Universal Fermi gases on the lattice

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Computational approaches to nuclear many-body problems and related quantum systems

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Outline

• Motivation
  • “unitary” Fermi gas in 3D
  • universal four-component Fermi gas in 1D
• Solution to the sign problem for nonrelativistic fermions in 1D
  • Mean-field results
• Numerical results for universal Fermi gas
  • few-body results: energy spectrum
  • many-body results: evidence for a “universality” between conformal theories in \textit{different} spatial dimensions
• Summary & Outlook
Unitary Fermi gas
(three dimensions)

A dilute mixture of spin 1/2 fermions at infinite scattering length
2-particle scattering from a short-range potential

\[ A(p) = \frac{4\pi}{M} \frac{1}{p \cot \delta(p) - ip} \]

\[ p = \sqrt{EM} \]

scattering phase shift

\[ p \cot \delta(p) = -\frac{1}{a} + \frac{1}{2} r_0 p^2 + \ldots \]

radial profile of spherically symmetric potential

\[ r = |x_{rel}| \]

\[ \lim_{p \to 0} \sigma_0(p) = 4\pi a^2 \]
2-particle scattering from a short-range potential

\[ E \sim \frac{1}{Ma^2} \]

\[ \psi(r) \sim \frac{1}{r} - \frac{1}{a} \]

weakly bound state

\[ r\psi(r) \]
2-particle scattering from a short-range potential

zero-energy bound state

$E$

$V$

$r \psi(r)$

$a = \infty$
2-particle scattering from a short-range potential

\[ V(r) \]

\[ r \psi(r) \]

(no bound state)
2-particle scattering from a short-range potential

\[ p \cot \delta = 0 \]

\[ a \to \infty \]

\[ R \to 0 \]

\[ \sigma_0 \leq \frac{4\pi}{p^2} \]

“unitarity bound” is saturated!

\[ \psi \sim \frac{1}{r} \]

s-waves can only “see” zero-range potential (angular momentum barrier)
Interacting Fermi gas

\[ \rho = \frac{N}{V} \]

\[ R \ll \rho^{-1/3} \ll |a| \]

\[ \psi \sim \frac{1}{r_{ij}} - \frac{1}{a} , \quad r_{ij} = x_i^\uparrow - x_j^\downarrow \]
Interacting Fermi gas

BCS

\[
\frac{1}{p_F a} < 0
\]

Cooper pairs

cross-over

\[
\frac{1}{p_F a} = 0
\]

BEC of dimers

BEC

\[
\frac{1}{p_F a} > 0
\]
Physical realization: ultra-cold atoms

$\rho^{-1/3} \sim 5000 - 10000a_0$

Bohr radius

$r_0(^{40}K) \sim 60a_0$

$r_0(^{6}Li) \sim 30a_0$

interacting gas of fermions

($^{6}Li$ or $^{40}K$ atoms often used)
Physical realization: ultra-cold atoms

\[ r_0(^{40}\text{K}) \sim 60a_0 \] \hspace{1cm} \text{Bohr radius}

\[ r_0(^6\text{Li}) \sim 30a_0 \]

\[ \rho^{-1/3} \sim 5000 - 10000a_0 \]

Scattering length tuned by exploiting properties of a Feshbach resonance
Effective field theory description

\[ S_{\text{cont}}(\mu) = \int d^4x \left[ \psi^\dagger \left( \partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi - C_0(\psi^\dagger \psi)^2 \right] \]

\[ \psi = (\psi_\uparrow, \psi_\downarrow) \]

zero-range contact interaction
Effective field theory description

\[
S_{\text{cont}}(\mu) = \int d^4 x \left[ \psi^\dagger \left( \partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi - C_0 (\psi^\dagger \psi)^2 \right]
\]

Relationship between coupling \((C_0)\) and scattering length:

\[
\begin{align*}
A^{-1}(p) & \bigg|_{p \to 0} = \frac{m}{4\pi a} \\
\end{align*}
\]
Effective field theory description

\[ S_{\text{cont}}(\mu) = \int d^4x \left[ \psi^\dagger \left( \partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi - C_0(\psi^\dagger \psi)^2 \right] \]

Relationship between coupling \((C_0)\) and scattering length:

\[ \hat{C}_0(\mu) = -\frac{m\mu}{4\pi} C_0(\mu) \]

Renormalization scale (not chemical potential)
Effective field theory description

\[ S_{\text{cont}}(\mu) = \int d^4x \left[ \psi^\dagger \left( \partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi - C_0(\psi^\dagger \psi)^2 \right] \]

Relationship between coupling (\( C_0 \)) and scattering length:

\[ \hat{C}_0(\mu) = -\frac{m\mu}{4\pi} C_0(\mu) \]

Renormalization scale (not chemical potential)

\( \hat{\beta} = \mu \frac{\partial \hat{C}_0}{\partial \mu} = -\hat{C}_0(\hat{C}_0 - 1) \)

IR: trivial, free
UV: unitary, conformal

nonperturbative
Unitary fermions: in a box and in a trap
Unitary fermions: in a box and in a trap

\[ L \]

\[ L_0 \]

free space

harmonic trap

\[ \rho^{-1/3} \]
Properties of unitary fermions

- Operator state correspondence
- Virial theorems
- Rich and fascinating physics!
  - universal few- and many-body physics
  - universal (Tan) relations
  - Efimov physics
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Example: energy of many-body system

\[ \frac{E}{E_{FG}} = \xi \]

free space

\[ \frac{E}{E_{FG}} = \sqrt{\xi} \]

harmonic trap
Bertsch parameter

0.376(4) - MIT group

0.372(5) - Carlson, et al.
Bertsch parameter

Universal four-component Fermi gas (one dimension)
Universal Fermi gases in lower dimensions

• “Universal Fermi gases in mixed dimensions”
  Y. Nishida and S. Tan

• “Universal four-component Fermi gas in one dimension”
  Y. Nishida and D.T. Son
Universal Fermi gases in lower dimensions

- “Universal Fermi gases in mixed dimensions”
  Y. Nishida and S. Tan

- “Universal four-component Fermi gas in one dimension”
  Y. Nishida and D. T. Son
Effective field theory

\[ S_{\text{cont}}(\mu) = \int d^2 x \left[ \psi^\dagger \left( \partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi - g(\psi^\dagger \psi)^4 \right] \]

\( \mu = (\mu_a, \mu_b, \mu_c, \mu_d) \)

\( m = (m_a, m_b, m_c, m_d) \)

\( \psi = (\psi_a, \psi_b, \psi_c, \psi_d) \)
Effective field theory

\[ S_{\text{cont}}(\mu) = \int d^2 x \left[ \psi^\dagger \left( \partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi - g(\psi^\dagger \psi)^4 \right] \]

Highly tuned action: lower-dimension ops. absent:

\[ (\psi^\dagger \psi)^2 \]

\[ (\psi^\dagger \psi)^3 \]
Effective field theory

\[ S_{\text{cont}}(\mu) = \int d^2x \left[ \psi^\dagger \left( \partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi - g(\psi^\dagger \psi)^4 \right] \]

Relationship between coupling (g) and “scattering length”:

\[ A^{-1}(p) \bigg|_{p \to 0} \overset{\text{def.}}{=} \frac{m}{4\pi a} \]

four-particle scattering amplitude
Effective field theory

\[ S_{\text{cont}}(\mu) = \int d^2 x \left[ \psi^\dagger \left( \partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi - g(\psi^\dagger \psi)^4 \right] \]

Relationship between coupling (g) and “scattering length”:

\[ a \to \infty \iff g \to g_c \]

UV fixed point: “universal”, conformal, O(1) coupling
...many identical properties with unitary fermions

• Operator state correspondence
• Virial theorems
• Rich and fascinating physics!
  • universal few- and many-body physics
• universal (Tan) relations
• Efimov physics
Example: energy of many-body system

\[ \frac{E}{E_{FG}} = \xi \]  

\[ \frac{E}{E_{FG}} = \sqrt{\xi} \]  

free space  
harmonic trap
Example: energy of many-body system

\[ \frac{E}{E_{FG}} = \xi \]

\[ \frac{E}{E_{FG}} = \sqrt{\xi} \]

1d Bertsch parameter

same 1d Bertsch parameter

free space

harmonic trap

1d and 3d Bertsch parameters need not be the same!
Objective

• Qualitative similarities of one- and three-dimensional systems make numerical studies of 1D Fermi gas an attractive possibility

• Advantages over the three-dimensional theory:
  • computationally inexpensive
  • no sign problem for imbalanced population, mass and repulsive interactions

• Disadvantages:
  • gain qualitative insights, but how about quantitative ones?
Lattice discretization

\[ S_{cont}(\mu) = \int d^2x \left[ \nabla^2 \left( \partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi - g(\psi^\dagger \psi)^4 \right] \]

\[ (\partial_\tau \psi - \mu \psi)_n = \frac{1}{b_\tau} (\psi_n - e^{b_\tau \mu} \psi_{n-b_\tau e_0}) \]

\[ (-\nabla^2 \psi)_n = \frac{1}{b_s^2} (2\psi_n - \psi_{n+b_s e_1} - \psi_{n-b_s e_1}) \]

\[ (\psi^\dagger \psi)_n = \psi_n^\dagger e^{b_\tau \mu} \psi_{n-b_\tau e_0} \]

\[ b_\tau = b_s = 1 \]

“lattice units”
Lattice discretization

Continuum & Infinite Volume limits:

\[ b_s \ll \rho^{-1} \ll L \]

dilute limit

therm. limit

\[ \rho = N/L \]

\[ a \to \infty \]
Path integral formulation

\[-S(\mu) = \sum_{n \in \Lambda} \left[ -\psi_n^\dagger \left( 1 + \frac{1}{m} \right) \psi_n + \psi_n^\dagger e^\mu \psi_{n-e_0} + \psi_n^\dagger \frac{1}{2m} (\psi_{n+e_1} + \psi_{n-e_1}) + g (\psi_n^\dagger e^\mu \psi_{n-e_0})^4 \right] \]

\[Z(\mu) = \int [d\psi^\dagger][d\psi] e^{-S(\mu)}\]
Path integral formulation

\[-S(\mu) = \sum_{n \in \Lambda} \left[ -\psi_n^\dagger \left(1 + \frac{1}{m}\right) \psi_n + \psi_n^\dagger e^\mu \psi_{n-e_0} + \psi_n^\dagger \frac{1}{2m} (\psi_{n+e_1} + \psi_{n-e_1}) + g \left(\psi_n^\dagger e^\mu \psi_{n-e_0} \right)^4 \right] \]

\[Z(\mu) = \int [d\psi^\dagger][d\psi] e^{-S(\mu)} \]

\[g^{1/4} \phi \psi^\dagger e^\mu \psi \]

(e.g., \(\phi = z_4\) field)

Conventional Hubbard-Stratonovich transformation results in a sign problem
(after integrating out fermions)
Path integral formulation

\[-S(\mu) = \sum_{n \in \Lambda} \left[ -\psi_n^\dagger \left( 1 + \frac{1}{m} \right) \psi_n + \psi_n^\dagger e^\mu \psi_{n-e_0} + \psi_n^\dagger \frac{1}{2m} (\psi_{n+e_1} + \psi_{n-e_1}) + g (\psi_n^\dagger e^\mu \psi_{n-e_0})^4 \right] \]

\[Z(\mu) = \int [d\psi^\dagger][d\psi] e^{-S(\mu)} \]

**Solution:** consider a different representation for the partition function based on a hopping parameter expansion
Path integral formulation

\[-S(\mu) = \sum_{n \in \Lambda} \left[ -\psi_n^\dagger \left( 1 + \frac{1}{m} \right) \psi_n + \psi_n^\dagger e^\mu \psi_{n-e_0} + \psi_n^\dagger \frac{1}{2m} \left( \psi_{n+e_1} + \psi_{n-e_1} \right) + g \left( \psi_n^\dagger e^\mu \psi_{n-e_0} \right)^4 \right] \]

\[Z(\mu) = \int [d\psi^\dagger] [d\psi] e^{-S(\mu)}\]

Ignore interaction to begin with...
Consider a hopping parameter expansion

\[-S(\mu) = \sum_{n \in \Lambda} \left[ -\psi_n^\dagger \left( 1 + \frac{1}{m} \right) \psi_n + \psi_n^\dagger e^\mu \psi_{n-e_0} + \psi_n^\dagger \frac{1}{2m} \left( \psi_{n+e_1} + \psi_{n-e_1} \right) \right] \]

\[Z(\mu) = \int [d\psi^\dagger][d\psi] e^{-S(\mu)} \]

Expand in powers of the action, integrate out the fermions term by term
Consider a hopping parameter expansion

\[ -S(\mu) = \sum_{n \in \Lambda} \left[ -\psi_n^\dagger \left( 1 + \frac{1}{m} \right) \psi_n + \psi_n^\dagger e^\mu \psi_{n-e_0} + \psi_n^\dagger \frac{1}{2m} (\psi_{n+e_1} + \psi_{n-e_1}) \right] \]

\[ Z(\mu) = \int [d\psi^\dagger][d\psi] e^{-S(\mu)} \]

\[ - \left( 1 + \frac{1}{m} \right) \]
Consider a hopping parameter expansion

\[-S(\mu) = \sum_{n \in \Lambda} \left[ -\psi_n^\dagger \left( 1 + \frac{1}{m} \right) \psi_n + \psi_n^\dagger e^\mu \psi_{n-e_0} + \psi_n^\dagger \frac{1}{2m} (\psi_{n+e_1} + \psi_{n-e_1}) \right] \]

\[Z(\mu) = \int [d\psi^\dagger][d\psi] e^{-S(\mu)}\]
Consider a hopping parameter expansion

\[-S(\mu) = \sum_{n \in \Lambda} \left[ -\psi_n^\dagger \left( 1 + \frac{1}{m} \right) \psi_n + \psi_n^\dagger e^\mu \psi_{n-e_0} + \psi_n^\dagger \frac{1}{2m} \left( \psi_{n+e_1} + \psi_{n-e_1} \right) \right] \]

\[Z(\mu) = \int [d\psi^\dagger][d\psi] e^{-S(\mu)}\]
Consider a hopping parameter expansion

\[ -S(\mu) = \sum_{n \in \Lambda} \left[ -\psi_n^\dagger \left( 1 + \frac{1}{m} \right) \psi_n + \psi_n^\dagger e^\mu \psi_{n-e_0} + \psi_n^\dagger \frac{1}{2m} (\psi_{n+e_1} + \psi_{n-e_1}) \right] \]

\[ Z(\mu) = \int [d\psi^\dagger][d\psi] e^{-S(\mu)} \]

- Fermion paths form closed loops (due to Grassmann integration)
- Fermion loops are self-avoiding (Pauli exclusion)
- Single-hop fermion “bubbles” allowed
Consider a hopping parameter expansion

\[-S(\mu) = \sum_{n \in \Lambda} \left[ -\psi_n^\dagger \left( 1 + \frac{1}{m} \right) \psi_n + \psi_n^\dagger e^{\mu} \psi_{n-e_0} + \psi_n^\dagger \frac{1}{2m} (\psi_{n+e_1} + \psi_{n-e_1}) \right] \]

\[Z(\mu) = \int [d\psi^\dagger][d\psi] e^{-S(\mu)} \]

- All fermion loops come with a minus sign
- Every winding in time comes with a minus sign (APBCs)
- Fermion loops in time are disjoint (Pauli exclusion)
Consider a hopping parameter expansion

\[
Z(\mu) = \sum_{\{c_\sigma\} \in C} \left[ \prod_{\sigma} \left( 1 + \frac{1}{m_\sigma} \right)^{S(c_\sigma)} \left( \frac{1}{2m_\sigma} \right)^{B_s(c_\sigma)} (-1)^{F(c_\sigma)} e^{\mu B_t(c_\sigma)} \right]
\]

- \( S = \# \) unvisited sites
- \( B_s = \# \) space-like links
- \( B_t = \# \) time-like links
- \( F = \# \) space-like fermion bubble loops
Consider a hopping parameter expansion

\[ Z(\mu) = \sum_{\{c_\sigma\} \in C} \left[ \prod_{\sigma} \left( 1 + \frac{1}{m_\sigma} \right)^{S(c_\sigma)} \left( \frac{1}{2m_\sigma} \right)^{B_s(c_\sigma)} (-1)^{F(c_\sigma)} e^{\mu_\sigma B_\tau(c_\sigma)} \right] \]

...but we still have a sign problem.
Solving the sign problem

**Observation:** configurations fall into classes designated by the time-like loops
Solving the sign problem

Idea: sum all up the fermion bubbles within each class
Evaluation of the fermion bubble sum

\[ z_n(m) = z_{n-1}(m) \left(1 + \frac{1}{m}\right) - \frac{1}{(2m)^2} z_{n-2}(m) \]

\[ z_0(m) = 1 \quad z_1(m) = 1 + \frac{1}{m} \]
Evaluation of the fermion bubble sum

\[ z_n(m) = \frac{1}{2^{n+1} \sqrt{1 + 2/m}} \left[ \left( 1 + \frac{1}{m} + \sqrt{1 + \frac{2}{m}} \right)^{n+1} - \left( 1 + \frac{1}{m} - \sqrt{1 + \frac{2}{m}} \right)^{n+1} \right] \]
Final result for free fermions

\[ Z(\mu) = \sum_{\{c_\sigma\} \in C^*} \left[ \prod_\sigma \left( \prod_{d \in \mathcal{D}(c_\sigma)} z_{\mathcal{L}(d)}(m_\sigma) \right) \left( \frac{1}{2m_\sigma} \right)^{B_s(c_\sigma)} e^{\mu_\sigma B_\tau(c_\sigma)} \right] \]

\[ \mathcal{D}(c) = \text{set of domains } d \text{ associated with } c \]

\[ \mathcal{L}(d) = \text{length of } d \]

\[ C^* = \text{set of all possible "bubble free" configurations} \]
Final result for free fermions

\[ Z(\mu) = \sum_{\{c_\sigma\} \in C^*} \left[ \prod_{\sigma} \left( \prod_{d \in D(c_\sigma)} z_{\mathcal{L}(d)}(m_\sigma) \right) \left( \frac{1}{2m_\sigma} \right)^{B_s(c_\sigma)} e^{\mu_\sigma B_t(c_\sigma)} \right] \]

Adding back the interaction...
Final result for interacting fermions

\[ Z(\mu) = \sum_{\{c_\sigma\} \in C^*} \left[ \prod_{\sigma} \left( \prod_{d \in D(c_\sigma)} z_{L(d)}(m_\sigma) \right) \left( \frac{1}{2m_\sigma} \right)^{B_s(c_\sigma)} e^{\mu_\sigma B_\tau(c_\sigma)} \right] (1 + g)^{B_\tau(\cap c_\sigma)} \]

- Resulting partition function free of sign problems even with:
  - mass imbalance
  - polarization imbalance
  - repulsive interactions (provided \( g > -1 \))
Mean field results
Mean-field results: $m-a^{-1}$ phase diagram

- **I & IV**: zero density regime
- **II**: inaccessible within variational approach (complex action)
- **III**: saturated lattice, density equals four

$$\frac{-m}{4\pi a} = \frac{1}{g} - \frac{1}{g_c}$$

$g = g_c$
Mean-field results: $m - a^{-1}$ phase diagram

- I & IV: zero density regime
- II: inaccessible within variational approach (complex action)
- III: saturated lattice, density equals four

\[
\frac{m}{4\pi a} = \frac{1}{g} - \frac{1}{g_c}
\]

$g = g_c$
Mean-field results: free energy & number density

- Number density at critical coupling jumps discontinuously from region of low(-ish) density to region in which lattice is saturated with fermions as a function of $\mu$.

- Continuum: $\rho \ll 1$ with $a\rho=\text{fixed}$

- exists within mean-field theory at low density
Numerical results
Numerical simulations


• Implemented Monte Carlo simulation of the canonical partition function for one-dimensional Fermi gas:
  • in a finite box
  • in a harmonic trap

• Studies include:
  • few-body energies
  • virial theorem
  • one-dimensional Bertsch parameter
Energy observable

\[ E = \lim_{\beta \to \infty} \frac{1}{\beta} \frac{d \log \hat{Z}(q)}{d \log \omega} \]

\[ \omega = \frac{1}{mL_0^2} \]

\[ = \lim_{\beta \to \infty} \frac{1}{\beta} \left[ \frac{\partial \log \hat{Z}(q)}{\partial \log m} + \frac{\partial \log \hat{Z}(q)}{\partial \log \kappa} + \left( -\frac{\partial \log g_c}{\partial \log m} \right) \frac{\partial \log \hat{Z}(q)}{\partial \log g_c} \right] \]

kinetic (T)  potential (V)  interaction (I)
Energy observable

\[ E = \lim_{\beta \to \infty} \frac{1}{\beta} \frac{d \log \hat{Z}(q)}{d \log \omega} \]

\[ \omega = \frac{1}{mL_0^2} \]

\[ = \lim_{\beta \to \infty} \frac{1}{\beta} \left[ \frac{\partial \log \hat{Z}(q)}{\partial \log m} + \frac{\partial \log \hat{Z}(q)}{\partial \log \kappa} + \left( -\frac{\partial \log g_c}{\partial \log m} \right) \frac{\partial \log \hat{Z}(q)}{\partial \log g_c} \right] \]

kinetic (T) \hspace{2cm} potential (V) \hspace{2cm} interaction (I)

\[ E = T + V + I \]

\[ E = 2V \text{ (Virial)} \]

\[ E = 2(T+I) \text{ (Virial)} \]
Continuum limit

- Symanzik action: lattice artifacts associated with higher-dimension operators in a *continuum* effective theory
- operator-state correspondence allows us to identify scaling dimensions of few-body operators
- lack of scales allows us to identify volume scaling via dimensional analysis in a perturbative expansion in couplings
- Non-trivial volume scaling for dimensionless observables:

\[
\mathcal{O}\left(\frac{b_s}{L_0}\right) = \mathcal{O}_{\text{cont}} + \mathcal{O}_1 \left(\frac{b_s}{L_0}\right) + \mathcal{O}_{1.6666} \left(\frac{b_s}{L_0}\right)^{1.6666} + \ldots
\]
Five-body system (trapped)

\[ q = (2,1,1,1) \]

(exact value = 2.333)

\[ E/\omega \]

\[ 1/L_0 \]

\[ (T+V+I)/\omega \]

\[ 2V/\omega \]

\[ 2(T+I)/\omega \]
Six-body system(s) (trapped)

\[ q = (3,1,1,1) \]

\[ E/\omega \]

\[ 1/L_0 \]

\[ q = (3,1,1,1) \]

\[ E/\omega \text{ (extrap.)} \]

\[ 1/L_0 \text{ (max.)} \]
Seven-body system(s) (trapped)
Few-body summary ($\leq 8$ trapped fermions)

$$Q = \sum_{\sigma} q_{\sigma}$$
Many-body systems (untrapped & trapped)

continuum extrapolated energies

thermodynamic limit extrapolation
Many-body systems (untrapped & trapped)

\[ \xi_{1d} = 0.370(4) \]
\[ \xi_{1d} = 0.372(1) \]
3d Bertsch parameter

1d result agrees within 1% errors of most recent 3d results!
Summary/Outlook
Summary

- Despite their simplicity, universal Fermi gases exhibit rich and fascinating physics!
- Found a solution to the “sign problem” for 1d system
- Simulated a universal four-component Fermi gas in one spatial dimension
  - few-body energies in a trap agree with exact results
  - demonstrated restoration of virial theorem
- 1d & 3d Bertsch parameters are equal to within 1% errors
Outlook/Future plans

• Theoretical understanding of Bertsch equality
  • dynamical in origin?
  • due to symmetries (conformal, scale invariance)?
• Continue few/many body simulations:
  • “integrated contact density”
  • imbalanced few- and many-body systems
Thank you!