Pairing wave functions for quantum Monte Carlo methods

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Auxiliary field formalism

- Represent importance sampled wave function by a set of “walkers” $|R_i\rangle$ sampled from $\langle\Psi_T|R\rangle\langle R|\psi(t)\rangle$.
- To order Δt

$$
\begin{aligned}
e^{-(H-E_T)\Delta t} &= e^{-\frac{P^2}{2m}\Delta t} e^{-(V-E_T)\Delta t} \\
&= \int \frac{dX}{(2\pi)^{d/2}} e^{-\frac{X^2}{2}} e^{-\frac{i}{\hbar}PX\sqrt{\frac{\hbar^2\Delta t}{m}}} e^{-(V-E_T)\Delta t} \qquad (1) \\
e^{-\frac{i}{\hbar}PA}|R\rangle &= |R+A\rangle
\end{aligned}
$$

- Propagation with importance sampling

$$
\begin{aligned}
&\int \frac{dX}{(2\pi)^{d/2}} e^{-\frac{X^2}{2}} \frac{\langle\Psi_T|e^{-\frac{i}{\hbar}PX\sqrt{\frac{\hbar^2\Delta t}{m}}}|R\rangle}{\langle\psi_T|R\rangle} e^{-\frac{i}{\hbar}PX\sqrt{\frac{\hbar^2\Delta t}{m}}}|R\rangle \\
&= \int \frac{dX}{(2\pi)^{d/2}} e^{-\frac{\left(X-\frac{i}{\hbar}\sqrt{\frac{\hbar^2\Delta t}{m}}P_L(R)\right)^2}{2}} e^{-(E_L(R)-E_T)\Delta t} e^{-\frac{i}{\hbar}PX\sqrt{\frac{\hbar^2\Delta t}{m}}}|R\rangle
\end{aligned}
\qquad (2)
$$

Auxiliary field formalism for other systems

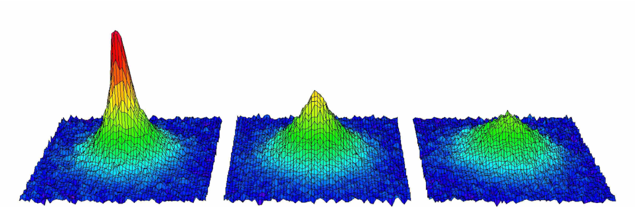
- In each case we typically write the Hamiltonian as a sum of squared operators O_n.
- We typically choose the walker basis such that $e^{-iO_n\sqrt{\Delta t}}$ operating on a walker gives one new walker possibly multiplied by a weight.
- For neutron matter the walkers are the positions as in diffusion Monte Carlo along with a spinor for each particle. The spin-dependent potential is written as the sum of squares of linear combinations of Pauli spin operators for each particle.
- For lattice Hamiltonians, the walkers are a set of orbitals, one for each particle, given by the amplitude for finding a single particle on each lattice site. The hamiltonian is written as the sum of squares of a linear combination of hopping operators.
- Importance sampling, drift, and the local energy are derived as for diffusion Monte Carlo.

Fermions can become superfluid

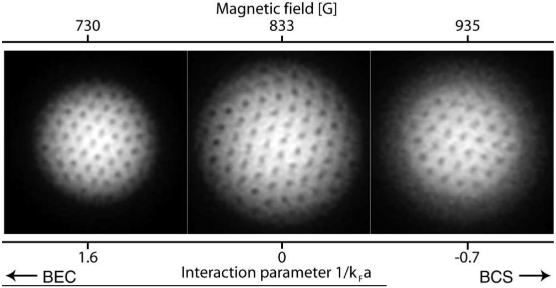
- Superconductivity is superfluidity of charged system (H. Kamerlingh Onnes 1911).
- Electronic superconductivity explained by J. Bardeen, L. Cooper, R. Schrieffer, (BCS) in 1957.
- You can think of this as fermions pairing to become Cooper pairs which are effectively bosons. These bosons Bose condense.
- John Bardeen hated this idea. In most superconductors the size of a Cooper pair is such that there are many other electrons between the paired electrons.
- Cold fermi atoms can be used to explore the regime from large Cooper pairs (BCS) to small Cooper pairs (BEC).

Fermion superfluidity in Cold Atoms

Cold Fermi atoms can become superfluid



Time of flight, ^{40}K.[1]



Superfluid Vortices[2]

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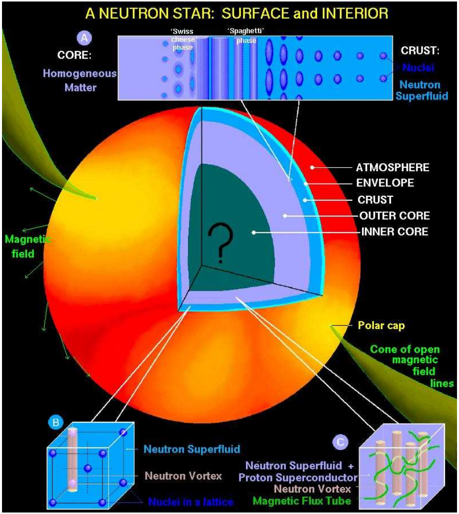
[1] C.A. Regal, M. Greiner, and D.S. Jin, PRL **92** 040403 (2004).

[2] Zwierlein et al.,Nature **435** 1047 (2005).

Superfluidity in Neutrons

Neutron matter in neutron star crusts should be superfluid.[3]



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[3] D. Page and S. Reddy, Annu. Rev. Nucl. Part. Sci. **56**, 327 (2006).

Slater determinants and BCS pairing

- Most Fermion trial wave functions are built out of Slater determinants of single-particle orbitals.

$$\Psi_T = \mathcal{A}[\psi_1(\boldsymbol{r}_1, s_1)\psi_2(\boldsymbol{r}_2, s_2)...\psi_N(\boldsymbol{r}_N, s_N)]$$

  - Linear combinations.
  - Backflow correlations $\Rightarrow \boldsymbol{r}_i \to \boldsymbol{r}_i + \sum_{j\neq i} \xi_{ij}\boldsymbol{r}_{ij}$.
- Fermion with pairing correlations are more efficiently described by BCS pairing wave functions,

$$\begin{aligned}\Psi_T &= \mathcal{A}[\phi(\boldsymbol{r}_1, s_1; \boldsymbol{r}_2, s_2)...\phi(\boldsymbol{r}_{N-1}, s_{N-1}; \boldsymbol{r}_N, s_N)] \\ &= \mathcal{A}[\phi_{12}\phi_{34}...\phi_{N-1\,N}] \,.\end{aligned}$$

General Properties

- For equal numbers of spin-up and spin-down fermions, the slater determinant can be written in the BCS form.
- An arbitrary BCS form corresponds to a large linear combination of slater determinants.
- Nodal Structure of the BCS form and Slater determinants can be quite different.

Relationship to Standard BCS

The BCS form used here is the standard BCS form projected onto N particles.

For a bulk system of spin singlet pairs,

$$\begin{aligned}
|BCS\rangle &= \prod_{\boldsymbol{k}} \left[u_k + v_k c^{+}_{\boldsymbol{k}\uparrow} c^{+}_{-\boldsymbol{k}\downarrow} \right] |0\rangle \\
\phi(\boldsymbol{r}_1, s_1; \boldsymbol{r}_2, s_2) &\propto \sum_{\boldsymbol{k}} \frac{v_k}{u_k} \cos\left(\boldsymbol{k} \cdot [\boldsymbol{r}_1 - \boldsymbol{r}_2]\right) \left[\langle s_1 s_2 | \uparrow\downarrow\rangle - \langle s_1 s_2 | \downarrow\uparrow\rangle \right]
\end{aligned}$$

In general

$$\begin{aligned}
|BCS\rangle &= \prod_{n} \left[u_n + v_n c^{+}_{n} c^{+}_{n'} \right] |0\rangle \\
\phi(\boldsymbol{r}_1, s_1; \boldsymbol{r}_2, s_2) &\propto \sum_{n} \frac{v_n}{u_n} \left[\psi_n(\boldsymbol{r}_1, s_1)\psi_{n'}(\boldsymbol{r}_2, s_2) - \psi_n(\boldsymbol{r}_2, s_2)\psi_{n'}(\boldsymbol{r}_1, s_1) \right]
\end{aligned}$$

Pairing wave functions as determinants and Pfaffians

First described by Lhuillier and coworkers, [4]
The Pfaffian is

$$\mathrm{Pf} A = \mathcal{A}[a_{12} a_{34} a_{45} \ldots a_{N-1,N}]$$

with the result normalized so that every equivalent term occurs only once, and $a_{ij} = -a_{ji}$.
For $N = 4$:

$$\mathrm{Pf} A = [a_{12} a_{34} - a_{13} a_{24} + a_{14} a_{23}]$$

The Pfaffian is zero if N is odd and has $(N-1)!!$ terms otherwise.

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[4] J. P. Bouchaud, A. Georges, and C. Lhuillier, “Pair Wave-functions for strongly correlated fermions and their determinantal representation,” J. Physique **49**, 553 (1988), and references therein.

Pfaffian properties

The Pfaffian can be constructed recursively as

$$\begin{aligned}\mathrm{Pf}A &= \sum_{\text{cyc perms of } 2\ldots N} a_{12}\mathcal{A}[a_{34}a_{56}\ldots a_{N-1,N}] \\ &\equiv \sum_{j=2}^{N} a_{1j}P_c(a_{1j})\end{aligned}$$

$P_c(a_{1j})$ is the Pfaffian cofactor of a_{1j}.
In general a skew-symmetric matrix A

$$A = \begin{pmatrix} 0 & a_{12} & a_{13} & a_{14} \\ -a_{12} & 0 & a_{23} & a_{24} \\ -a_{13} & -a_{23} & 0 & a_{34} \\ -a_{14} & -a_{24} & -a_{34} & 0 \end{pmatrix},$$

has the Pfaffian given above.
The determinant of A is the square of the Pfaffian.

Pfaffian computation

I. Exchange of particle *i* and *j* corresponds to interchanging rows *i* and *j* *and* interchanging colummns *i* and *j*.
    a. The Pfaffian changes sign.
    b. The determinant is invariant.
    c. We can use this to pivot the matrix for better roundoff.

II. Adding a multiple of row *j* to row *k* while adding the same multiple of column *j* to column *k* keeps the matrix in skew-symmetric form.
    a. Substituting into the recursion definition of the Pfaffian shows that the additional terms are not antyisymmetric and cancel.
    b. The determinant is also invariant.

Pfaffian computation

Using the column containing a_{12} to eliminate a_{13} and a_{14}. Exactly the same operations are used with the row containing $-a_{12}$ to eliminate $-a_{13}$ and $-a_{14}$.

Using these rules, a 6x6 matrix can be reduced to a form

$$A' = \begin{pmatrix} 0 & a'_{12} & 0 & 0 & 0 & 0 \\ -a'_{12} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & a'_{34} & 0 & 0 \\ 0 & 0 & -a'_{34} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & a'_{56} \\ 0 & 0 & 0 & 0 & -a'_{56} & 0 \end{pmatrix}.$$

The pfaffian is the product $a'_{12}a'_{34}a'_{56}$, and the determinant is the square.

Pfaffian updates

Cayley showed[4]

$$
\mathrm{Det}\begin{pmatrix} 0 & b_{12} & b_{13} & \cdots & b_{1,N} \\ -a_{12} & 0 & a_{23} & \cdots & a_{2,N} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ -a_{1N} & -a_{2N} & -a_{3N} & \cdots & 0 \end{pmatrix}
$$

$$
= \mathrm{Pf}\begin{pmatrix} 0 & a_{12} & a_{13} & \cdots & a_{1,N} \\ -a_{12} & 0 & a_{23} & \cdots & a_{2,N} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ -a_{1N} & -a_{2N} & -a_{3N} & \cdots & 0 \end{pmatrix} \mathrm{Pf}\begin{pmatrix} 0 & b_{12} & b_{13} & \cdots & b_{1,N} \\ -b_{12} & 0 & a_{23} & \cdots & a_{2,N} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ -b_{1N} & -a_{2N} & -a_{3N} & \cdots & 0 \end{pmatrix}.
$$

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[4] A. Cayley, *Sur les déterminants gauches*, Journal für die reine angewandte Mathematik **38**, 93 (1849)

Pfaffian updates

The Pfaffian obtained by changing the space or spin coordinates of one particle can be calculated from the inverse, determinant and Pfaffian of *A* in order *N* operations.
Calling *B* the matrix with the first row and column changed, its Pfaffian is

$$\mathrm{Pf}B = \frac{\mathrm{Det}A \sum_j b_{1j} A^{-1}_{j1}}{\mathrm{Pf}A}$$

or since the square of the Pfaffian is the determinant,

$$\mathrm{Pf}B = \mathrm{Pf}A \sum_j b_{1j} A^{-1}_{j1}$$

which shows that the inverse transpose times the Pfaffian is the Pfaffian cofactor.

The determinant as bipartite Pfaffian

If the skew symmetric matrix is bipartite in the sense that if $a_{ij} \neq 0$ and $a_{i'j'} \neq 0$, then $a_{ii'} = a_{j,j'} = 0$, and we can pivot the matrix into the form

$$\begin{pmatrix} 0 & B \\ -B^T & 0 \end{pmatrix} .$$

Here B is the matrix of nonzero elements of A, B^T is the transpose of B, and 0 is the zero matrix. The Pfaffian of this matrix is the deteminant of B.

Pairing Wave Functions

A pairing wave function can be written in the form

$$a_{12} = \phi(\boldsymbol{r}_1, s_1; \boldsymbol{r}_2 s_2) \, .$$

Often better coordinates would be the relative and center of mass positions along with the spin singlet and triplet state amplitudes. Notice that with spin singlet pairing, evaluating the Pfaffian with particles 1 through $N/2$ up and $N/2+1$ through N down gives a bipartite matrix as in Eq. 3, and the singlet pairing function can be written as a determinant.

Combinations of paired and unpaired orbitals

A general state with n paired and o unpaired orbitals for a total of $N = 2n + o$ particles can be written as

$$\mathcal{A}[\phi_{12}\phi_{34}...\phi_{2n-1,2n}...\psi_1(2n+1)...\psi_o(N)]$$

which is the Pfaffian of the $(N+o) \times (N+o)$ matrix

$$\begin{pmatrix}
0 & \phi_{12} & \phi_{13} & \cdots & \phi_{1N} & \psi_1(1) & \cdots & \psi_o(1) \\
-\phi_{12} & 0 & \phi_{23} & \cdots & \phi_{2N} & \psi_1(2) & \cdots & \psi_o(2) \\
-\phi_{13} & \phi_{23} & 0 & \cdots & \phi_{3N} & \psi_1(3) & \cdots & \psi_o(3) \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
-\phi_{1N} & -\phi_{2N} & -\phi_{3N} & \cdots & 0 & \psi_1(N) & \cdots & \psi_o(N) \\
-\psi_1(1) & -\psi_1(2) & -\psi_1(3) & \cdots & -\psi_1(N) & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
-\psi_o(1) & -\psi_o(2) & -\psi_o(3) & \cdots & -\psi_o(N) & 0 & \cdots & 0
\end{pmatrix},$$

where the lower $o \times o$ section is all zeroes.
Notice that if all the $\phi_{ij} = 0$, the result is bipartite and reduces to the usual Slater determinant. Spin singlet pairing again reduces to a determinant.

Electronic Structure Examples

Work done by M. Bajdich, L. Mitas, L.K. Wagner, G. Drobny and KES.

Since the coulomb interaction does not flip spins, we can assign spins to the particles.
A singlet/triplet/unpaired (STU) orbital pfaffian wave function is given by

$$\Psi_{STU} = \mathrm{pf}\begin{bmatrix} \boldsymbol{\chi}^{\uparrow\uparrow} & \boldsymbol{\Phi}^{\uparrow\downarrow} & \boldsymbol{\varphi}^{\uparrow} \\ -\boldsymbol{\Phi}^{\uparrow\downarrow T} & \boldsymbol{\chi}^{\downarrow\downarrow} & \boldsymbol{\varphi}^{\downarrow} \\ -\boldsymbol{\varphi}^{\uparrow T} & -\boldsymbol{\varphi}^{\downarrow T} & 0 \end{bmatrix} \tag{3}$$

The bold symbols are block matrices/vectors of corresponding orbitals and T denotes transposition.

Single Pfaffian Results

Table: Total energies (a.u.) for N atom and dimer with amounts of correlation energy recovered, in VMC and DMC methods.

WF	N	E_{corr}[%]	N_2	E_{corr}[%]
HF	-9.628915	0	-19.44946	0
VMC/HF	-9.7375(1)	83.3(1)	-19.7958(5)	80.1(1)
VMC/BCS	-9.7427(3)	87.3(2)	-19.8179(6)	85.2(1)
VMC/STU	-9.7433(1)	87.8(1)	-19.821(1)	86.0(2)
DMC/HF	-9.7496(2)	92.6(2)	-19.8521(3)	93.1(1)
DMC/BCS	-9.7536(2)	95.7(2)	-19.8605(6)	95.1(1)
DMC/STU	-9.7551(2)	96.8(1)	-19.8607(4)	95.2(1)
Exact/est.	-9.759215	100	-19.88196	100

Mulitple Pfaffian results

Table: Percentages of correlation energies recovered for C, N and O atoms by VMC and DMC methods with different trial wave functions. Corresponding number of pfaffians/determinants *n* for each wave function is also shown. The estimated exact correlation energies for C,N,O are 0.1031, 0.1303, 0.1937 a.u., M. Dolg, Chem. Phys. Lett. **250**, 75 (1996)

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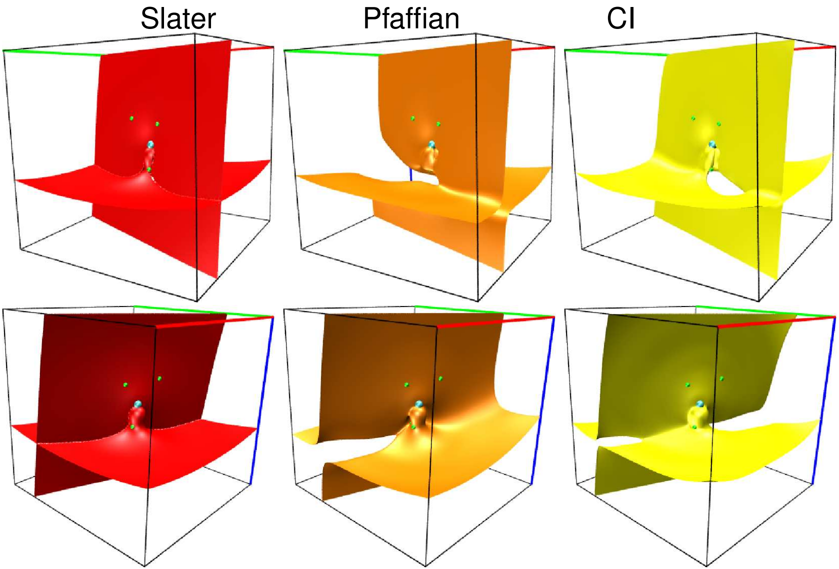
WF	*n*	C	*n*	N	*n*	O
VMC(MPF)	3	92.3(1)	5	90.6(1)	11	93.6(2)
VMC(CI)	98	89.7(4)	85	91.9(2)	136	89.7(4)
DMC(MPF)	3	98.9(2)	5	98.4(1)	11	97.5(1)
DMC(CI)	98	99.3(3)	85	98.9(2)	136	98.4(2)

Nodal Structure Differences – Oxygen Atom



Slater

Pfaffian

CI

Superfluid cold atoms

Experiments are ^{6}Li or ^{40}K atoms (fermions) in a trap cooled below the BCS/BEC (Bose-Einstein condensation) temperature.
Atomic potential is short ranged.
Scattering length can be tuned using a Feshbach resonance.

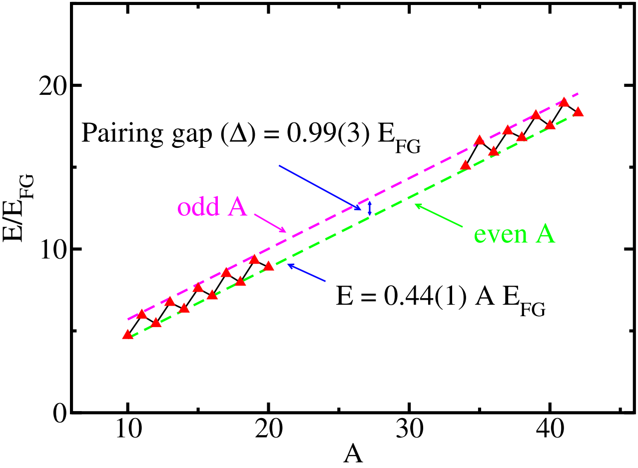
Unitary limit

- Infinite scattering length
$$a^{-1} = 0$$
is called unitary limit or at unitarity.
- Cross section has its maximum value (bigger means S-matrix is not unitary)
- Only length scale in homogeneous gas is interparticle spacing.
- Equation of state at unitarity is described by one number ξ,
$$\frac{E}{N} = \xi E_{FG} = \xi \frac{3}{5} \frac{\hbar^2 k_F^2}{2m}$$

Our First DMC calculations

Energy at unitarity

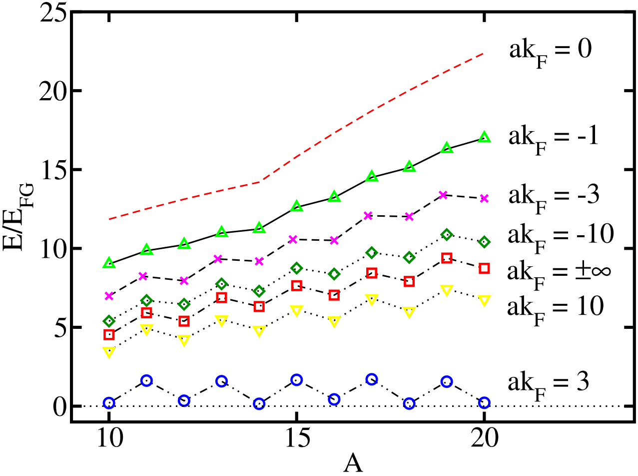
Slater determinant nodes give an energy of $E/N = 0.54 E_{FG}$.



From J. Carlson, S-Y Chang, V.R. Pandharipande, and KES PRL **91** 050401 (2003).

Our First DMC calculations

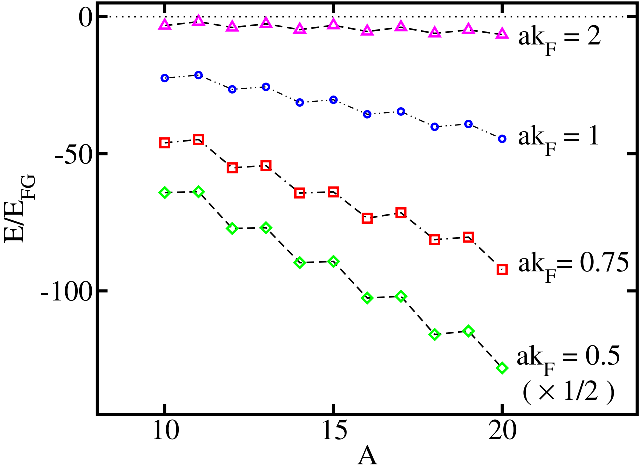
Energy away from unitarity



From S-Y Chang, V.R. Pandharipande, J. Carlson, and KES, PRA **70**,043602 (2004)

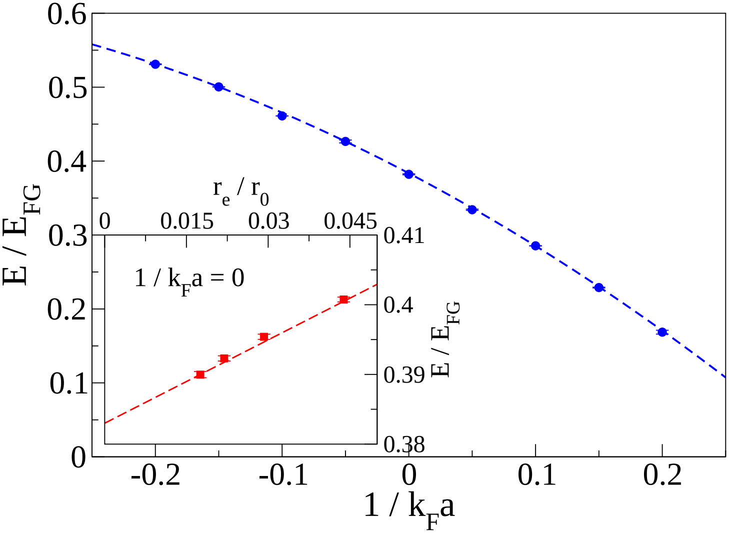
Our First DMC calculations

Energy away from unitarity



From S-Y Chang, V.R. Pandharipande, J. Carlson, and KES, PRA **70**,043602 (2004)

Energy per particle near unitarity

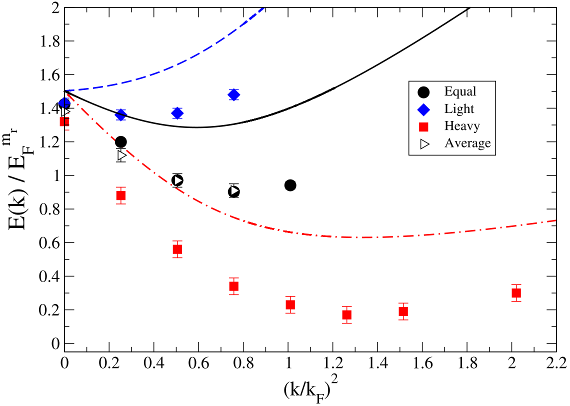


$\xi = 0.383(1)$, $\zeta = 0.901(2)$, $\nu = 0.49(2)$.

S. Gandolfi, KES, J. Carlson, Phys. Rev. A **83**, 041601 (2011).

Excitation spectrum

We add an extra particle with momentum $\hbar k$.



A. Gezerlis, S. Gandolfi, KES, and J. Carlson, Phys. Rev. Lett. **103**, 060403 (2009).

Superfluidity with auxiliary field quantum Monte Carlo

- Diffusion in space of Slater determinants.
- With attractive interactions up-spin determinant and down-spin determinant are always identical – no fermion sign problem!
- Uses a truncated plane-wave basis – Equivalent to a lattice in real space.
- Use a BCS wave function to help sample the random walk. Same mathematics as in electronic structure.

Lattice Hamiltonian

- A kinetic energy for the particle ϵ_k for momentum $\hbar k$. Get correct continuum limit if it goes to $\frac{\hbar^2 k^2}{2m}$ for wavelengths much greater than lattice spacing.
- An attractive onsite interaction $U < 0$.
- Becomes attractive Hubbard model for a particular choice of ϵ_k.
- Previous best Hubbard calculations used 14 particles and an 8^3 lattice ,D. Lee, Phys. Rev. C **78**, 024001(2008). We find more than a 100 fold speed up for this system with a BCS guiding function.
- This speed up grows exponentially for larger systems. Our largest simulations have 27^3 lattices. We use up to 66 particles.

$$H = \frac{1}{N_k^3} \sum_{\boldsymbol{k},\boldsymbol{j},\boldsymbol{m},s} \psi^\dagger_{\boldsymbol{j}s} \psi_{\boldsymbol{m}s} \epsilon_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_{\boldsymbol{j}} - \boldsymbol{r}_{\boldsymbol{m}})} + U \sum_{\boldsymbol{i}} n_{\boldsymbol{i}\uparrow} n_{\boldsymbol{i}\downarrow} \,. \tag{4}$$

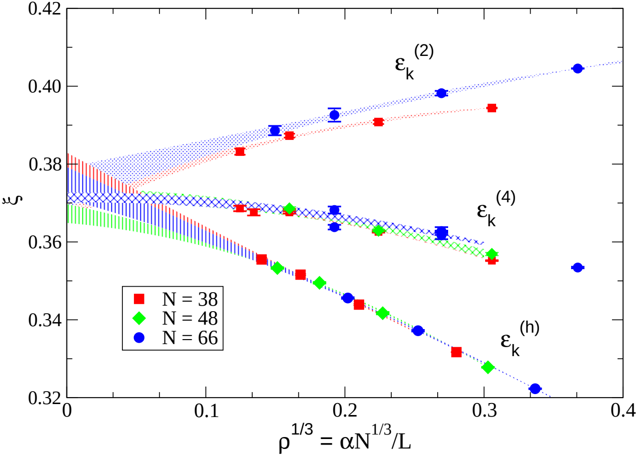
Different kinetic energy forms at unitarity

α is lattice spacing.

$$\begin{aligned}
\epsilon_k^{(h)} &= \frac{\hbar^2}{m\alpha^2}[3 - \cos(k_x\alpha) - \cos(k_y\alpha) - \cos(k_z\alpha)] \\
\epsilon_k^{(2)} &= \frac{\hbar^2 k^2}{2m} \\
\epsilon_k^{(4)} &= \frac{\hbar^2 k^2}{2m}\left[1 - \beta^2 k^2 \alpha^2\right]
\end{aligned} \tag{5}$$

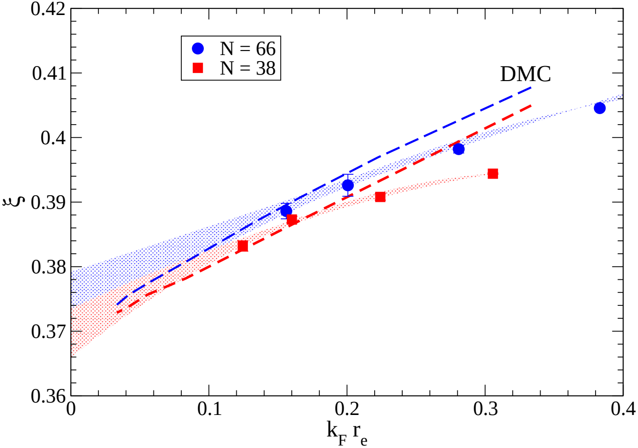
Energy	$U\frac{2m\alpha^2}{\hbar^2}$	β	$r_e\alpha^{-1}$
$\epsilon_{\boldsymbol{k}}^{(h)}$	-7.91355	-	-0.3057
$\epsilon_k^{(2)}$	-10.2887	-	0.3369
$\epsilon_k^{(4)}$	-8.66605	0.16137	0

Energy results



J. Carlson, S. Gandolfi, KES, S. Zhang, Phys. Rev. A **84**, 061602 (2011).

Universality of the equation of state on effective range



$\frac{E}{E_{FG}} = \xi + Sk_f r_e + \ldots$ with $\xi = 0.372 \pm 0.005$, $S = 0.12 \pm 0.03$, universal parameters at unitarity.

J. Carlson, S. Gandolfi, KES, S. Zhang, Phys. Rev. A **84**, 061602 (2011).

Argonne v_{18} family

- The Argonne[5], were developed for integral equation methods. They have weak nonlocality and substantially more local repulsion at short distances than other potentials. This makes them popular for integral equations and Monte Carlo calculations, but less popular for shell model and coupled-cluster calculations.
- They have the form:

$$V = \sum_{p=1}^{N_{\rm op}} v_p(r_{ij}) O^p_{ij} \tag{6}$$

- The first 14 operators are $(1,\ \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j,\ t_{ij},\ \boldsymbol{L}_{ij} \cdot \boldsymbol{S}_{ij},\ L^2,\ L^2(\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j),\ (\boldsymbol{L}_{ij} \cdot \boldsymbol{S}_{ij})^2$ and these multiplied by $\tau_i \cdot \tau_j$. The last 4 operators break isospin invariance. Defining $T_{ij} \equiv 3\tau_{iz}\tau_{jz} - \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$, they are $T_{ij},\ T_{ij}\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j,\ T_{ij}t_{ij}, \tau_{iz} + \tau_{jz}$. $\boldsymbol{L} \cdot \boldsymbol{S}$ is the spin orbit operator $\boldsymbol{L}_{ij} = \frac{1}{2}\boldsymbol{r}_{ij} \times (\nabla_i - \nabla_j)$, $\boldsymbol{S}_{ij} = \frac{1}{2}(\boldsymbol{\sigma}_i + \boldsymbol{\sigma}_j)$.

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[5] R. B. Wiringa, V. G. J. Stoks, R. Schiavilla, *Accurate nucleon-nucleon potential with charge-independence breaking*, Phys. Rev C **51**, 38-51, (1995).

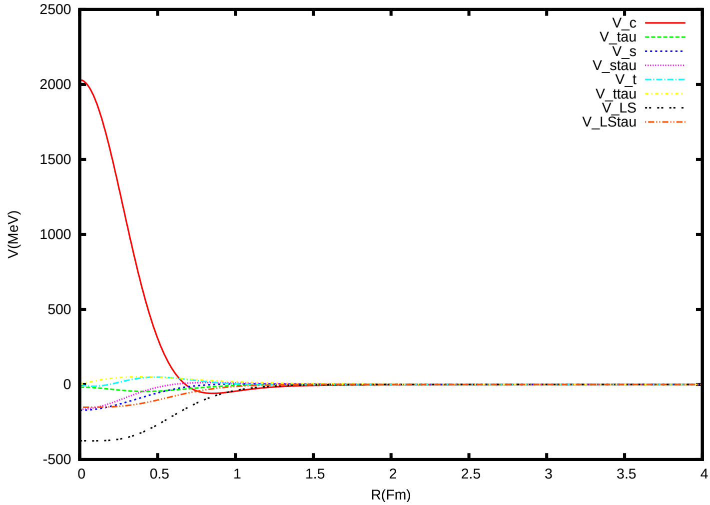
Argonne v_{18} terms

Physics:

- 1 (central) potential
- $(\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)$ is 1 in spin triplet $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, $|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$ states, -3 in spin singlet $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$ states.
- t_{ij} tensor (spin dipole-dipole) operator as in one pion exchange.
- $\boldsymbol{L} \cdot \boldsymbol{S}$, couples spin and orbital angular momentum – interaction conserves total $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$. This term is momentum dependent.
- $(\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j)$ acts like $(\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)$ except on proton-neutron states.

Other terms are weaker and can often be included with perturbation theory.

Potential graph



The first 8 operators of Argonne v_{18}.

Basic Hamiltonian

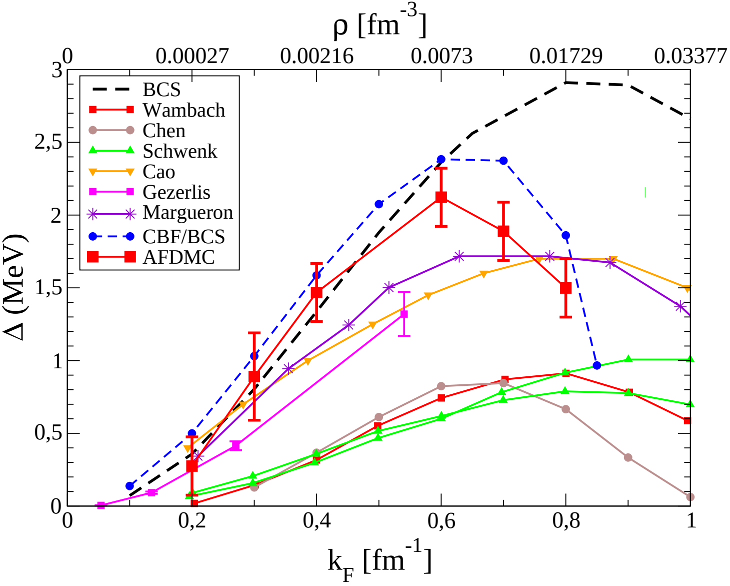
The Hamiltonian that nuclear Monte Carlo uses contains:

- Nonrelativistic kinetic energy

$$\sum_i \frac{p_i^2}{2m}$$

- Sum over pairs of a two-body potential such as Argonne v_{18}
- Sum over triplets of a three-body potential ...

Neutron energy gap calculations



Beyond pairing; Three- and four-body clusters of fermions

- Both of these require the hyperdeterminant (or hyperpfaffian) of a 4 index hypermatrix.
- Examples are:

$$\mathcal{A}\left[\phi(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3, \boldsymbol{r}_4)\phi(\boldsymbol{r}_5, \boldsymbol{r}_6, \boldsymbol{r}_7, \boldsymbol{r}_8)...\right]$$

or

$$\mathcal{A}\left[\phi_1(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3)\phi_2(\boldsymbol{r}_4, \boldsymbol{r}_5, \boldsymbol{r}_6)...\right]$$

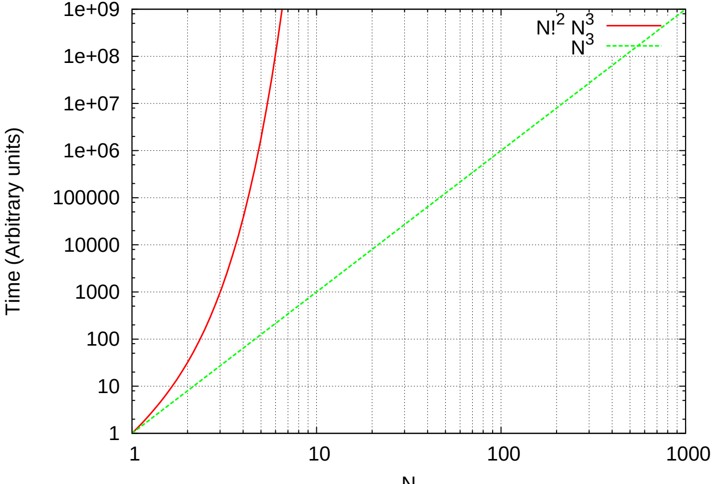
- If all the variables are antisymmetrized it is a hyperpfaffian.
- If the particles in the different slots are distinguishable (like different spins with a central potential) it is a hyperdeterminant.
- These were studied by Cayley and others but I know of no polynomial method for their evaluation.

Beyond pairing; Three- and four-body clusters of fermions

- The 4 index hyperdeterminant can be evaluated in $N!^2 N^3$ operations. That is direct summation over the permutations of 2 indices leaves the last two indices a determinant.
- There are possibly efficient stochastic methods for the evaluation.

Beyond pairing; Three- and four-body clusters of fermions

QMC with 20 or 24 particle clusters possible by brute force.
Work in progress...



Conclusions

- Pairing wave functions can be efficiently calculated for a variety of quantum systems.
- Adding pairing correlations can dramatically speed up quantum Monte Carlo calculations
- Pairing correlations can reproduce the nodal structure in electronic systems.
- Carefully optimized fixed-node DMC calculations and selected AFQMC calculations can extract the universal parameters for Cold atoms.
- Agreement with condensed matter experiments gives us some confidence that our neutron star matter calculations are accurate.
- Small systems with three- and four-body clustering can be simulated. More efficient methods for hyperdeterminants/hyperpfaffians are needed for larger systems.

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Figure Description

A three-dimensional cut through the fermion node hypersurface of oxygen atom obtained by scanning the wave function with a spin-up and -down (singlet) pair of electrons at equal positions, while keeping the rest of electrons at a given VMC snapshot positions (small green spheres). Nucleus is depicted in the center of the cube by the blue sphere. The three colors (from left to right) show nodes of: Hartree-Fock (red/dark gray); multi-pfaffian nodes (orange/medium gray); and the nodes of the CI wave function (yellow/light gray) in two different views (upper and lower rows). The CI nodal surface is very close to the exact one (see text). The HF node clearly divides the space into four nodal cells while pfaffian and CI wave functions partitioning leads to the minimal number of two nodal cells. The changes in the nodal topology occur on the appreciable spatial scale of the order of 1 a.u.