Lattice Methods for Nuclear Physics

Lecture 2: Worldlines and Quantum Fields

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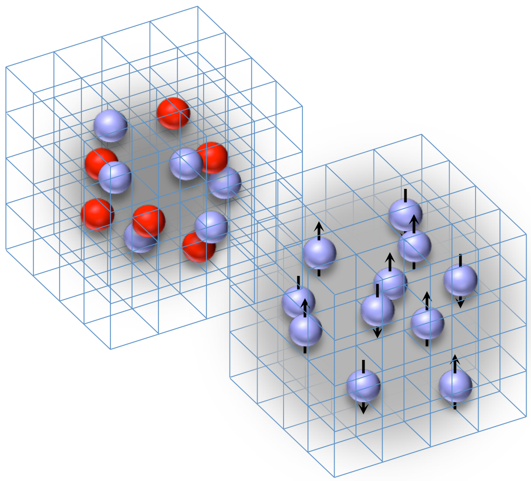
Nuclear Lattice EFT Collaboration



TALENT School
on Nuclear Quantum Monte Carlo Methods
North Carolina State University
July 21, 2016

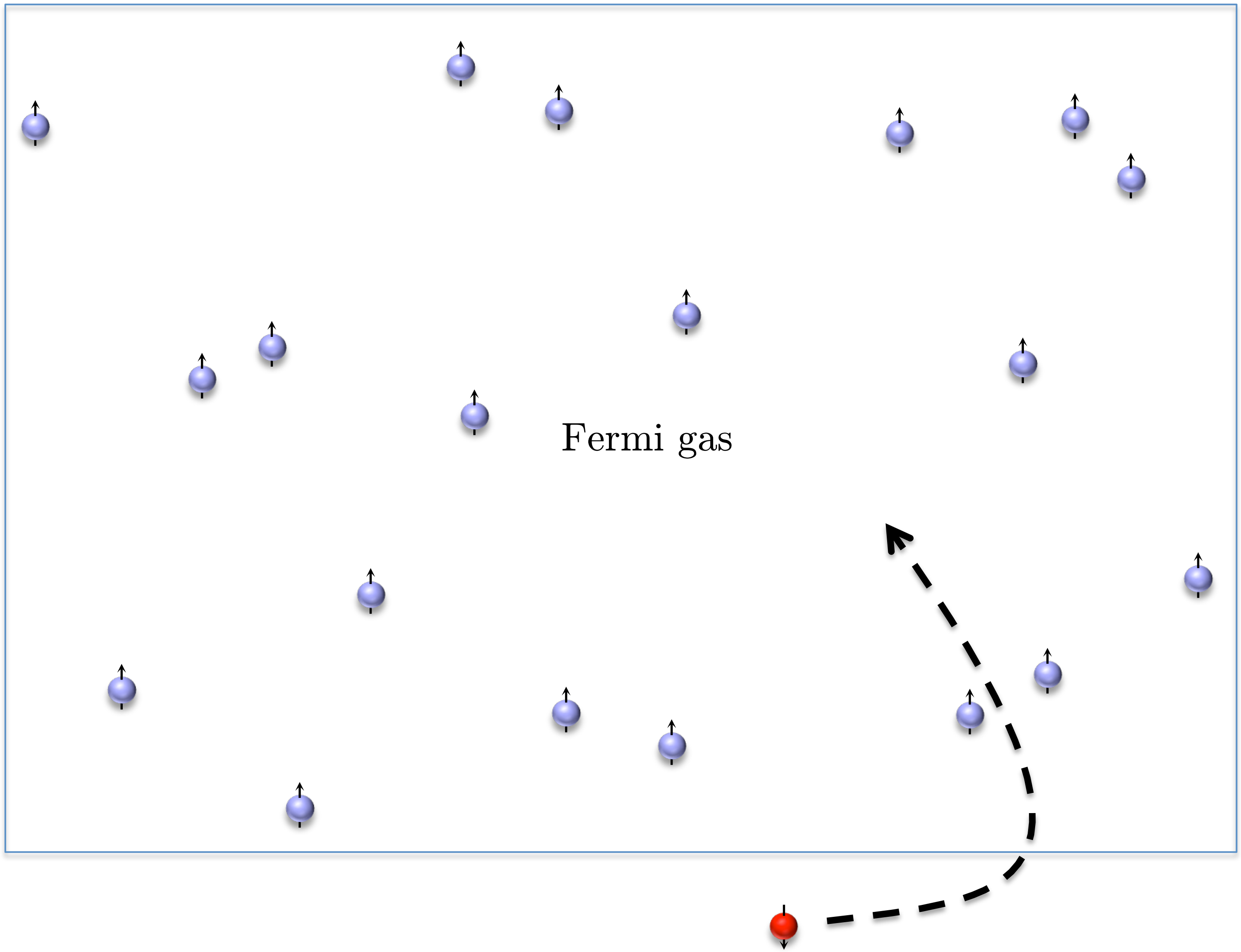
Worldline simulations

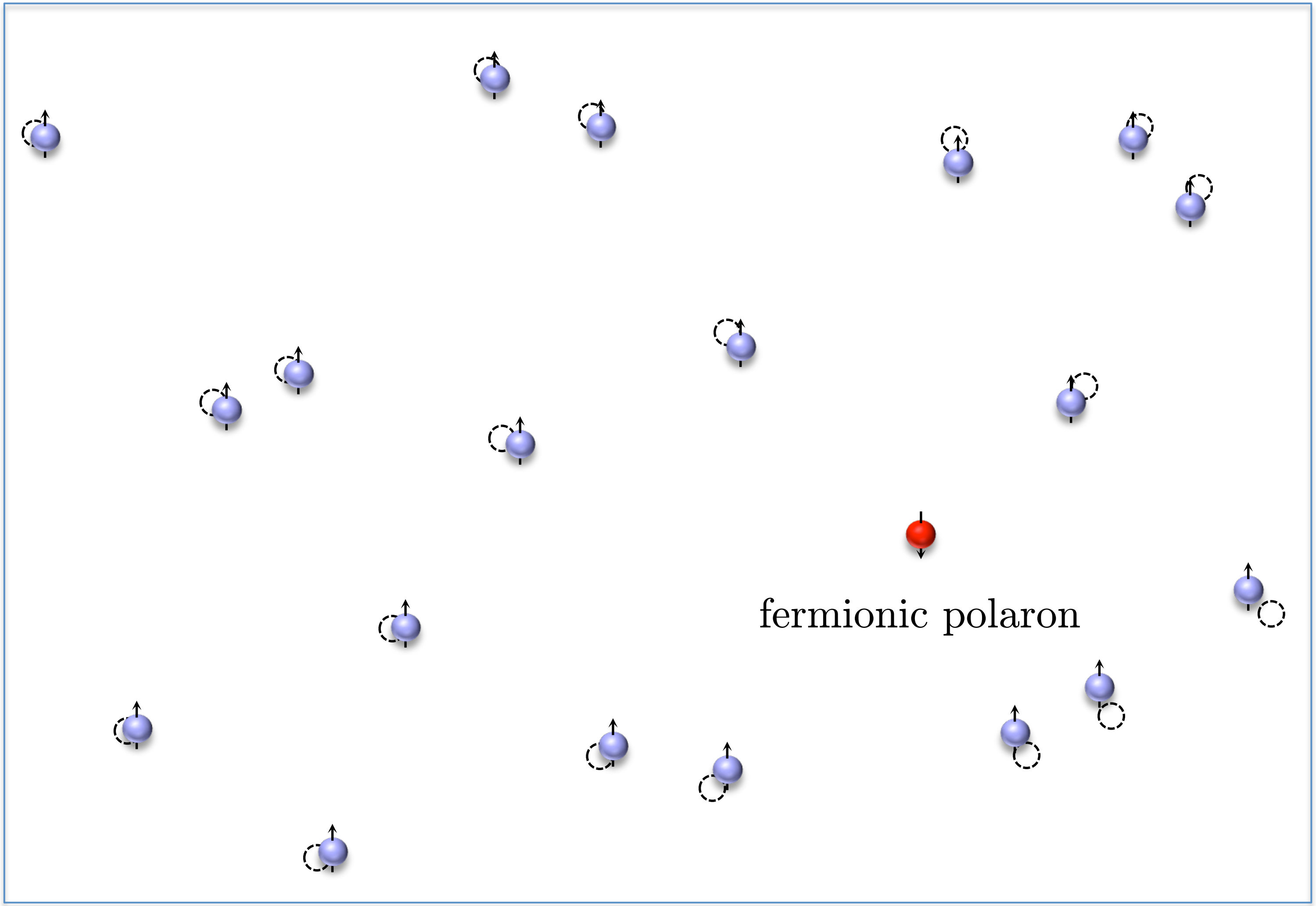
As an example of lattice worldline methods, we discuss a rather new many-body technique called impurity lattice Monte Carlo. Impurity lattice Monte Carlo is a method which treats an impurity in our quantum system by explicit sampling of its lattice worldline. If the other particles in the system have interactions in addition to the coupling to the impurity, then these are treated using auxiliary field Monte Carlo.

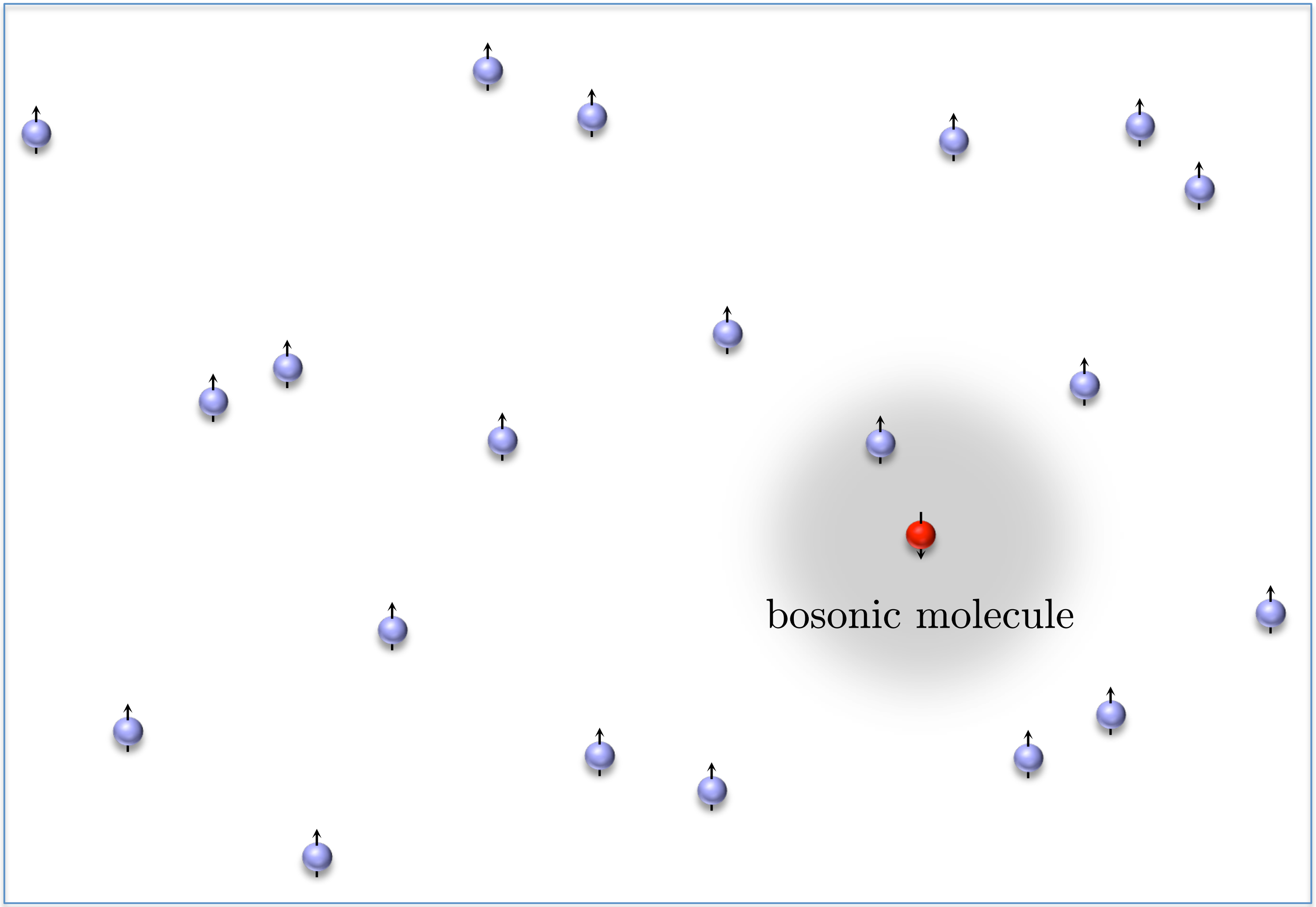
We apply impurity lattice Monte Carlo to the problem of attractive Fermi polarons in two spatial dimensions. We first describe what are attractive Fermi polarons.

Elhatisari, D.L., PRC 90, 064001 (2014)
Bour, D.L, Hammer, Meißner, PRL 115, 185301 (2015)

Attractive Fermi polarons




fermionic polaron


bosonic molecule

Impurity lattice Monte Carlo

Impurity lattice Monte Carlo is a hybrid method which treats the impurity using explicit sampling of its lattice worldline. We demonstrate using two-component fermions in d spatial dimensions with zero-range interactions. The spatial lattice spacing is denoted as a.

$$H_{\text{free}} = H_{\text{free}}^{\uparrow} + H_{\text{free}}^{\downarrow} =$$

$$\frac{-\hbar^2}{2ma^2} \sum_{\mu=1}^{d} \sum_{\vec{n},i=\uparrow,\downarrow} \underbrace{\boxed{a_i^{\dagger}(\vec{n})\left[a_i(\vec{n}+\hat{\mu}) - 2a_i(\vec{n}) + a_i(\vec{n}-\hat{\mu})\right]}}_{\to\, a_i^{\dagger}\partial_{\mu}^2 a_i},$$

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

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

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

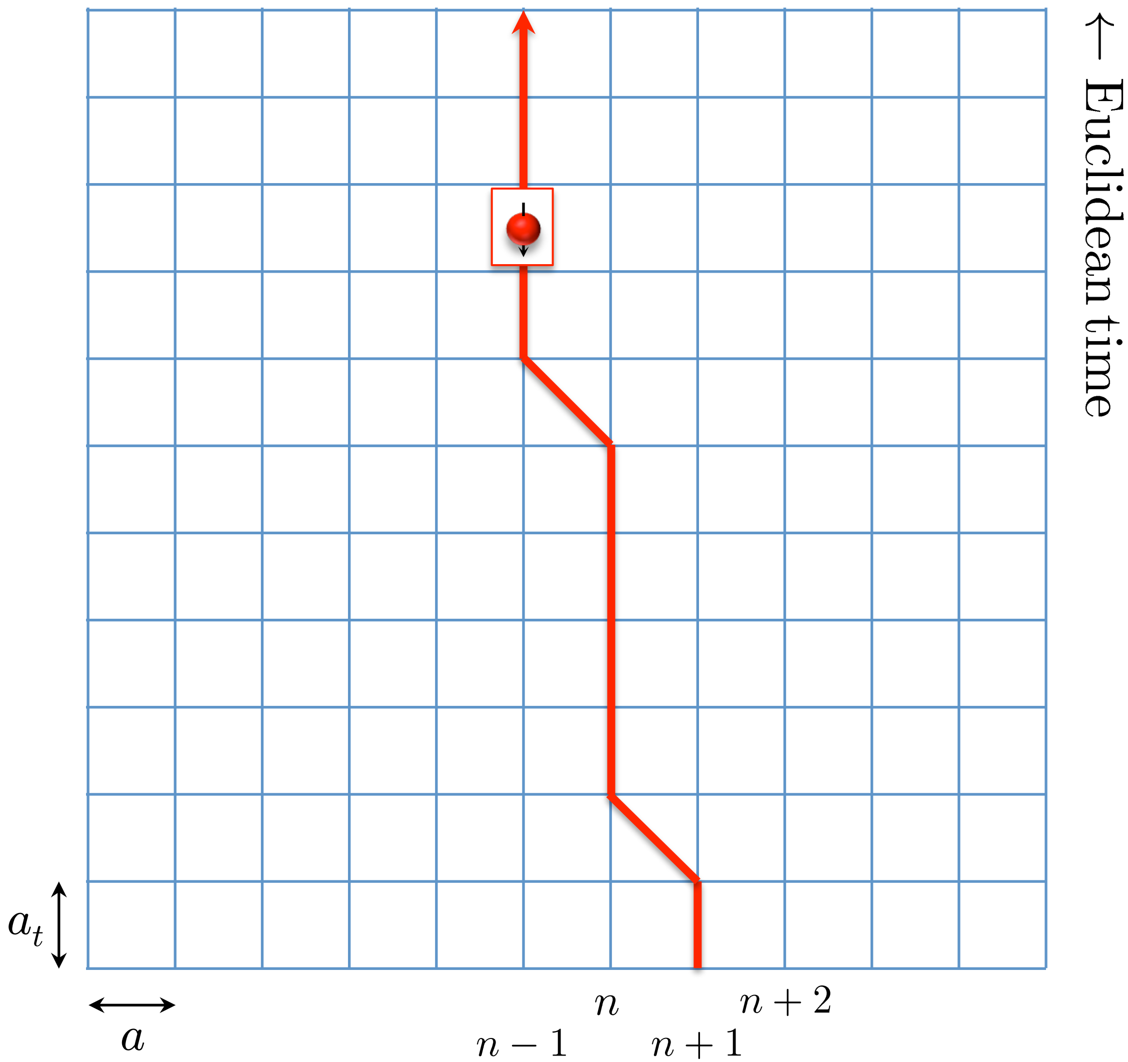
We now consider a system where we have N up-spin particles and just one down-spin particle. Since we only have one down-spin particle we can write the normal-ordered transfer matrix as

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

$$=: (1 - a_t H^{\downarrow}_{\text{free}}/\hbar - a_t C \sum_{\vec{n}} \rho_{\uparrow}(\vec{n})\rho_{\downarrow}(\vec{n})/\hbar)e^{-a_t H^{\uparrow}_{\text{free}}/\hbar} :$$

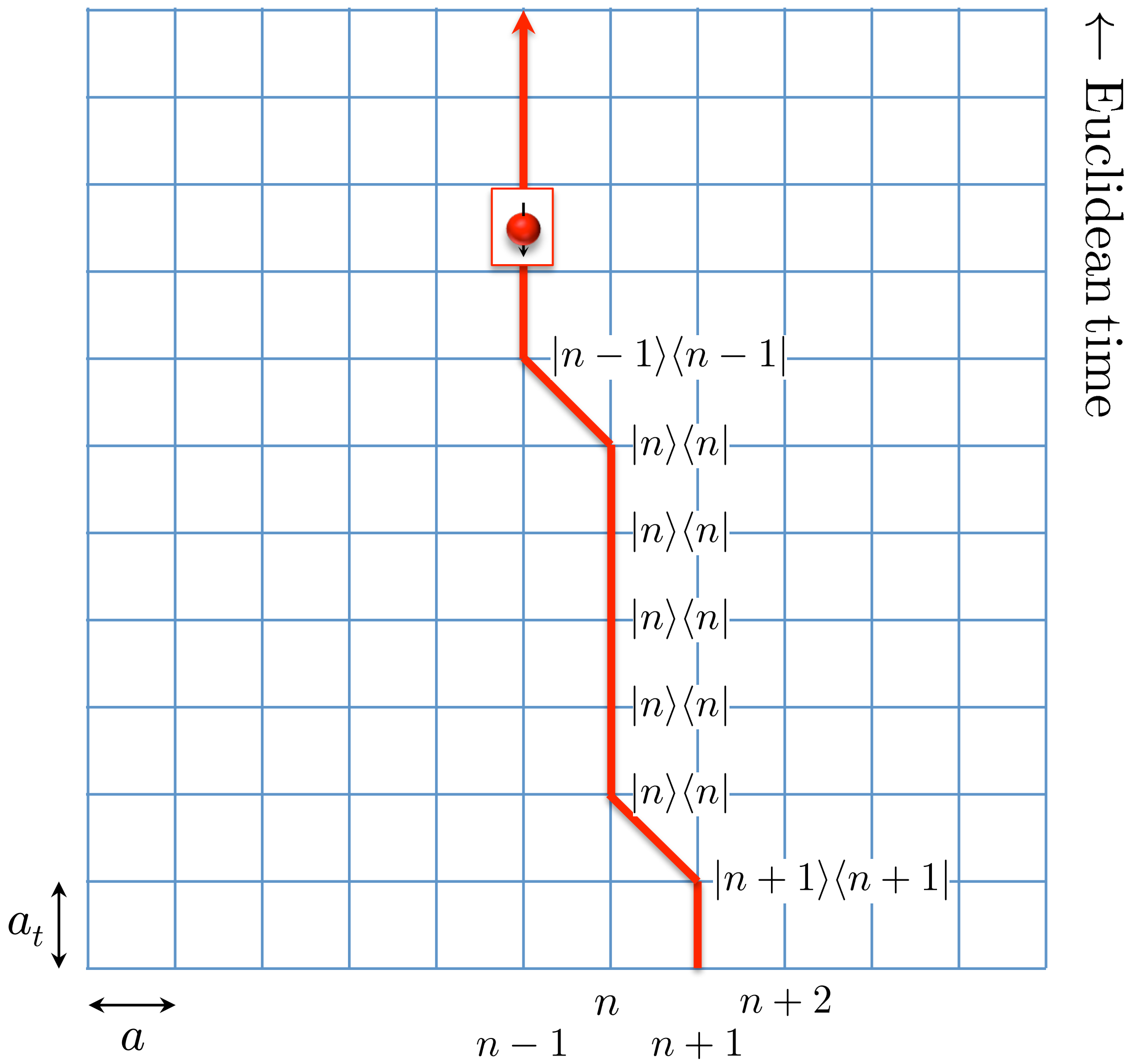
We now consider any worldline for the down-spin particle. For simplicity we show the case for one spatial dimension.

$$M =: (1 - a_t H^{\downarrow}_{\text{free}}/\hbar - a_t C \sum_{\vec{n}} \rho_{\uparrow}(\vec{n})\rho_{\downarrow}(\vec{n})/\hbar) e^{-a_t H^{\uparrow}_{\text{free}}/\hbar} :$$



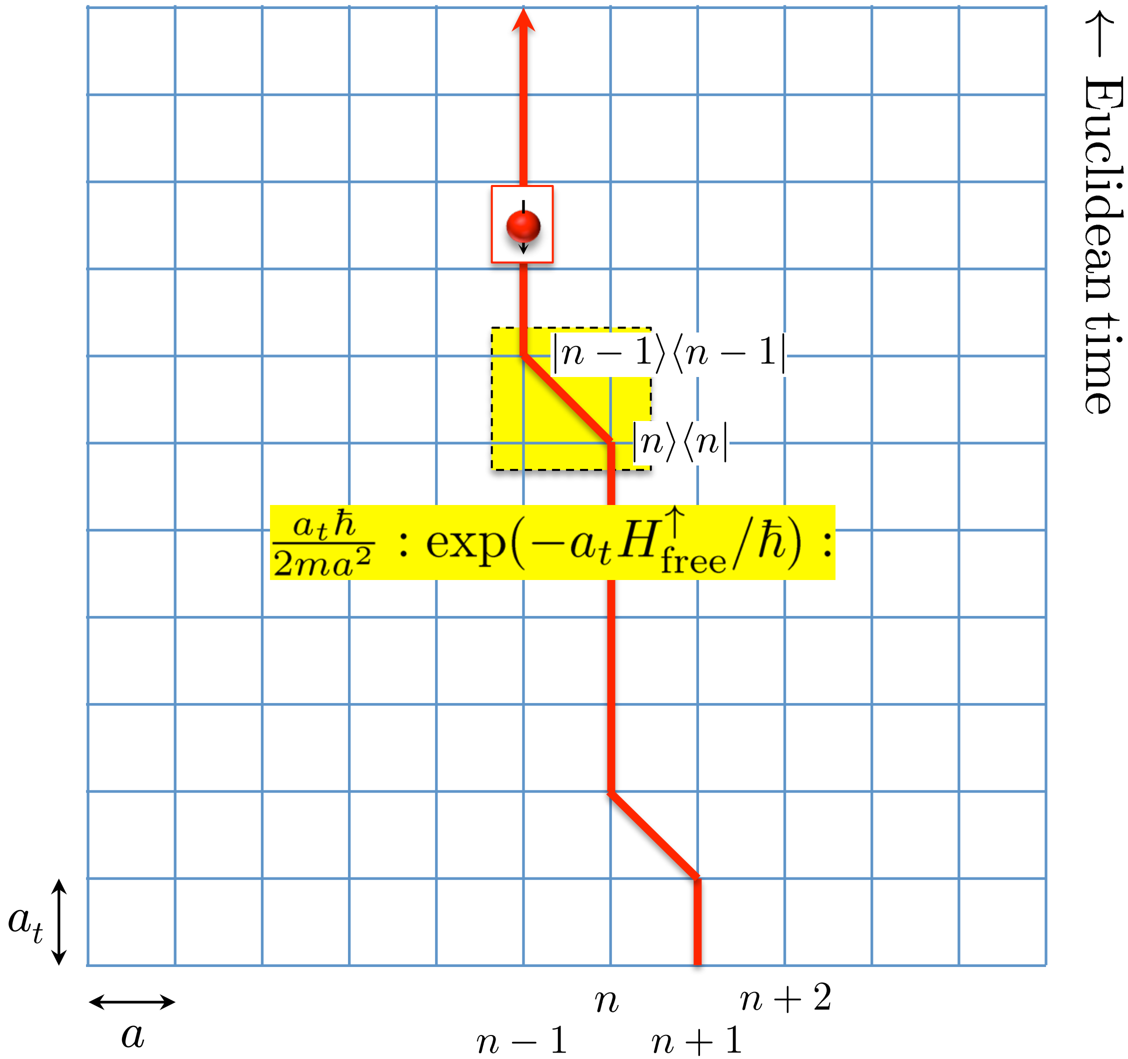
$$H^{\downarrow}_{\text{free}} = \frac{-\hbar^2}{2ma^2} \sum_{\mu=1}^{d} \sum_{\vec{n}} a^{\dagger}_{\downarrow}(\vec{n}) \left[a_{\downarrow}(\vec{n}+\hat{\mu}) - 2a_{\downarrow}(\vec{n}) + a_{\downarrow}(\vec{n}-\hat{\mu}) \right]$$

$$M =: (1 - a_t H_{\text{free}}^{\downarrow}/\hbar - a_t C \sum_{\vec{n}} \rho_{\uparrow}(\vec{n})\rho_{\downarrow}(\vec{n})/\hbar) e^{-a_t H_{\text{free}}^{\uparrow}/\hbar} :$$



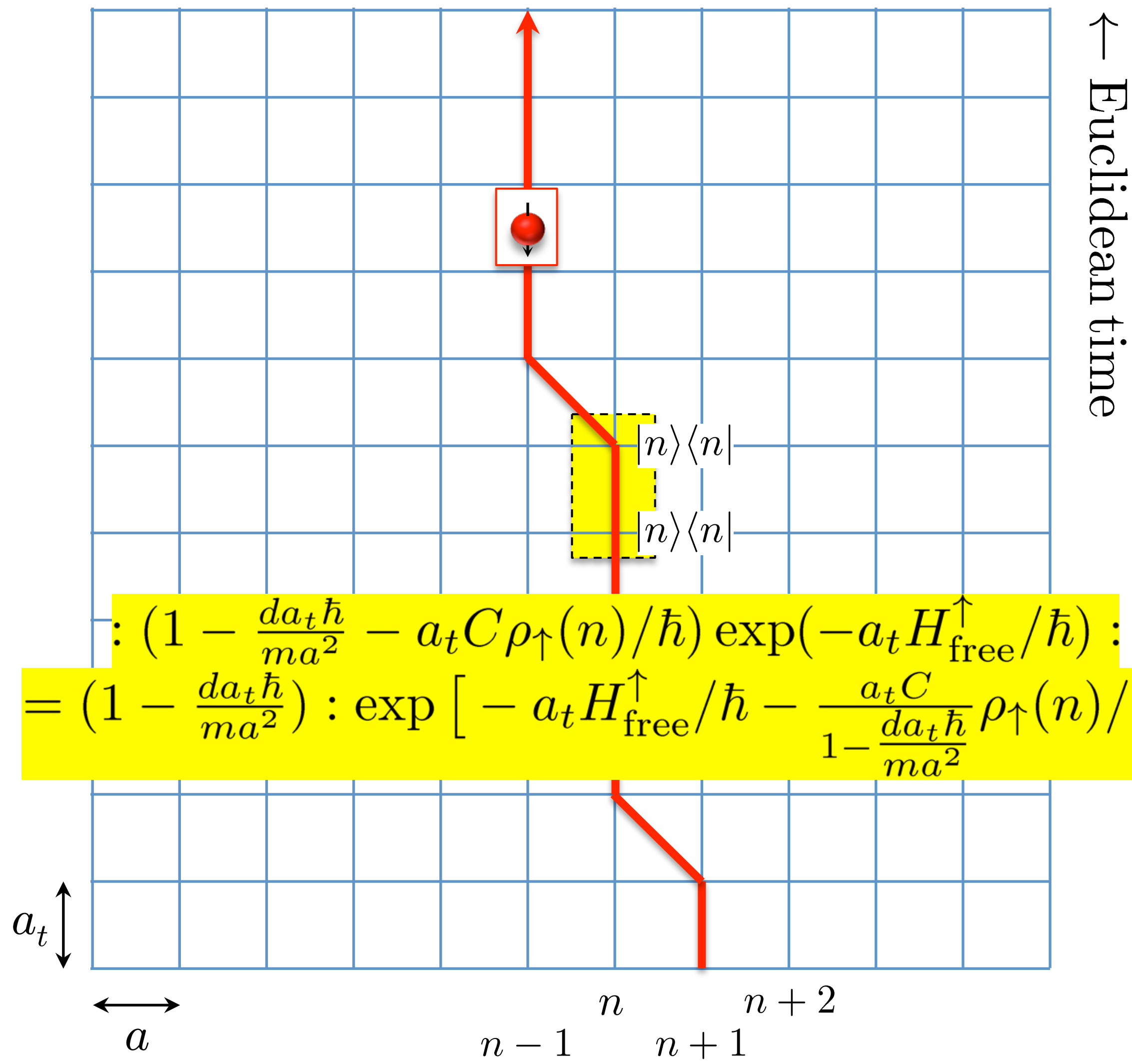
$$H_{\text{free}}^{\downarrow} = \frac{-\hbar^2}{2ma^2} \sum_{\mu=1}^{d} \sum_{\vec{n}} a_{\downarrow}^{\dagger}(\vec{n}) \left[a_{\downarrow}(\vec{n}+\hat{\mu}) - 2a_{\downarrow}(\vec{n}) + a_{\downarrow}(\vec{n}-\hat{\mu}) \right]$$

$$M =: (1 - a_t H^{\downarrow}_{\text{free}}/\hbar - a_t C \sum_{\vec{n}} \rho_{\uparrow}(\vec{n})\rho_{\downarrow}(\vec{n})/\hbar) e^{-a_t H^{\uparrow}_{\text{free}}/\hbar} :$$



$$H^{\downarrow}_{\text{free}} = \frac{-\hbar^2}{2ma^2} \sum_{\mu=1}^{d} \sum_{\vec{n}} a^{\dagger}_{\downarrow}(\vec{n}) \left[a_{\downarrow}(\vec{n}+\hat{\mu}) - 2a_{\downarrow}(\vec{n}) + a_{\downarrow}(\vec{n}-\hat{\mu}) \right]$$

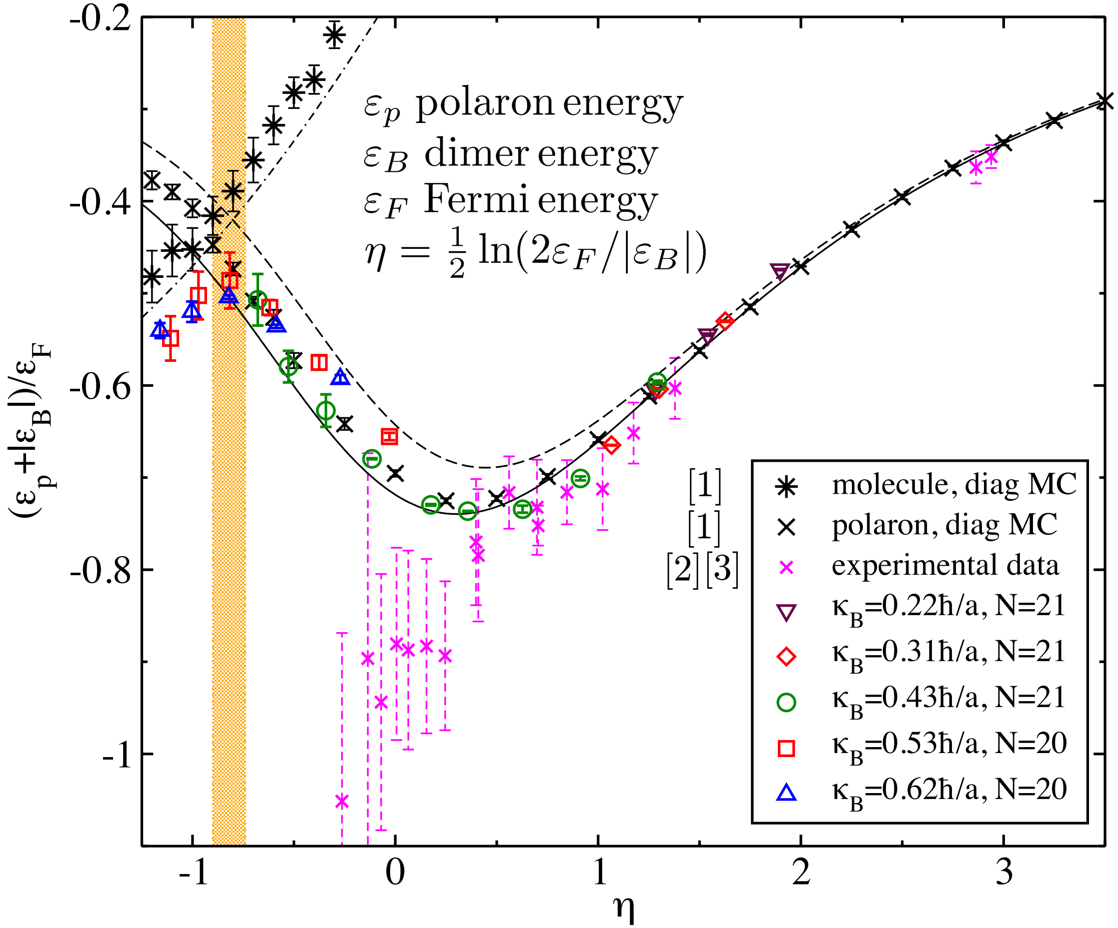
$$M =: (1 - a_t H^{\downarrow}_{\text{free}}/\hbar - a_t C \sum_{\vec{n}} \rho_{\uparrow}(\vec{n})\rho_{\downarrow}(\vec{n})/\hbar) e^{-a_t H^{\uparrow}_{\text{free}}/\hbar} :$$



$$: (1 - \frac{d a_t \hbar}{m a^2} - a_t C \rho_{\uparrow}(n)/\hbar) \exp(-a_t H^{\uparrow}_{\text{free}}/\hbar) :$$

$$= (1 - \frac{d a_t \hbar}{m a^2}) : \exp\left[- a_t H^{\uparrow}_{\text{free}}/\hbar - \frac{a_t C}{1 - \frac{d a_t \hbar}{m a^2}} \rho_{\uparrow}(n)/\hbar \right] :$$

$$H^{\downarrow}_{\text{free}} = \frac{-\hbar^2}{2 m a^2} \sum_{\mu=1}^{d} \sum_{\vec{n}} a^{\dagger}_{\downarrow}(\vec{n}) \left[a_{\downarrow}(\vec{n} + \hat{\mu}) - 2 a_{\downarrow}(\vec{n}) + a_{\downarrow}(\vec{n} - \hat{\mu}) \right]$$



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

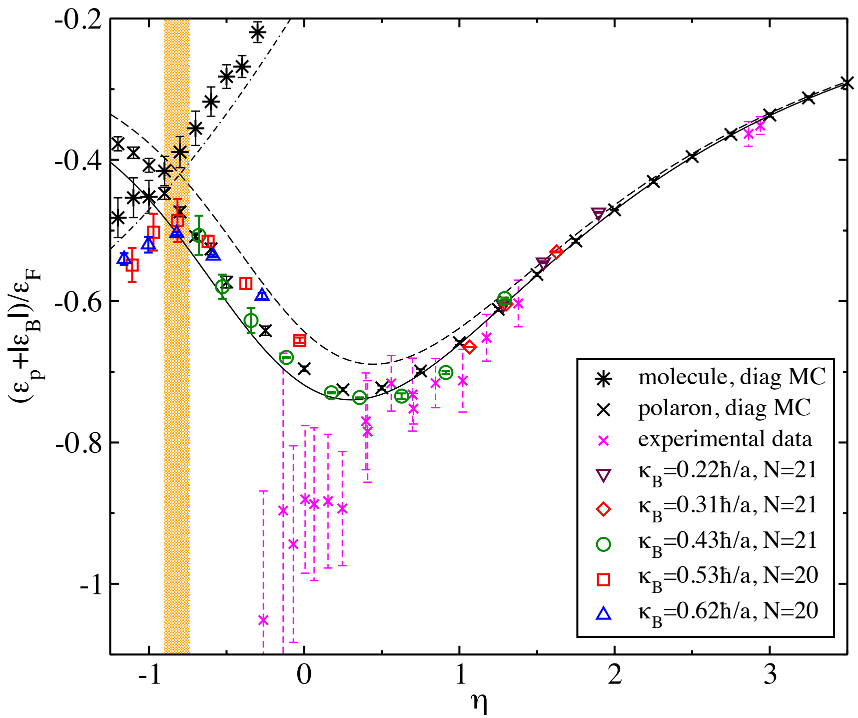
Solid: [5] Polaron variational calculation including two particle-hole pairs

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



Smooth crossover transition at

$$\eta \approx -0.8$$

Bour, D.L, Hammer, Meißner, PRL 115, 185301 (2015)

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

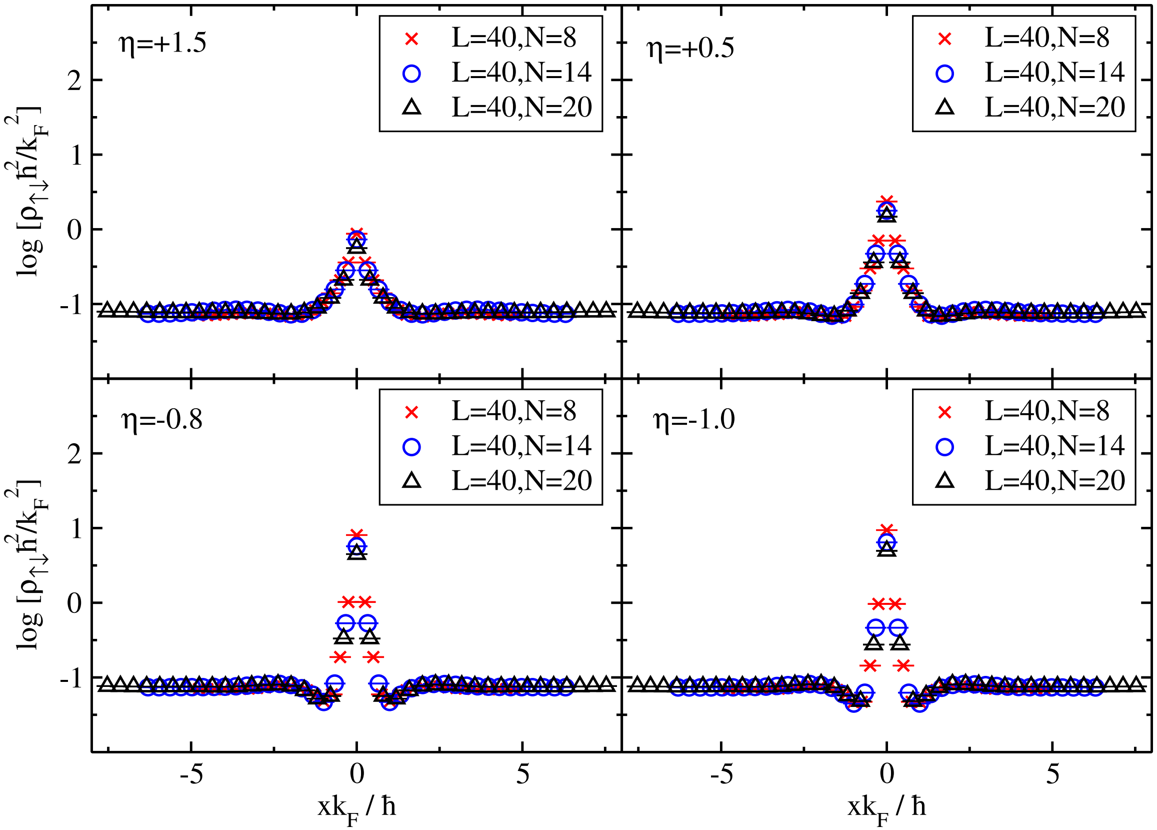
Analysis of experimental data with conversion from quasi 2D to pure 2D gives a transition at

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

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

Density-density correlations

$$\rho_{\uparrow\downarrow}(\vec{r}) = \int d^2r' \, \langle \rho_{\uparrow}(\vec{r}+\vec{r}\,')\rho_{\downarrow}(\vec{r}\,')\rangle$$



Evidence for smooth crossover transition

Bour, D.L, Hammer, Meißner, PRL 115, 185301 (2015)

Free scalar quantum field

We consider a relativistic free scalar quantum field in $3+1$ dimensions, three spatial dimensions plus time. We work in Euclidean space where time t is replaced by Euclidean or imaginary time x_4.

$$x = (\vec{x}, x_4)$$

The Euclidean action for the free scalar field is

$$S_E[\phi] = \frac{1}{2}\int d^4x \phi(x)(-\Box + M^2)\phi(x)$$

where

$$\Box = \sum_\mu \partial_\mu \partial_\mu$$

Rothe, Lattice Gauge Theories, Second Edition,
World Scientific Lecture Notes in Physics, Vol. 59, 1997

We can calculate any expectation value of products of quantum fields by computing the ratio of path (or functional) integrals

$$\langle \phi(x)\phi(y)\cdots\rangle = \frac{\int D\phi\phi(x)\phi(y)\cdots e^{-S_E[\phi]}}{\int D\phi e^{-S_E[\phi]}}$$

where the path integral measure is

$$D\phi = \prod_x d\phi(x)$$

We now put this system on a lattice with periodic boundary conditions

$$L \times L \times L \times L_t \ \text{ lattice}$$

$$x_\mu \to n_\mu a$$

$$\phi(x) \to \phi(na)$$

$$\phi(na + \hat{1}La) = \phi(na)$$

$$\phi(na + \hat{2}La) = \phi(na)$$

$$\phi(na + \hat{3}La) = \phi(na)$$

$$\phi(na + \hat{4}L_t a) = \phi(na)$$

The Euclidean time duration, $L_t a$, will be the inverse temperature β. On the lattice we also make the replacements

$$\int d^4x \to a^4 \sum_n$$

$$D\phi(x) \to \prod_n d\phi(na)$$

$$\Box\phi(x) \to \frac{1}{a^2}\hat{\Box}\phi(na)$$

where

$$\hat{\Box}\phi(na) = \sum_\mu (\phi(na + \hat{\mu}a) - 2\phi(na) + \phi(na - \hat{\mu}a))$$

To simplify the notation further we redefine the fields and mass parameter multiplied by the lattice spacing to render it dimensionless.

$$\hat{\phi}_n = a\phi(na)$$

$$\hat{M} = aM$$

Then the expectation value of products of quantum fields can be written as

$$\langle \hat{\phi}_n \hat{\phi}_m \cdots \rangle = \frac{\int \prod_l d\hat{\phi}_l \hat{\phi}_n \hat{\phi}_m \cdots e^{-S_E[\hat{\phi}]}}{\int \prod_l d\hat{\phi}_l e^{-S_E[\hat{\phi}]}}$$

where

$$S_E = -\sum_{n,\mu} \hat{\phi}_n \hat{\phi}_{n+\hat{\mu}} + \frac{1}{2}(8 + \hat{M}^2) \sum_n \hat{\phi}_n \hat{\phi}_n$$

We can also write

$$S_E = \frac{1}{2} \sum_{n,m} \hat{\phi}_n K_{n,m} \hat{\phi}_m$$

where

$$K_{n,m} = -\sum_{\mu}[\delta_{n+\hat{\mu},m} + \delta_{n-\hat{\mu},m} - 2\delta_{n,m}] + \hat{M}^2\delta_{n,m}$$

Using this notation, the two-field expectation value called the Euclidean propagator is given by

$$\langle\hat{\phi}_n\hat{\phi}_m\rangle = \frac{\int\prod_l d\hat{\phi}_l\hat{\phi}_n\hat{\phi}_m e^{-\frac{1}{2}\sum_{n,m}\hat{\phi}_n K_{n,m}\hat{\phi}_m}}{\int\prod_l d\hat{\phi}_l e^{-\frac{1}{2}\sum_{n,m}\hat{\phi}_n K_{n,m}\hat{\phi}_m}}$$

$K_{n,m}$ is a symmetric positive-definite matrix which only depends on the vector difference $n - m$. We can compute the square root and define

$$\hat{\phi}'_n = \sum_m K^{\frac{1}{2}}_{n,m}\hat{\phi}_m$$

We can also invert to get

$$\hat{\phi}_n = \sum_m K_{n,m}^{-\frac{1}{2}} \hat{\phi}'_m$$

We now do a change of variables in the path integration and get

$$\langle \hat{\phi}_n \hat{\phi}_m \rangle = \frac{\int \prod_l d\hat{\phi}_l \hat{\phi}_n \hat{\phi}_m e^{-\frac{1}{2}\sum_{n,m} \hat{\phi}_n K_{n,m} \hat{\phi}_m}}{\int \prod_l d\hat{\phi}_l e^{-\frac{1}{2}\sum_{n,m} \hat{\phi}_n K_{n,m} \hat{\phi}_m}}$$

$$= \frac{\int \prod_l d\hat{\phi}'_l \sum_{n'} K_{n,n'}^{-\frac{1}{2}} \hat{\phi}'_{n'} \sum_{m'} K_{m,m'}^{-\frac{1}{2}} \hat{\phi}'_{m'} e^{-\frac{1}{2}\sum_j \hat{\phi}'_j \hat{\phi}'_j}}{\int \prod_l d\hat{\phi}'_l e^{-\frac{1}{2}\sum_j \hat{\phi}'_j \hat{\phi}'_j}}$$

It is straightforward to calculate the second moments of this simple Gaussian distribution

$$\frac{\int \prod_l d\hat{\phi}'_l \hat{\phi}'_{n'} \hat{\phi}'_{m'} e^{-\frac{1}{2}\sum_j \hat{\phi}'_j \hat{\phi}'_j}}{\int \prod_l d\hat{\phi}'_l e^{-\frac{1}{2}\sum_j \hat{\phi}'_j \hat{\phi}'_j}} = \delta_{n',m'}$$

The Euclidean propagator is then

$$\langle \hat{\phi}_n \hat{\phi}_m \rangle = \sum_{n'} K^{-\frac{1}{2}}_{n,n'} K^{-\frac{1}{2}}_{m,n'} = \sum_{n'} K^{-\frac{1}{2}}_{n,n'} K^{-\frac{1}{2}}_{n',m} = K^{-1}_{n,m}$$

In order to compute this inverse matrix, we first compute the Fourier transform of

$$K_{n,m} = -\sum_{\mu} [\delta_{n+\hat{\mu},m} + \delta_{n-\hat{\mu},m} - 2\delta_{n,m}] + \hat{M}^2 \delta_{n,m}$$

and get the momentum-space function

$$\begin{aligned} \tilde{K}(k) = \sum_l K_{m+l,m} e^{-ik\cdot l} &= -\sum_{\mu} [e^{-ik\cdot\hat{\mu}} + e^{+ik\cdot\hat{\mu}} - 2] + \hat{M}^2 \\ &= 2\sum_{\mu} [1 - \cos(k_\mu)] + \hat{M}^2 \end{aligned}$$

The allowed momentum modes on the lattice in our periodic box are

$$k_1 = 0, 2\pi/L, 4\pi/L, \cdots 2(L-1)\pi/L$$

$$k_2 = 0, 2\pi/L, 4\pi/L, \cdots 2(L-1)\pi/L \quad k_4 = 0, 2\pi/L_t, 4\pi/L_t, \cdots 2(L_t-1)\pi/L_t$$

$$k_3 = 0, 2\pi/L, 4\pi/L, \cdots 2(L-1)\pi/L$$

To convert back to coordinate space, we compute the inverse Fourier transform

$$K_{n,m} = \frac{1}{L^3 L_t} \sum_k \tilde{K}(k) e^{ik\cdot(n-m)}$$

and we can construct the inverse matrix as

$$K^{-1}_{n,m} = \frac{1}{L^3 L_t} \sum_k \frac{1}{\tilde{K}(k)} e^{ik\cdot(n-m)}$$

We can check that this definition is in fact the matrix inverse

$$\sum_l K^{-1}_{n,l} K_{l,m} = \frac{1}{L^3 L_t} \sum_l \sum_k \frac{1}{\tilde{K}(k)} e^{ik\cdot(n-l)} \frac{1}{L^3 L_t} \sum_{k'} \tilde{K}(k') e^{ik'\cdot(l-m)}$$

$$= \frac{1}{L^3 L_t} \sum_k \frac{1}{\tilde{K}(k)} \tilde{K}(k) e^{ik\cdot(n-m)}$$

$$= \frac{1}{L^3 L_t} \sum_k e^{ik\cdot(n-m)} = \delta_{n,m}$$

We conclude that the Euclidean propagator is

$$\langle \hat{\phi}_n \hat{\phi}_m \rangle = K^{-1}_{n,m} = \frac{1}{L^3 L_t} \sum_k \frac{1}{2\sum_\mu [1-\cos(k_\mu)] + \hat{M}^2} e^{ik\cdot(n-m)}$$

Exercise 3

Use a Markov chain Monte Carlo simulation to compute the Euclidean propagator for a real scalar field on the lattice in $3+1$ dimensions.

$$\langle \hat{\phi}_n \hat{\phi}_m \rangle = \frac{\int \prod_l d\hat{\phi}_l \hat{\phi}_n \hat{\phi}_m e^{-S_E[\hat{\phi}]}}{\int \prod_l d\hat{\phi}_l e^{-S_E[\hat{\phi}]}}$$

$$S_E = -\sum_{n,\mu} \hat{\phi}_n \hat{\phi}_{n+\hat{\mu}} + \frac{1}{2}(8 + \hat{M}^2) \sum_n \hat{\phi}_n \hat{\phi}_n$$

Take the size of the periodic box to be $L = L_t = 10$ and also set

$$\hat{M} = 1$$

Check that your simulation gives the same result as the expression we had derived analytically

$$\langle \hat{\phi}_n \hat{\phi}_m \rangle = \frac{1}{L^3 L_t} \sum_k \frac{1}{2\sum_\mu [1-\cos(k_\mu)] + \hat{M}^2} e^{ik\cdot(n-m)}$$

for the cases where the separation between n and m is pointing along the x-axis:

$$n - m = 0, 1\hat{1}, 2\hat{1}, \cdots (L-1)\hat{1}$$