New approach for studying large numbers of fermions in the unitary regime

Michael G. Endres*

Columbia University

Lattice 2010
Villasimius, Sardinia
June 18, 2010

*in collaboration with David B. Kaplan, Jong-Wan Lee and Amy N. Nicholson

Motivation

Unitary fermions

- *strongly coupled system of two-component nonrelativistic fermions*
- *two particle s-wave phase shift:* $p \cot \delta = 0$

- Such systems can be explored experimentally using ultra-cold atoms
- Natural starting point for lattice effective field theory approach to nuclear physics
  - nucleon-nucleon s-wave scattering lengths are large compared to the range of interaction

Quantum Monte Carlo methods for unitary fermions

- **Fixed Node Greens Function Monte Carlo** – variational

  Chang, Pandharipande, Carlson, and Schmidt (2004)
- **Diagrammatic Determinant Monte Carlo**

  Bourovski, Prokof'ev and Svistunov (2004)
- **Determinantal Monte Carlo**

  Bulgac, Drut and Magierski (2006)
- **Fixed Node Diffusion Monte Carlo** – variational

  Blume, von Stecher, and Greene (2007)
- $\vdots$

Can we apply lattice QCD techniques to study strongly interacting nonrelativistic fermions?

Action

Starting point:

- *non-relativistic action for spin 1/2 fermions*
- *zero-range 2-body (3-body) interactions*
- *no chemical potential; finite density from many fermion correlators*

$$\mathcal{L} = \bar{\psi}\left(\partial_\tau - \frac{\nabla^2}{2M}\right)\psi + C_0(\bar{\psi}\psi)^2$$

Naive discretization à la Kaplan & Chen (2003):

- $\partial_\tau \longrightarrow$ *standard forward difference*
- $\nabla^2 \longrightarrow$ *standard lattice Laplacian*
- *attractive split-point interaction:* $(\bar{\psi}\psi)^2 \longrightarrow (\bar{\psi}_\tau \psi_{\tau-1})^2$

Action

Starting point:

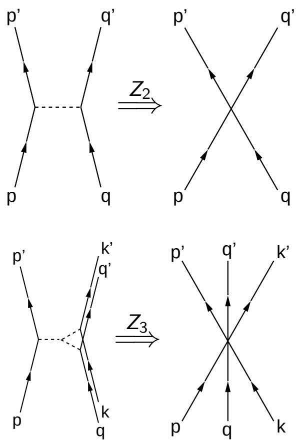
- *non-relativistic action for spin 1/2 fermions*
- *zero-range 2-body (3-body) interactions*
- *no chemical potential; finite density from many fermion correlators*

$$\mathcal{L} = \bar{\psi}\left(\partial_\tau - \frac{\nabla^2}{2M}\right)\psi + C_0(\bar{\psi}\psi)^2$$

Parameter tuning à la Kaplan & Chen (2003):

- *coupling C_0 related to two particle s-wave scattering length by evaluating 2-fermion scattering amplitude at zero momentum*

Interactions



p-body interactions introduced via Z_p ($p = 2, 3 \ldots$) auxiliary fields (ϕ)

- reduce action to fermion bilinears (necessary for Monte Carlo studies)
- *p*-body interactions requires at least *p* fermion species

$$\mathcal{L} \to \bar{\psi} \underbrace{\left(\partial_\tau - \frac{\nabla^2}{2M} + \sqrt{C_0}\phi \right)}_{K(\phi)} \psi$$

Fermion operator

$$K(\phi) = \begin{pmatrix} D & X(0) & 0 & 0 & \dots & 0 \\ 0 & D & X(1) & 0 & \dots & 0 \\ 0 & 0 & D & X(2) & \dots & 0 \\ 0 & 0 & 0 & D & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & X(T-1) \\ -X(T) & 0 & 0 & 0 & \dots & D \end{pmatrix}$$

$$D = 1 - \frac{\nabla^2}{2M} \qquad X(\tau) = 1 - \phi(\tau)$$

Auxiliary field dependence in off-diagonal components of fermion matrix

Fermion operator

$$K(\phi) = \begin{pmatrix} D & X(0) & 0 & 0 & \dots & 0 \\ 0 & D & X(1) & 0 & \dots & 0 \\ 0 & 0 & D & X(2) & \dots & 0 \\ 0 & 0 & 0 & D & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & X(T-1) \\ \cancelto{0}{-X(T)} & 0 & 0 & 0 & \dots & D \end{pmatrix}$$

$$D = 1 - \frac{\nabla^2}{2M} \qquad X(\tau) = 1 - \phi(\tau)$$

Key ingredient to our approach: *instead of anti-periodic boundary conditions in time direction, impose open boundary conditions*

Fermion determinant & propagators

- Auxiliary field-independent fermions determinant

  $\Longrightarrow$ full simulation = quenched simulation
  (auxiliary fields are action-less)

$$\det K(\phi) = \det D^T$$

- No fermion loops in time direction

  $\Longrightarrow$ simple form for propagators

$$K^{-1}(\tau,0) = D^{-1}X(\tau-1)D^{-1}\ldots D^{-1}X(0)D^{-1}$$

Simulation method

Procedure: *Time evolution of single particle wave functions on random background configurations*

For each configuration:

Initialize N sources at time zero ψ_i^{source} $(i = 1, \ldots, N)$

For each source:

Compute $\psi_i(0) = D^{-1}\psi_i^{source}$

For each time slice τ thereafter:

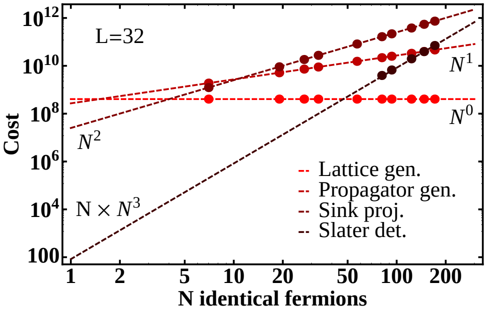
Generate random auxiliary fields at time slice

Compute $\psi_i(\tau) = D^{-1}X(\tau)\psi_i(\tau - 1)$ using FFTs

Project propagators onto single/multi-particle sinks

Perform contractions (e.g. Slater determinants)

Simulation cost



- Scaling with space-time volume: $T \times L^3 \log L^3$
- Trivial parallelization: sequential configurations have zero correlation $\Longrightarrow$ can run independent streams on different nodes

Understanding dependence on b_s and b_τ

Free fermion spectrum:

$$E_{1-particle} = \frac{\mathbf{p}^2}{2M} - \left(\frac{b_\tau}{8M^2} + \frac{b_s^2}{24M} \right) \sum_j p_j^4 + \dots$$

Two particle ground state (infinite volume limit, $a >> r_0$):

$$E_{2-particle}^{(gnd)} = \frac{1}{Ma^2} \left[1 + \frac{r_0}{a} + \frac{5}{4} \left(\frac{r_0^2}{a^2} + \frac{b_s^2}{5a^2} + \frac{b_\tau}{Ma^2} \right) + \dots \right]$$

$$a \leftrightarrow C_0 \ , \qquad r_0 \sim \mathcal{O}(b_s)$$

Understanding dependence on b_s and b_τ

Free fermion spectrum:

$$E_{1-particle} = \frac{\mathbf{p}^2}{2M} - \left(\frac{b_\tau}{8M^2} + \frac{b_s^2}{24M} \right) \sum_j p_j^4 + \dots$$

Two particle ground state (infinite volume limit, $a >> r_0$):

$$E^{(gnd)}_{2-particle} = \frac{1}{Ma^2} \left[1 + \frac{r_0}{a} + \frac{5}{4} \left(\frac{r_0^2}{a^2} + \frac{b_s^2}{5a^2} + \frac{b_\tau}{Ma^2} \right) + \dots \right]$$

Can we eliminate all discretization errors?

Understanding dependence on b_s and b_τ

Free fermion spectrum:

$$E_{1-particle} = \frac{\mathbf{p}^2}{2M} - \left(\frac{b_\tau}{8M^2} + \frac{b_s^2}{24M} \right) \sum_j p_j^4 + \ldots$$

Two particle ground state (infinite volume limit, $a >> r_0$):

$$E_{2-particle}^{(gnd)} = \frac{1}{Ma^2} \left[1 + \frac{r_0}{a} + \frac{5}{4} \left(\frac{r_0^2}{a^2} + \frac{b_s^2}{5a^2} + \frac{b_\tau}{Ma^2} \right) + \ldots \right]$$

Can we control sub-leading terms in the effective range expansion?

Understanding dependence on b_s and b_τ

Can we eliminate all discretization errors? **YES!**

- Simulation strategy allows us to use a "perfect" dispersion relation

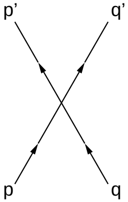
$$\frac{-\nabla^2}{2M} \longrightarrow e^{\mathbf{p}^2/(2M)} - 1$$

Can we control sub-leading terms in the effective range expansion? **YES!**

- Simulation strategy allows us to incorporate appropriate derivative interactions to all orders in $\mathbf{p}^2$

$$\mathcal{L} \supset \bar{\psi}\sqrt{C(\nabla^2)}\psi\bar{\psi}\sqrt{C(\nabla^2)}\psi$$

Improved two-body interaction

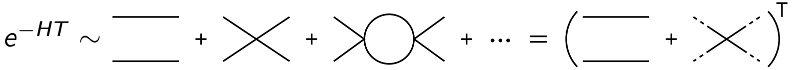


$$\sim \sqrt{C(\mathbf{p}')}\sqrt{C(\mathbf{q}')}\delta_{\mathbf{p}+\mathbf{q},\mathbf{p}'+\mathbf{q}'}$$

- Express C as a power series in $\mathbf{p}^2$
- Any basis set of operators acceptable; we choose:

$$C(\mathbf{p}) = \frac{4\pi}{M}\sum_n C_{2n}O_{2n}(\mathbf{p}) \ , \quad O_{2n}(\mathbf{p}) = M^n\left(1 - e^{-\mathbf{p}^2/M}\right)^n \approx \mathbf{p}^{2n}$$

Two fermion transfer matrix



- RHS may be interpreted as a two-fermion transfer matrix $\mathcal{T} = e^{-H}$
- $\mathcal{T}$ can be diagonalized giving us the two-fermion spectrum

Zero center of momentum eigenvalues ($p = \sqrt{ME}$) satisfy:

$$\sum_n C_{2n} I_{2n}(p) = 1 \ , \quad I_{2n}(p) = \frac{1}{V} \sum_{\mathbf{q}} \frac{O_{2n}(\mathbf{q})}{e^{(-p^2+\mathbf{q}^2)/M} - 1}$$

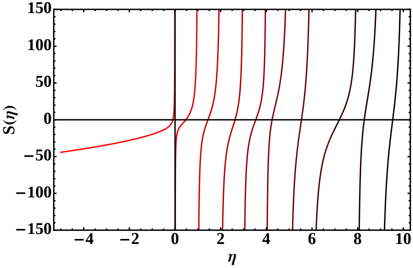
$\Longrightarrow$ *Now we only need a strategy for tuning Cs...*

Luscher's formula

Goal: *Relate C-coefficients to s-wave scattering parameters (a, r_0, etc.)*

$$p \cot \delta = -\frac{1}{a} + \frac{1}{2} r_0 p^2 + \ldots$$

Method: *Use Luscher's formula to relate the exact zero CM solutions to two-fermion transfer matrix to continuum Luscher energies*



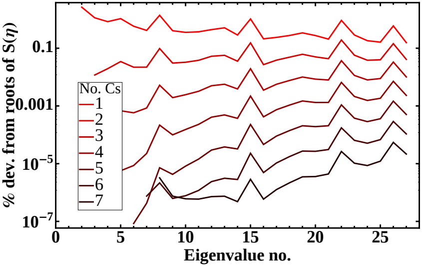
$$p\cot\delta = \frac{1}{\pi L} S(\eta) \quad \eta = \left(\frac{pL}{2\pi}\right)^2$$

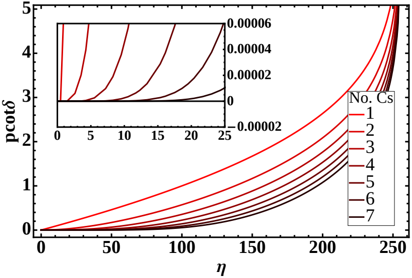
$$S(\eta) = \lim_{\Lambda\to\infty} \left[\sum_{|\mathbf{n}|<\Lambda} \frac{1}{\mathbf{n}^2 - \eta} - 4\pi\Lambda\right]$$

Parameter tuning: one of several methods

- *Determine first k solutions p_i^* $(i = 1, \dots k)$ to Luscher's formula*
- *Solve the linear set of equations: $\sum_{n=0}^{k-1} C_{2n} I_{2n}(p_i^*) = 1$ for each i*

Example: $p \cot \delta = 0$ (unitary fermions)





Unitary fermions

Talk by J-W. Lee (Next-to-Next!)

- *unitary fermions in a finite box*
- *measurement of energies for up to 38 paired fermions (first three shells filled)*
- *measurement of a universal quantities known as the Bertsch parameter and pairing gap*

Talk by A. N. Nicholson (Next!)

- *unitary fermions in a harmonic trap*
- *precision measurement of energies for up to 20 paired fermions*
- *independent measurement of the Bertsch parameter and pairing gap*

Conclusion

- New approach for numerically simulating strongly interacting nonrelativistic fermions
  - full simulation same as a quenched simulation
  - discretization errors removed to all orders
  - $p \cot \delta$ tunable to arbitrary order in p^2
- Ideal for numerical studies of unitary fermions in a finite box and harmonic trap (both underway)
- Possible future applications in nuclear physics
  - start with small nuclei: deuteron, triton, alpha, etc.
  - requires introduction of physical effective range, spin flip interactions, three-body interactions, etc.