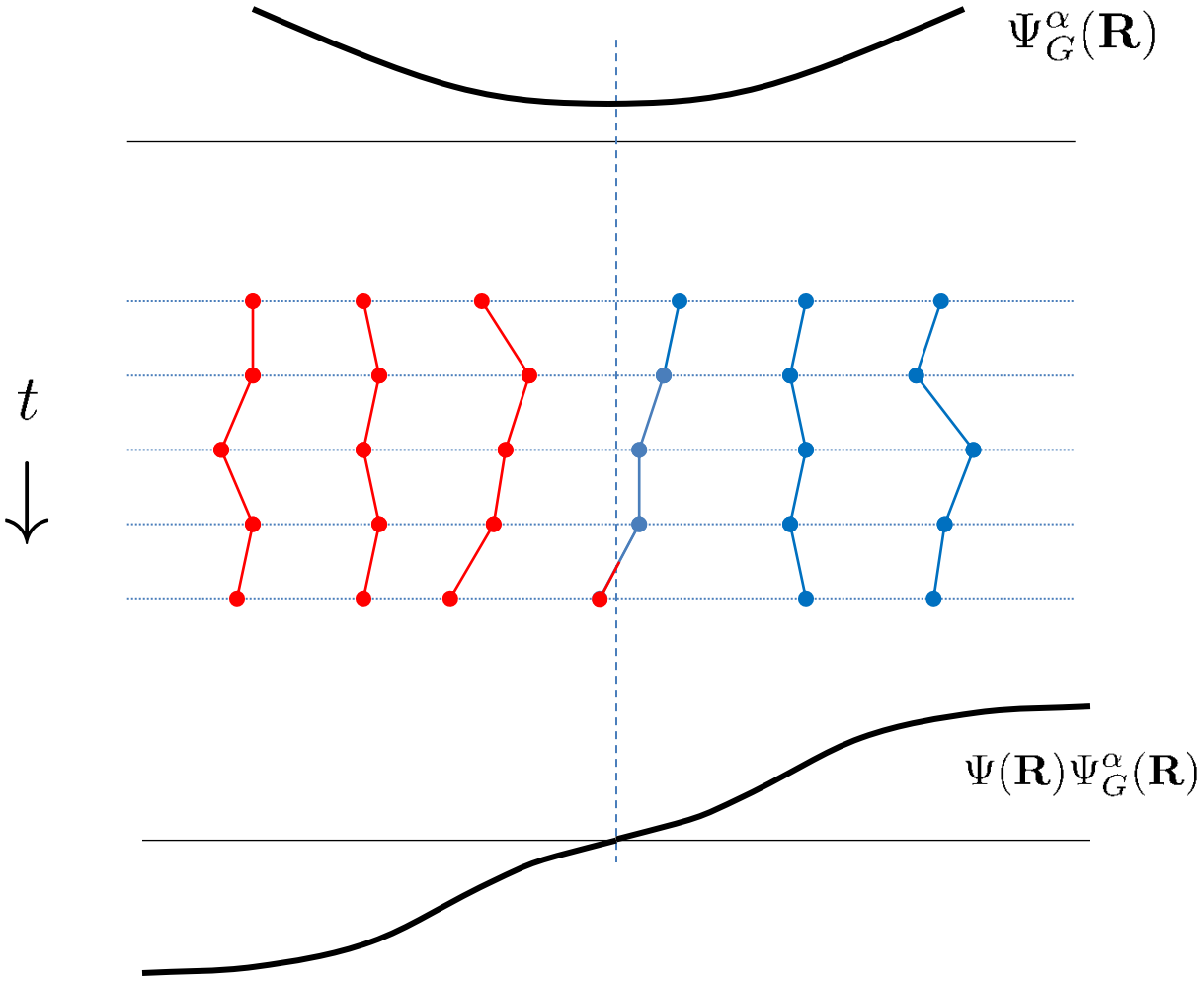
For the released-node diffusion Monte Carlo, we importance sample using a positive-definite guiding function

$$\Psi_G^{\alpha}(\mathbf{R}) = \sqrt{\Psi_T^2(\mathbf{R}) + \alpha \langle \Psi_T^2 \rangle}$$

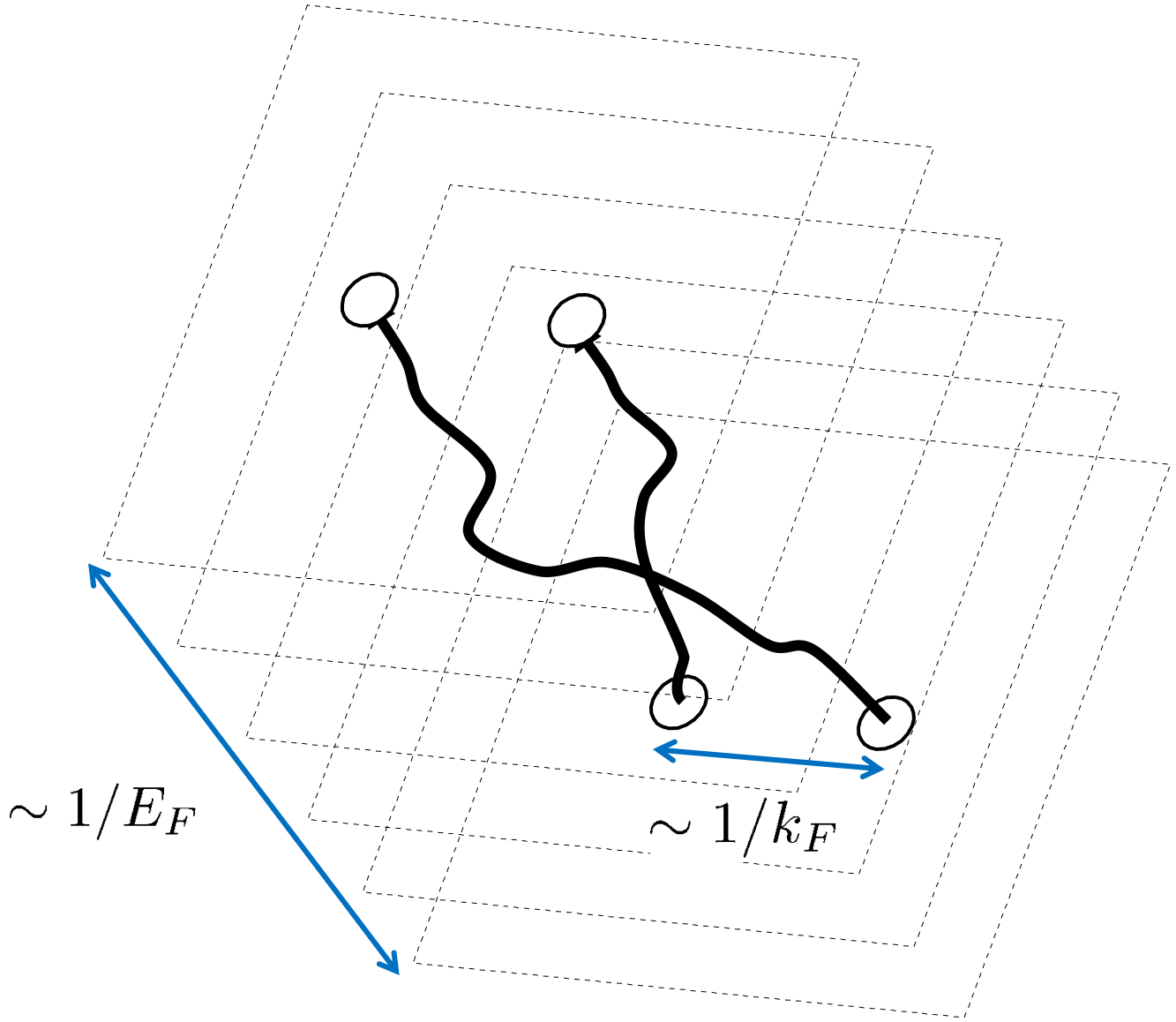
We vary the control parameter α. The average squared trial wavefunction is evaluated at the beginning of the released-node propagation time.

During the released-node propagation, we assign weight factors to the individual walkers rather than using birth-death branching processes.

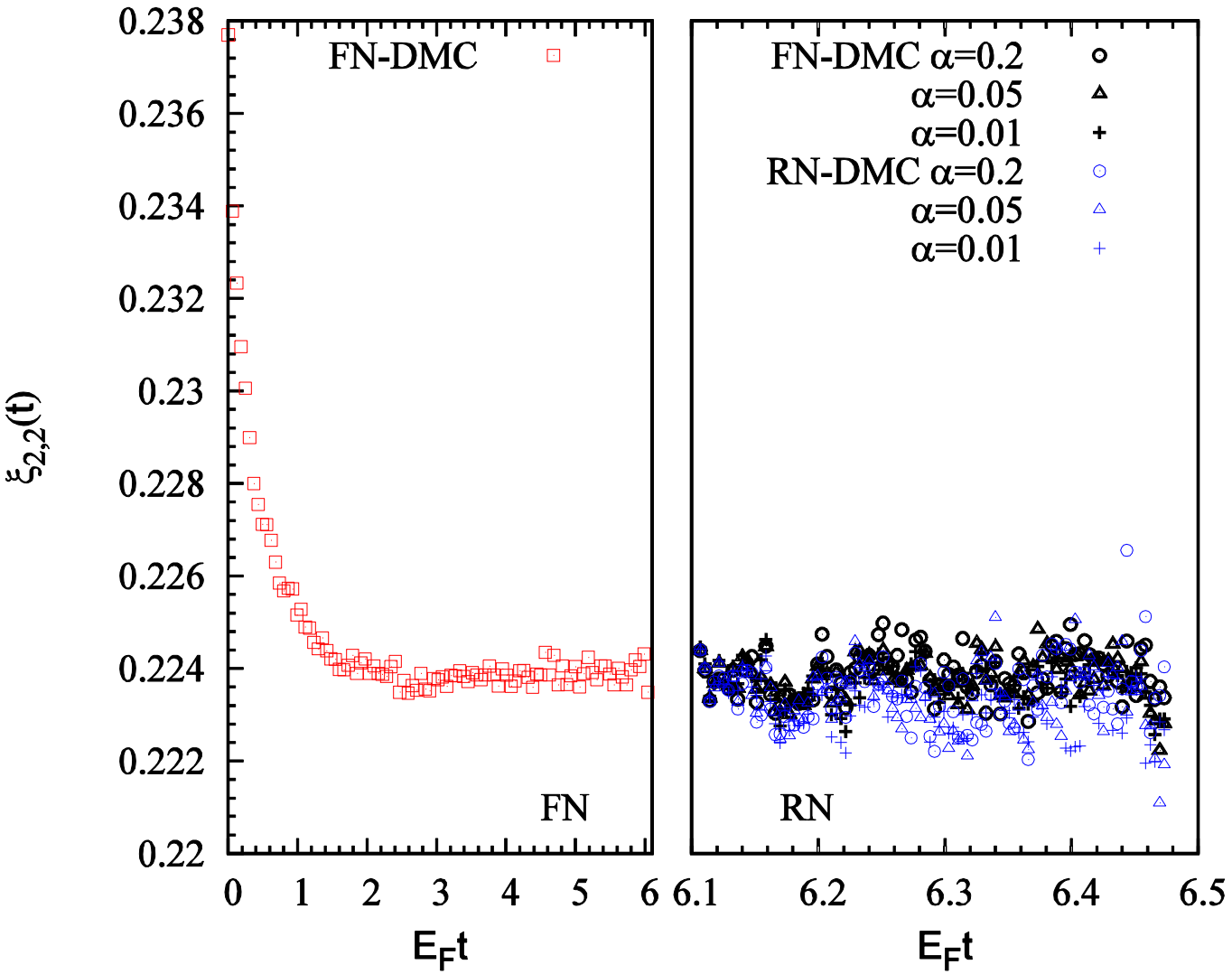
Released-node diffusion Monte Carlo

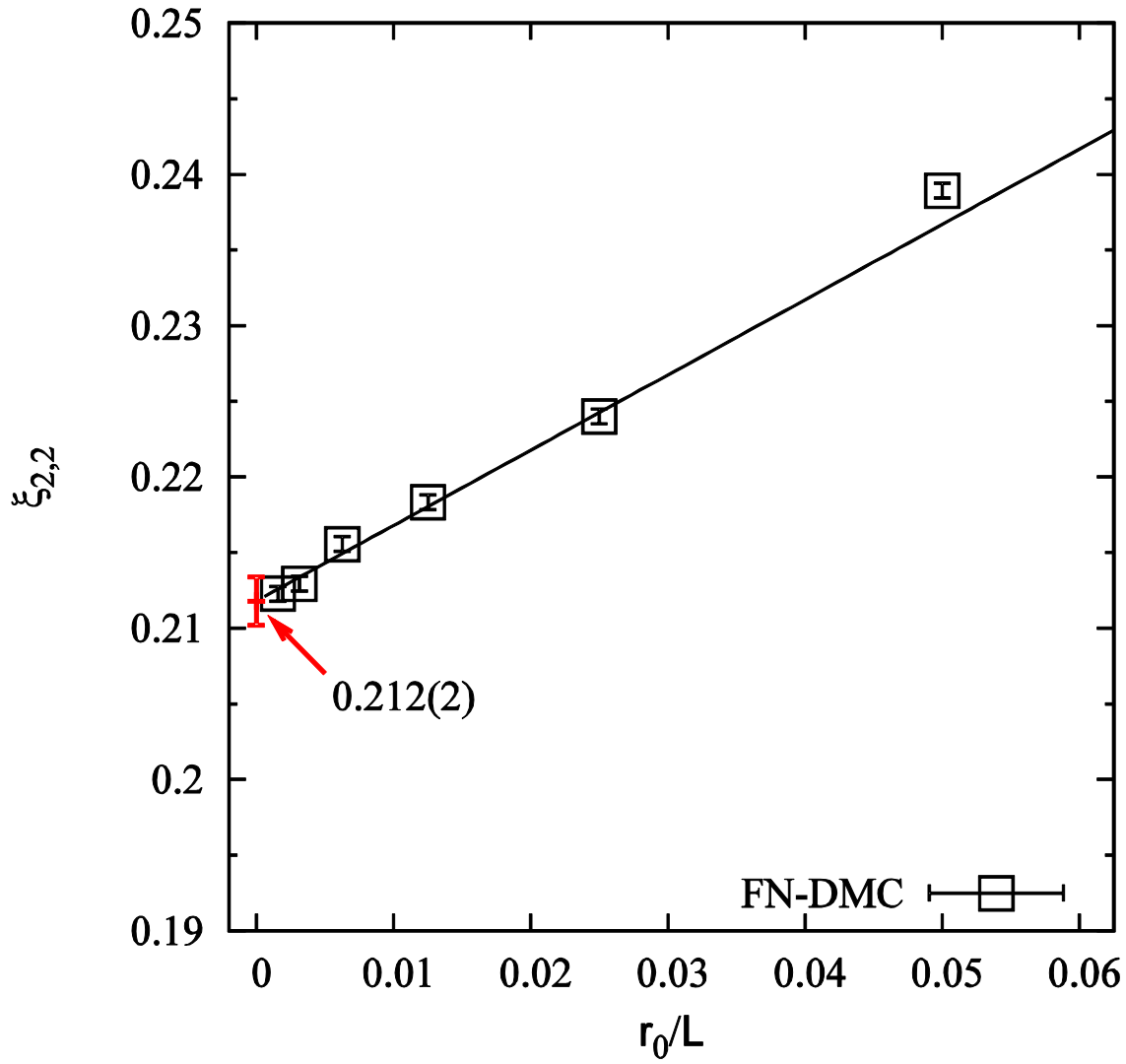


Nodal crossing diffusion time



$r_0/L = 0.025$


FN-DMC
FN
RN
FN-DMC α=0.2
α=0.05
α=0.01
RN-DMC α=0.2
α=0.05
α=0.01
ξ2,2(t)
EFt
EFt
0.238
0.236
0.234
0.232
0.23
0.228
0.226
0.224
0.222
0.22
0
1
2
3
4
5
6
6.1
6.2
6.3
6.4
6.5


0.25
0.24
0.23
0.22
0.21
0.2
0.19
$\xi_{2,2}$
0.212(2)
FN-DMC
0
0.01
0.02
0.03
0.04
0.05
0.06
r_0/L

Summary of benchmark results

Hamiltonian lattice using Lanczos iteration

$$\xi_{2,2} = 0.211(2)\ (H_1) \qquad\qquad \xi_{2,2} = 0.210(2)\ (H_2)$$

Euclidean lattice Monte Carlo

$$\xi_{2,2} = 0.206(9)$$

Fixed-node diffusion Monte Carlo

$$\xi_{2,2} = 0.212(2)$$

Released-node diffusion Monte Carlo

$$0.207(2) \leq \xi_{2,2} \leq 0.212(2)$$