Lattice Methods for Nuclear Physics

Lecture 4: Chiral Effective Field Theory on the Lattice I

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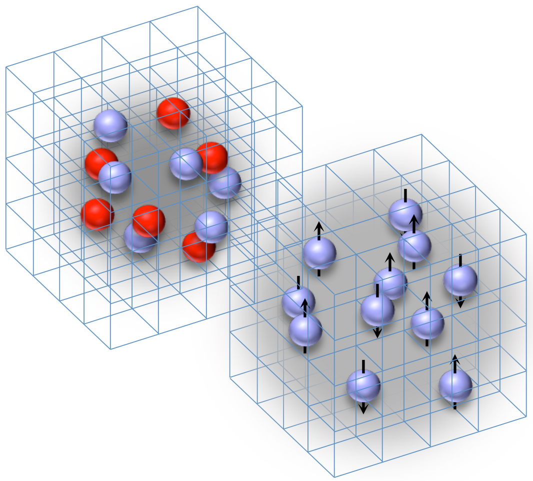

TALENT School
on Nuclear Quantum Monte Carlo Methods
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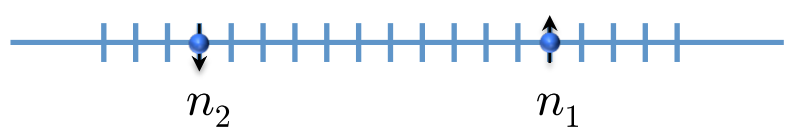
Example: Two fermions in one-dimension

Let us consider a system with one up-spin particle and one down-spin particle on a one-dimensional periodic lattice with L sites. For the interactions we choose zero-range attractive interactions as we discussed previously. We can label the two-body system with a basis corresponding with the positions of the particles.

$$|n_1, n_2\rangle$$



The transfer matrix has the form

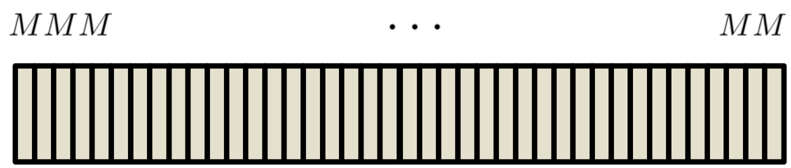
$$M =: \exp\left[-H_{\text{free}}\alpha_t - C\alpha_t \sum_{n_x} \rho_{\uparrow}(n_x)\rho_{\downarrow}(n_x)\right]:$$

where the free lattice Hamiltonian in its simplest possible form is

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

$$= -\frac{1}{2m} \sum_{n_x, i=\uparrow,\downarrow} a_i^{\dagger}(n_x)\big[a_i(n_x+1) - 2a_i(n_x) + a_i(n_x-1)\big]$$

We compute the projection amplitude

$$Z(L_t) = \langle \psi_{\text{init}}|$$


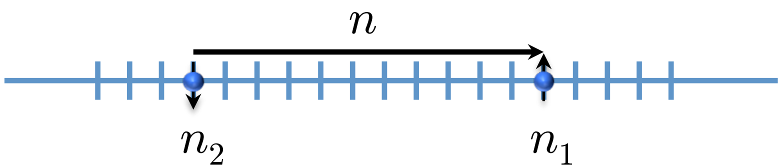
$$|\psi_{\text{init}}\rangle$$

in order to get the ground state energy in the subspace that is not orthogonal to our initial state

$$\lim_{L_t \to +\infty} Z(L_t)/Z(L_t-1) = \lambda_{\max} = e^{-E_0 \alpha_t}$$

Since the system has translational symmetry, we can set the total momentum to zero and label only the relative separation between the two particles

$$|n\rangle = \frac{1}{\sqrt{L}} \sum_{m=0}^{L-1} |n+m, m\rangle$$



We need to compute the action of the transfer matrix on such states

$$M|n\rangle = \left[(1 - H_{\text{free}}^{\uparrow}\alpha_t)(1 - H_{\text{free}}^{\downarrow}\alpha_t) - C\alpha_t \sum_{n_x} \rho_{\uparrow}(n_x)\rho_{\downarrow}(n_x)\right] |n\rangle$$

The matrix elements of interest are

$$\langle n'|H_{\text{free}}^{\uparrow}|n\rangle = \langle n'|H_{\text{free}}^{\downarrow}|n\rangle = -\frac{1}{2m}\delta_{n',n+1} - \frac{1}{2m}\delta_{n',n-1} + \frac{2}{2m}\delta_{n',n}$$

$$\langle n'| \sum_{n_x} \rho_{\uparrow}(n_x)\rho_{\downarrow}(n_x)|n\rangle = \delta_{n',0}\delta_{n,0}$$

As an example we take the initial state to have zero relative momentum (in addition to the total momentum being zero).

$$|\psi_{\rm init}\rangle = \frac{1}{\sqrt{L}} \sum_n |n\rangle$$

We can then compute products of the transfer matrix acting upon the initial state

$$|v(n_t)\rangle = M^{n_t} |\psi_{\rm init}\rangle$$

and determine the amplitude

$$Z(L_t) = \langle \psi_{\rm init} | M^{L_t} | \psi_{\rm init} \rangle = \langle \psi_{\rm init} | v(L_t) \rangle$$

```fortran
      do nx = 0,L-1
         vrel(nx,0) = 1.D0/dsqrt(1.D0*L)
      enddo
      overlap(0) = 1.D0

      do nt = 1,Lt
         do nx = 0,L-1
            temp(nx) =
     $           vrel(nx,nt-1)*(1.D0 - 1.D0/am*alphat)
     $           + vrel(mod(nx-1+L,L),nt-1)/(2.D0*am)*alphat
     $           + vrel(mod(nx+1,L),nt-1)/(2.D0*am)*alphat
         enddo
         do nx = 0,L-1
            vrel(nx,nt) =
     $           temp(nx)*(1.D0 - 1.D0/am*alphat)
     $           + temp(mod(nx-1+L,L))/(2.D0*am)*alphat
     $           + temp(mod(nx+1,L))/(2.D0*am)*alphat
         enddo
         vrel(0,nt) = vrel(0,nt) - c*alphat*vrel(0,nt-1)
         overlap(nt) = 0.D0
         do nx = 0,L-1
            overlap(nt) = overlap(nt) + vrel(nx,nt)/dsqrt(1.D0*L)
         enddo
      enddo
```

$$M|n\rangle = \left[(1-H^{\uparrow}_{\text{free}}\alpha_t)(1-H^{\downarrow}_{\text{free}}\alpha_t) - C\alpha_t \textstyle\sum_{n_x} \rho_{\uparrow}(n_x)\rho_{\downarrow}(n_x)\right]|n\rangle$$

$$Z(L_t) = \langle\psi_{\text{init}}|M^{L_t}|\psi_{\text{init}}\rangle = \langle\psi_{\text{init}}|v(L_t)\rangle$$

$$e^{-E(L_t)\alpha_t} = Z(L_t)/Z(L_t - 1)$$

L_t	Energy (MeV)
30	-17.6412
31	-17.7085
32	-17.7650
33	-17.8125
34	-17.8523
35	-17.8856
36	-17.9135
37	-17.9369
38	-17.9564
39	-17.9728
40	-17.9864
41	-17.9978
42	-18.0074
43	-18.0153
44	-18.0220
45	-18.0275
46	-18.0322
47	-18.0360
48	-18.0393
49	-18.0420
50	-18.0442

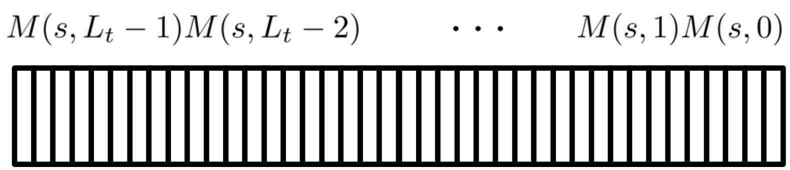
For $L = 6$, $C = -0.200$, $m = 938.92$ MeV, $a = a_t = (100 \text{ MeV})^{-1}$

We can calculate the same observables using auxiliary field Monte Carlo. The amplitude we want to calculate is

$$Z(L_t) = \prod_{\vec{n},n_t} \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} ds(n_x, n_t) e^{-\frac{1}{2}s^2(n_x,n_t)} \right] Z(s, L_t)$$

where the auxiliary field amplitude is

$Z(s, L_t) = \langle \psi_{\text{init}} |$



$| \psi_{\text{init}} \rangle$

and the auxiliary field transfer matrix given by

$$M(s, n_t) =: \exp \left\{ -H_{\text{free}} \alpha_t + \textstyle\sum_{n_x} \sqrt{-C\alpha_t} s(n_x, n_t) \rho(n_x) \right\} :$$

For our initial state we again choose both the up and down spin particles to have zero momentum

$$|\psi_{\text{init}}\rangle = \tfrac{1}{L}\sum_{n_1=0}^{L-1}\sum_{n_2=0}^{L-1}|n_1, n_2\rangle$$

We should note that this is not an efficient starting point to reach the ground state, but it is a simple initial state we can use to benchmark the Monte Carlo code with the exact transfer matrix calculation.

In terms of our single-particle initial state coefficient functions f_1 and f_2, we have

$$|\psi_{\text{init}}\rangle = |f_1, f_2\rangle = \left[\sum_{n_x,i} a_i^\dagger(n_x) f_1(n_x,i)\right]\left[\sum_{n_x,i} a_i^\dagger(n_x) f_2(n_x,i)\right]|0\rangle$$

$$f_1(n_x,i) = \delta_{i,\uparrow}\frac{1}{\sqrt{L}}$$

$$f_2(n_x,i) = \delta_{i,\downarrow}\frac{1}{\sqrt{L}}$$

We store the set of vectors for each single-particle initial state at each time step

$$|v_j(s,n_t)\rangle = M(s,n_t-1)\cdots M(s,0)|f_j\rangle$$

as well as the dual vectors at each time step propagating in the reverse temporal direction

$$\langle v_i(s,n_t)| = \langle f_i|M(s,L_t-1)\cdots M(s,n_t)$$

These are useful in computing the update to an auxiliary field value at time step n_t, using the following relation:

$$\mathbf{Z}_{i,j}(s,L_t) = \langle v_i(s,n_t+1)|M(s,n_t)|v_j(s,n_t)\rangle$$

$$Z(s,L_t) = \det \mathbf{Z}(s,L_t)$$

change here
and re-evaluate

```fortran
      dimension v(0:L-1,0:Lt)
      dimension dualv(0:L-1,0:Lt)

          :

      accept = 0.D0
      ratio_bin = 0.D0

c     since we have the same initial vector for both up
c     and down spins and the auxiliary-field transfer matrix
c     is independent of spin, we can use the same single-particle
c     states for up and down spins

      do nx = 0,L-1
         v(nx,0) = 1.D0/dsqrt(1.D0*L)
         dualv(nx,Lt) = 1.D0/dsqrt(1.D0*L)
      enddo
```

```
      subroutine getv(v,s,ntm,ntp,c,am,alphat,L,Lt)

      implicit integer(i-n)
      implicit double precision(a-h,o-y)
      implicit complex*16(z)
      dimension v(0:L-1,0:Lt)
      dimension s(0:L-1,0:Lt-1)

      do nt = ntm+1,ntp
         do nx = 0,L-1
            v(nx,nt) =
     $           v(nx,nt-1)*(1.D0 - 1.D0/am*alphat
     $           + dsqrt(-c*alphat)*s(nx,nt-1))
     $           + v(mod(nx-1+L,L),nt-1)/(2.D0*am)*alphat
     $           + v(mod(nx+1,L),nt-1)/(2.D0*am)*alphat
         enddo
      enddo

      return
      end
```

$$M(s,n_t-1) =: \exp\left\{-H_{\text{free}}\alpha_t + \textstyle\sum_{n_x}\sqrt{-C\alpha_t}\,s(n_x,n_t-1)\rho(n_x)\right\}:$$

```fortran
      subroutine getdualv(dualv,s,ntm,ntp,c,am,alphat,L,Lt)

      implicit integer(i-n)
      implicit double precision(a-h,o-y)
      implicit complex*16(z)
      dimension dualv(0:L-1,0:Lt)
      dimension s(0:L-1,0:Lt-1)

      do nt = ntp,ntm+1,-1
         do nx = 0,L-1
            dualv(nx,nt-1) =
     $           dualv(nx,nt)*(1.D0 - 1.D0/am*alphat
     $           + dsqrt(-c*alphat)*s(nx,nt-1))
     $           + dualv(mod(nx-1+L,L),nt)/(2.D0*am)*alphat
     $           + dualv(mod(nx+1,L),nt)/(2.D0*am)*alphat
         enddo
      enddo

      return
      end
```

$$M(s,n_t-1) =: \exp\left\{-H_{\mathrm{free}}\alpha_t + \sum_{n_x}\sqrt{-C\alpha_t}\,s(n_x,n_t-1)\rho(n_x)\right\}:$$

We initialize the auxiliary field configuration s, and compute the bosonic part of the action

$$\sum_{n_x,n_t} \tfrac{1}{2} s^2(n_x, n_t)$$

which is needed in the calculation of

$$Z(L_t) = \prod_{\vec{n},n_t} \left[\tfrac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} ds(n_x, n_t) e^{-\frac{1}{2}s^2(n_x,n_t)} \right] Z(s, L_t)$$

```
bose = 0.D0
do nt = 0,Lt-1
   do nx = 0,L-1
      s(nx,nt) = grnd()-0.5D0
      bose = bose + 0.5D0*s(nx,nt)*s(nx,nt)
   enddo
enddo
```

We compute the auxiliary-field amplitude $Z(s, L_t)$ for the initial configuration of s

```
call getv(v,s,0,Lt,c,am,alphat,L,Lt)
amp = 0.D0
do nx = 0,L-1
   amp = amp + dualv(nx,Lt)*v(nx,Lt)
enddo
```

We now set up our Markov chain with target probability given by

$$p_{\text{target}}(s) = e^{-\frac{1}{2}\sum_{n_x,n_t} s^2(n_x,n_t)} Z(s, L_t)$$

We do Metropolis updates of the auxiliary field. Note the square of the single-particle amplitude since there are contributions from both the up spin and the down spin.

```
      do ntrial = 1,numtrials

         call getdualv(dualv,s,0,Lt,c,am,alphat,L,Lt)

         do nt = 0,Lt-1
            do nx = 0,L-1
               s_old = s(nx,nt)
               s_new = s(nx,nt) + grnd() - 0.5D0
               bosediff = 0.5D0*(s_new*s_new-s_old*s_old)
               ampnew = amp
     $              + dualv(nx,nt+1)*v(nx,nt)
     $              *dsqrt(-c*alphat)*(s_new-s_old)
               if (grnd() .lt.
     $              (ampnew/amp)**2.D0*dexp(-bosediff)) then
                  accept = accept + 1.D0
                  amp = ampnew
                  s(nx,nt) = s_new
                  bose = bose + bosediff
               endif
            enddo
            call getv(v,s,nt,nt+1,c,am,alphat,L,Lt)
         enddo

               ⋮
```

While doing the Metropolis updates, we also compute $Z(s, L_t - 1)$. We collect data which properly samples the numerator and denominator of the ratio

$$\frac{Z(L_t-1)}{Z(Lt)} = \frac{\prod_{n_x,n_t}\left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} ds(\vec{n},n_t)e^{-\frac{1}{2}s^2(n_x,n_t)}\right]Z(s,L_t-1)}{\prod_{n_x,n_t}\left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} ds(\vec{n},n_t)e^{-\frac{1}{2}s^2(n_x,n_t)}\right]Z(s,L_t)}$$

And from this ratio we get our estimate of the energy

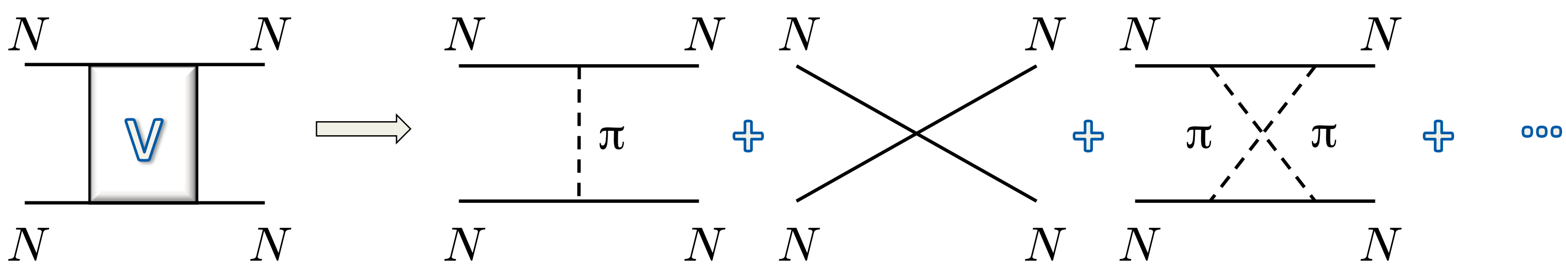
$$e^{-E(L_t)\alpha_t} = Z(L_t)/Z(L_t - 1)$$

```
     ⋮

   mtrial = ntrial - nwarmup

   if (mtrial .gt. 0) then
      amp1 = 0.D0
      do nx = 0,L-1
         amp1 = amp1 + dualv(nx,Lt)*v(nx,Lt-1)
      enddo
      ratio_bin = ratio_bin + amp1/amp
      energy = -dlog(mtrial/ratio_bin)/alphat
      if (mod(mtrial,nprintevery) .eq. 0) then
         write(*,*)
         write(*,*)'mtrial',mtrial,'energy (MeV)',energy*ainv
         write(*,*)'accept',accept/(ntrial*L*Lt)
      endif
   endif

enddo
```

Chiral EFT for low-energy nucleons

Weinberg, PLB 251 (1990) 288; NPB 363 (1991) 3

Construct the effective potential order by order

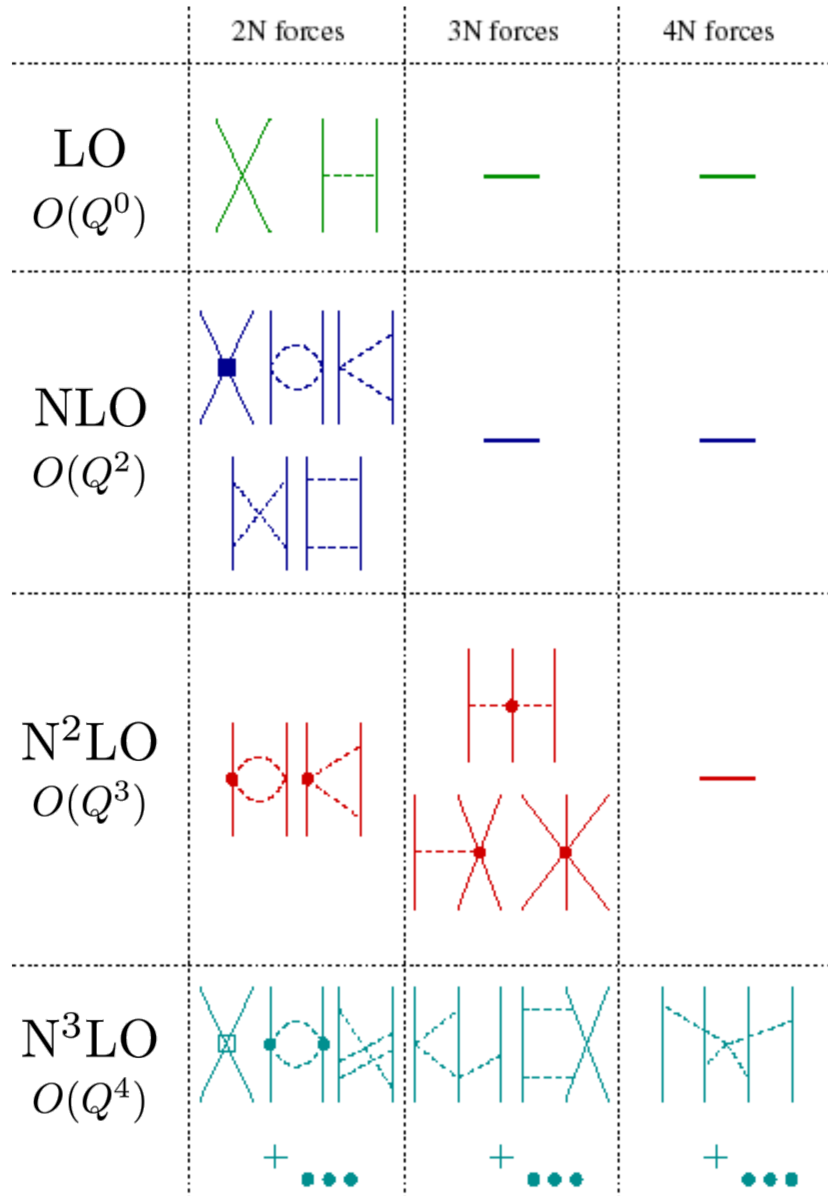


$$\underbrace{V^{\mathrm{OPEP}} \quad \text{Contact interactions } 1,\ \boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2}_{\text{Leading order (LO)}} \qquad \underbrace{V^{\mathrm{TPEP}}}_{\text{Next-to-leading order (NLO)}}$$

Nuclear
Scattering Data

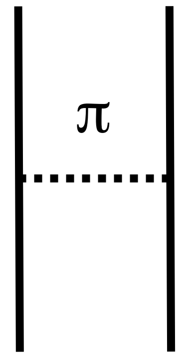
Effective Field Theory
Operator Coefficients

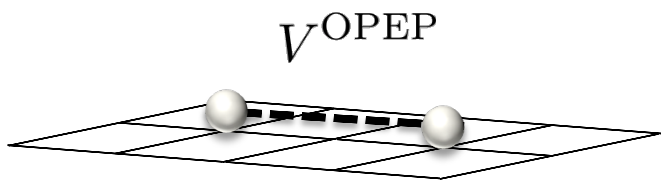
Ordonez et al. ’94; Friar & Coon ’94;
Kaiser et al. ’97; Epelbaum et al. ’98, ‘03;
Kaiser ’99-’01; Higa et al. ’03; ⋯

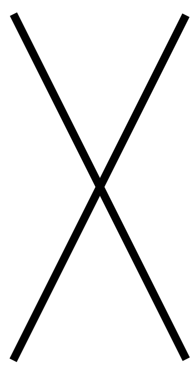


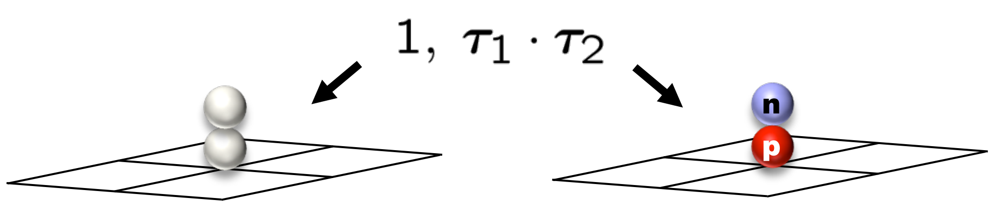
Lattice interactions

<u>Leading order on the lattice</u>

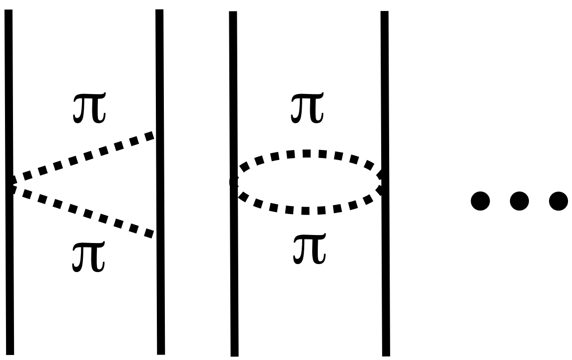




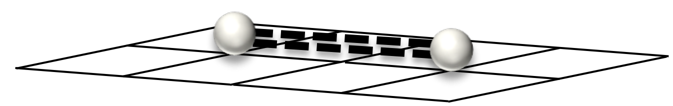


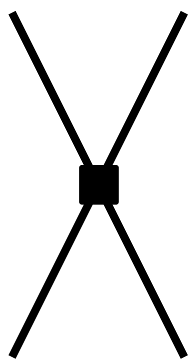


Next-to-leading order on the lattice

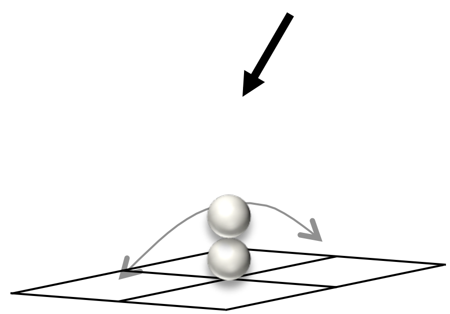


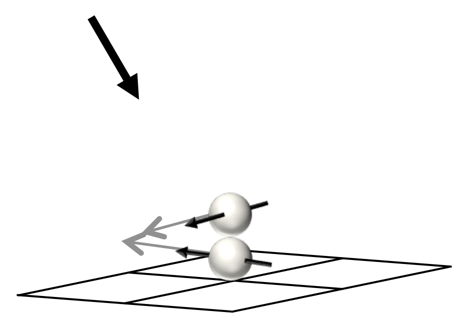
V^{TPEP}



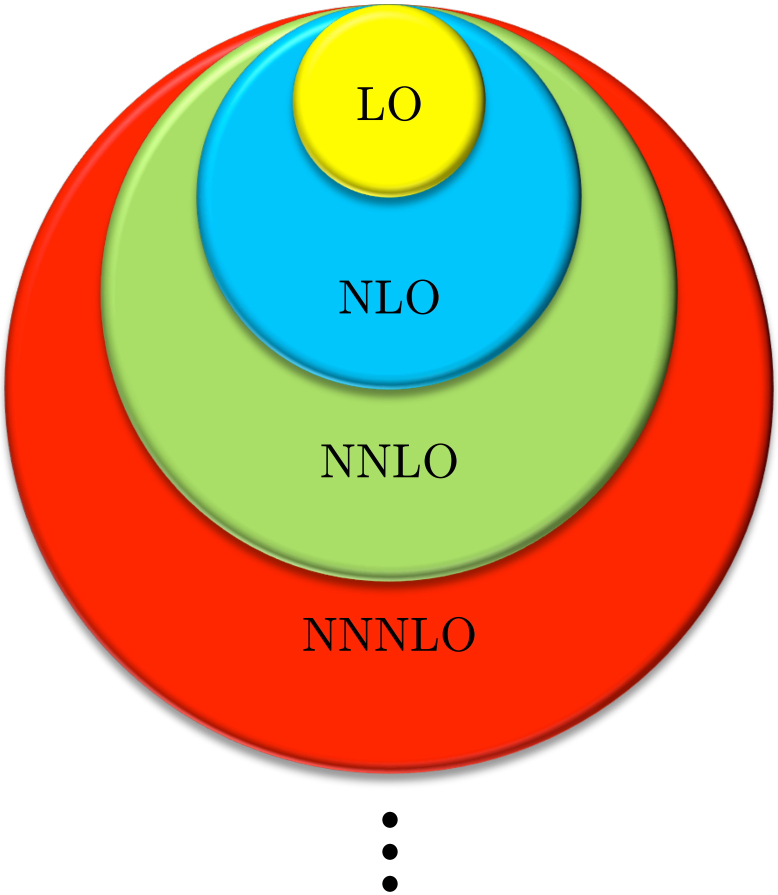


$\vec{\nabla}_1 \cdot \vec{\nabla}_2 \qquad (\vec{\sigma}_1 \cdot \vec{\nabla}_1)\,(\vec{\sigma}_2 \cdot \vec{\nabla}_2) \qquad \cdots$

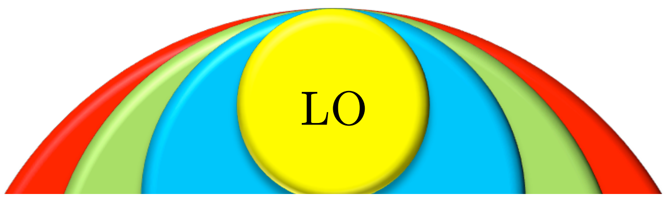




Computational strategy

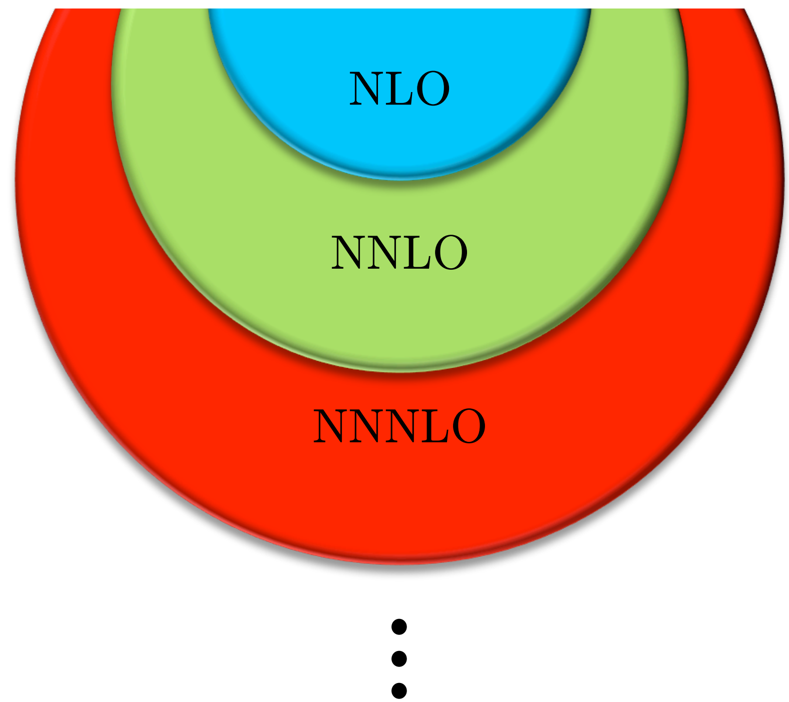


Non-perturbative – Monte Carlo



“Improved LO”

Perturbative corrections



Exercise 4

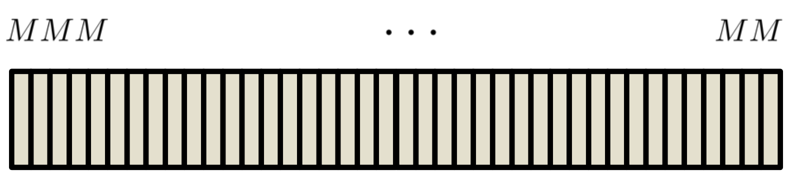
Consider the system of two-component fermions with zero-range attractive interactions.

$$M =: \exp\left[-H_{\text{free}}\alpha_t - C\alpha_t \textstyle\sum_{n_x} \rho_\uparrow(n_x)\rho_\downarrow(n_x)\right] :$$

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

$$= -\frac{1}{2m} \sum_{n_x, i=\uparrow,\downarrow} a_i^\dagger(n_x)\left[a_i(n_x+1) - 2a_i(n_x) + a_i(n_x-1)\right]$$

We consider one up spin and one down spin. Take the size of the periodic box to be $L = 6$ and choose $L_t = 50$. Do an exact (i.e., not Monte Carlo) calculation of the amplitude

$Z(L_t) = \langle \psi_{\text{init}} |$  $| \psi_{\text{init}} \rangle$

for the initial state with one up spin and down spin, each with zero momentum in the periodic box. For the parameters take

$$C = -0.200,\ m = 938.92\ \text{MeV},\ a = a_t = (100\ \text{MeV})^{-1}$$

Use the ratio of amplitudes with L_t and $L_t - 1$ time steps to determine an estimate for the energy using the relation

$$e^{-E(L_t)\alpha_t} = Z(L_t)/Z(L_t - 1)$$

Exercise 5

Consider exactly the same two-fermion system as in Exercise 4. Use the same initial state where both particles are at zero momentum and compute everything once again using auxiliary fields,

$$Z(L_t) = \prod_{\vec{n},n_t} \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} ds(n_x, n_t) e^{-\frac{1}{2}s^2(n_x,n_t)} \right] Z(s, L_t)$$

$$Z(s, L_t) = \langle \psi_{\text{init}} | \, M(s, L_t - 1) M(s, L_t - 2) \cdots M(s,1) M(s,0) \, | \psi_{\text{init}} \rangle$$

As in Exercise 4, take the size of the periodic box to be $L = 6$ and the number of time steps to be $L_t = 50$. Use the Metropolis algorithm to calculate the energy using the estimate

$$e^{-E(L_t)\alpha_t} = Z(L_t)/Z(L_t - 1)$$

for the parameter values

$$C = -0.200,\ m = 938.92\ \text{MeV},\ a = a_t = (100\ \text{MeV})^{-1}$$