Lattice Monte Carlo Simulation of a Dilute Fermi Gas: Theory and Numerical Exploration

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Outline

- Motivation
- Chen and Kaplan's Proposal
- Overview of Lattice Method
- Preliminary Tests
- Future Plan

Scenario

Recent proposal by J-W. Chen and D.B. Kaplan (hep-lat/0308016) to use lattice field theory to study a Fermi gas with

- 2 spin components
- Dilute limit: $k_F^{-1} \gg R$, the range of the potential
  - S wave scattering
  - Details of potential irrelevant
- Large scattering length: $|a| \to \infty$
  - Most interesting application
  - Necessary for nontrivial continuum limit
    * Continuum limit: lattice spacing (b) smaller than relevant physical scales $\frac{b}{\lambda_{phys}} \to 0$, so $k_F b \to 0$
    * Keep $k_F|a| = (k_F b)\left(\frac{|a|}{b}\right) > 1$
- Generalizations possible, but further down the road
  - Must keep a nonnegative fermion determinant (you'll see)

Specifically: Numerical Solution of Field Theory Path Integrals with a Lattice Regulator – Mature method for attacking QCD

Advantages

- Systematic
  - Finite spacing, size, and source effects can be improved
  - Nonperturbative in $k_F a$
  - No guesswork required
- $T \neq 0$ and $\mu \neq 0$ straightforward
  - Grand Canonical Ensemble
- Large $\langle N \rangle$ possible
  - If $k_F^{-1} \approx 4b$ then 40^3 volume implies max $\langle N \rangle = 1000$

Possible pitfalls

- It may crash and burn
  - Is there a continuum limit?
  - Should be obvious. First glances have me optimistic
- It may be computationally expensive
  - Infinite volume limit
  - SciDAC Lattice QCD initiative

Partition Function Path Integral

$$Z = \mathrm{Tr}\; e^{-\beta(H-\mu N)}$$

$$= \int \mathcal{D}\psi^\dagger \mathcal{D}\psi\; e^{-\int_0^\beta dx_4 \int d^3x\; \left(\mathcal{L}[\psi,\psi^\dagger]-\mu\psi^\dagger\psi\right)}$$

Discretize

$$\int d^4x\; \psi^\dagger \left(\partial_4 - \frac{\nabla^2}{2M} - \mu\right)\psi \;\longrightarrow\; S_0 = \sum_x \psi_x^\dagger (K_0\psi)_x$$

where

$$(K_0\psi)_x \;\equiv\; \left(\psi_x - e^{\mu}\psi_{x-\hat{t}}\right) - \sum_j \frac{\psi_{x+\hat{j}} - 2\psi_x + \psi_{x-\hat{j}}}{2M}$$

This time difference suppresses propagation backward in time

Tech. aside: $\mu\; \psi^\dagger(x)\psi(x) \;\rightarrow\; \psi_x^\dagger(e^\mu - 1)\psi_{x-\hat{t}}$ required to avoid divergent free energy – Hasenfratz & Karsch (1983)

$$\mathcal{L}_{int}(x) \;=\; -\,g^2\;\left(\psi^\dagger(x)\psi(x)\right)^2$$

Auxiliary scalar field – Hubbard/Stratonovich

$$\mathcal{L}_{int}(x) \;=\; -\,g\;m\;\phi(x)\left(\psi^\dagger(x)\psi(x)\right)$$

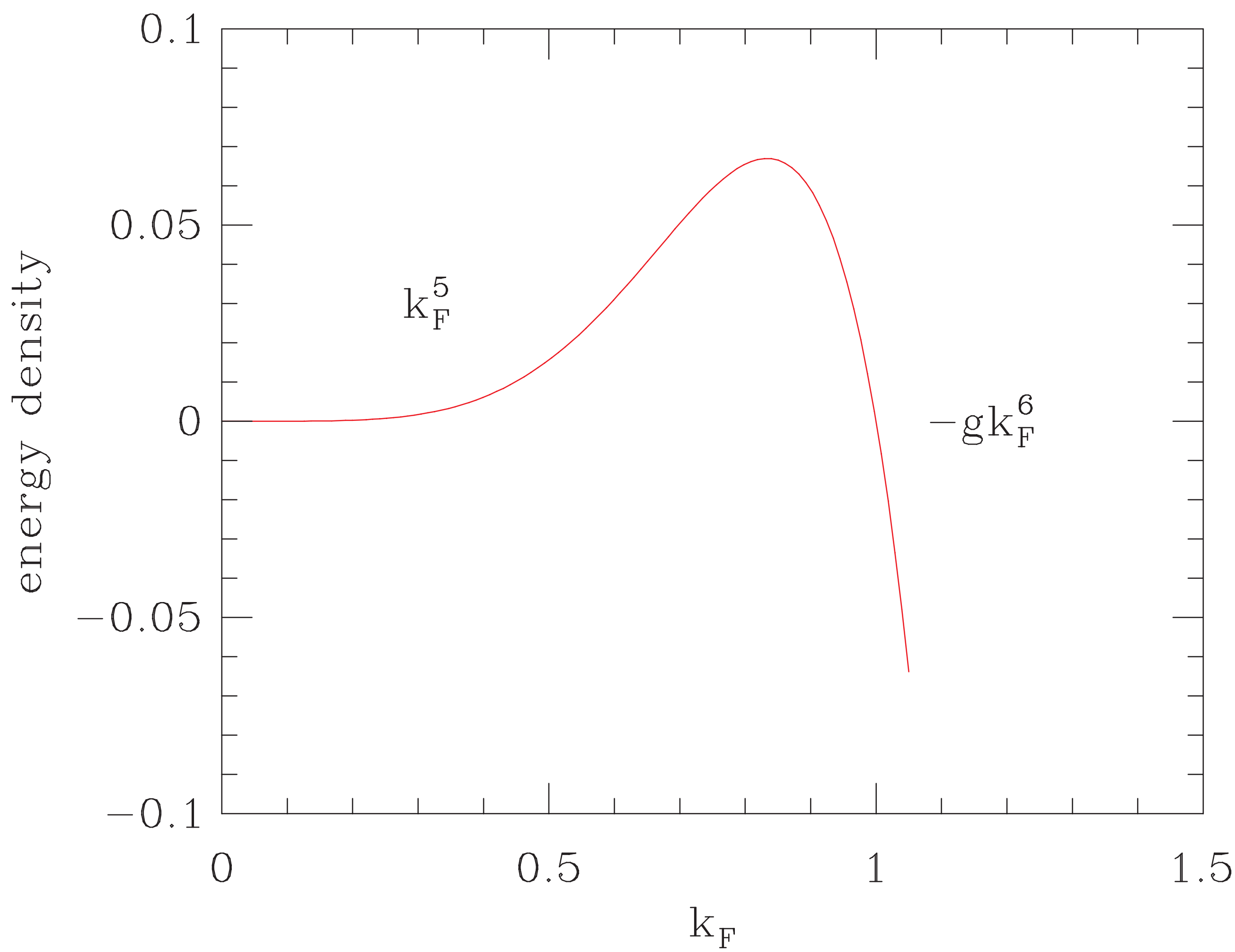
Lattice form

$$\begin{aligned}\psi_x^\dagger(K_0\psi)_x - \psi_x^\dagger\phi_x e^\mu\psi_{x-\hat{t}} + \frac{1}{2}m^2\phi_x^2 \\ \equiv\;\psi_x^\dagger(K\psi)_x + \frac{1}{2}m^2\phi_x^2\end{aligned}$$

Source for fermion pairs

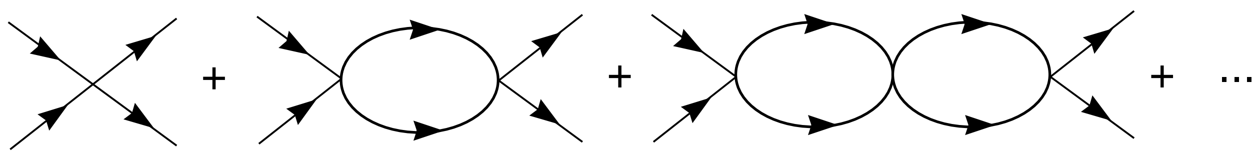
$$\frac{1}{2}\left(J\;\psi_x^T\sigma_2\psi_x\;+\;J^*\;\psi_x^\dagger\sigma_2\psi_x^{\dagger T}\right)$$

$\mu = 0$

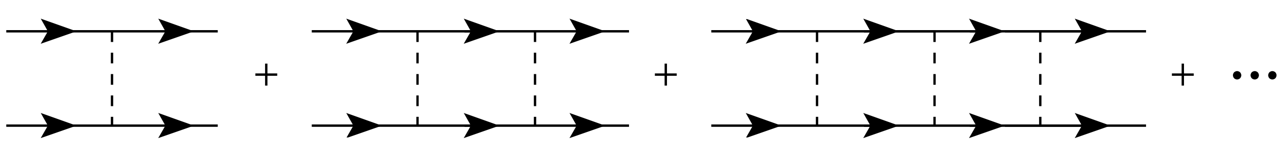


Need to keep lattice spacing b large enough so that $1/b$ is smaller than k_F where instability sets in

Relationship between coupling constants m^2, M and scattering length determined by 2 body scattering



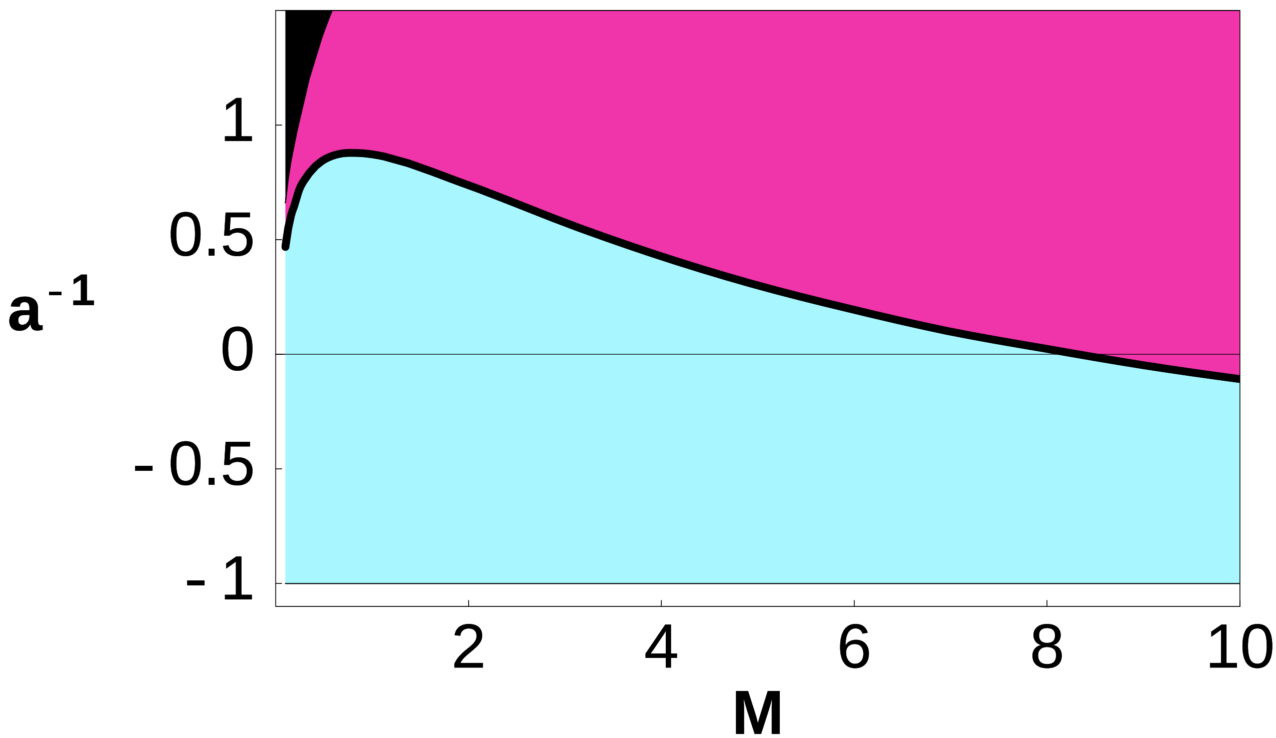
Or with auxiliary scalar



$$\frac{m^2}{M} = -\frac{1}{4\pi a} + L(M)$$

Here we see why interaction is split over a time slice: to suppress

$T = \mu = 0$ phase diagram



- Black = unaccessible: corresponds to $m^2 g^2 < 0$
- Magenta = Bad: $\langle n \rangle = \mathcal{O}(1)$ in lattice units, or $\mathcal{O}\left(1/b^3\right)$
- Cyan = Good: $\langle n \rangle = 0$. Implies $k_F b = 0$ and good continuum limit

$$
\begin{aligned}
\int \mathcal{D}\psi^\dagger \mathcal{D}\psi \quad & \exp\left[-\psi_x (K[\phi]\psi)_x - \frac{1}{2}\left(J\, \psi_x^T \sigma_2 \psi_x + \text{h.c.}\right)\right] \\
&= \int \mathcal{D}\Psi\ \exp\left[-\frac{1}{2}\Psi^T \mathcal{A}[\phi]\Psi\right] \\
&= \text{Pf}\ \mathcal{A}[\phi] \\
&= \det \widetilde{\mathcal{A}}[\phi] \\
&= \det\left(|J|^2 + \widetilde{K}^\dagger \widetilde{K}\right) \geq 0 \\
&\equiv \det\ Q
\end{aligned}
$$

where

$$
\Psi \equiv \begin{pmatrix} \psi \\ i\sigma_2 \psi^{\dagger T} \end{pmatrix}, \quad \mathcal{A} \equiv \begin{pmatrix} -iJ & K^\dagger \\ K & -iJ^* \end{pmatrix} \begin{pmatrix} i\sigma_2 & 0 \\ 0 & i\sigma_2 \end{pmatrix}
$$

- Numerically evaluate

$$\int \mathcal{D}\phi \, \det Q[\phi] \; e^{-\sum_x \frac{1}{2} m^2 \phi_x^2}$$

- Use Importance Sampling to find dominant field configurations
- Need a Markov process to generate a chain of important configurations
- $\det Q[\phi]$ makes local updating algorithms (Metropolis, heat bath) scale like $(N_s^3 N_t)^2$

Duane, Kennedy, Pendleton, Roweth, PLB **195**, 216 (1987)

- Pseudofermions

$$\int \mathcal{D}\phi\,\mathcal{D}\chi^\dagger\mathcal{D}\chi\; e^{-\sum_x\left(\frac{1}{2}m^2\phi_x^2 + \chi^\dagger Q^{-1}\chi\right)}$$

- Hamiltonian for evolution in "Monte Carlo time" τ

$$H[\pi,\phi] \;=\; \frac{1}{2}\pi^2 + \frac{1}{2}m^2\phi^2 + \chi^\dagger Q^{-1}\chi$$

- Use heatbath to generate $\chi(\tau), \chi^\dagger(\tau)$ and $\pi(\tau)$
- Evolve ϕ and π from τ to $\tau+\delta\tau$: Leapfrog

$$\begin{aligned}
\pi(\tau+\frac{\Delta\tau}{2}) \;&=\; \pi(\tau-\frac{\Delta\tau}{2}) \;-\; \frac{\delta H}{\delta\phi}\,\Delta\tau \\
\phi(\tau+\Delta\tau) \;&=\; \phi(\tau) \;+\; \pi(\tau)\,\Delta\tau
\end{aligned}$$

- Monte Carlo accept/reject step: $\mathcal{P}(\mathrm{accept}) = \min(1, e^{-\Delta H})$
- Test $\langle e^{-\Delta H}\rangle = 1$. Also $e^{-\langle\Delta H\rangle} \leq 1$ or $\langle\Delta H\rangle \geq 0$

On $4^3 \times 4$ lattice, with $J = 1.0$, $n\Delta\tau = 1$ on a Pentium 4
1000 Monte Carlo steps

$\Delta\tau$	$\langle e^{-\Delta H} \rangle$	A/R (%)	time (min)
0.5	0.992(16)	81.2	12
0.25	1.000(4)	95.9	15
0.2	1.000(2)	97.2	15
0.1	0.9998(6)	99.4	21

Computation will get harder as V gets large and J gets small

Future Plan

- Firm up continuum limit picture
- Thermodynamic quantities F, p, n in (T, μ) plane
- Pairing condensate $\langle \psi^T \sigma_s \psi \rangle$ in $V \to \infty, |J|^2 \to 0$ limit
- Correlation functions?
- You tell me