Quantum Monte Carlo
J. Carlson - LANL

- Simple Explanation
- History
- Some Applications
- Ground-States
  - Weak Binding
  - Efimov Regime
- Low-Energy Scattering
- Static Response
- Dynamic Response
- Challenges
<table>
<thead>
<tr>
<th>GFMC/DMC</th>
<th>AFMC/SMMC</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\exp[-Ht]$ Evolve Particle Coordinates</td>
<td>$\exp[-Ht]$ Evolve Single-Particle Orbitals</td>
</tr>
<tr>
<td><strong>MC for kinetic term</strong></td>
<td><strong>MC for interaction</strong></td>
</tr>
<tr>
<td>$\exp[-T\delta\tau] = \exp[-\frac{(R-R')^2}{4\frac{\hbar^2}{2m} \delta\tau}]$</td>
<td>$\exp \left{ -\frac{a}{2}x^2 \right} = \sqrt{\frac{1}{2\pi a}} \int_{-\infty}^{\infty} \exp \left[ -\frac{y^2}{2a} - ixy \right] dy,$</td>
</tr>
<tr>
<td>$\exp[-Vt]$ explicitly</td>
<td>$\exp[-Tt]$ explicitly</td>
</tr>
</tbody>
</table>

Some Applications:
- Electron Gas
- Liquid He
- Light Nuclei
- Cold Atoms

Some Applications:
- Hubbard Model, ...
- Shell Model of Nuclei
- Cold Atoms
Quantum Monte Carlo methods

- **Stochastic Green function (SGF) algorithm**: An algorithm designed for bosons that can simulate any complicated lattice Hamiltonian that does not have a sign problem. Used in combination with a directed update scheme, this is a powerful tool.
- **Variational Monte Carlo**: A good place to start; it is commonly used in many sorts of quantum problems.
- **Diffusion Monte Carlo**: The most common high-accuracy method for electrons (that is, chemical problems), since it comes quite close to the exact ground-state energy fairly efficiently. Also used for simulating the quantum behavior of atoms, etc.
- **Path integral Monte Carlo**: Finite-temperature technique mostly applied to bosons where temperature is very important, especially superfluid helium.
- **Auxiliary field Monte Carlo**: Usually applied to lattice problems, although there has been recent work on applying it to electrons in chemical systems.
- **Reptation Monte Carlo**: Recent zero-temperature method related to path integral Monte Carlo, with applications similar to diffusion Monte Carlo but with some different tradeoffs.
- **Gaussian quantum Monte Carlo**

Implementations

- ALPS
- CASINO
- CHAMP
- Monte Python
- PIMC++
- pi-qmc
- QMcBeaver
- QmcMol
- QMCPACK
- Qumax
- Qwalk
- TurboRVB
- Zori
(some) History:
MC calculation of the ground state of 3- and 4-body nuclei, M. H. Kalos, PR 128, 1797 (1962).


DMC Algorithm (shortest version)

- Start with a set of ‘configurations’
  each configuration with coordinates $R$
  (spin-isospin amplitudes $\alpha_i$),
  initially from VMC with probability $|\sum \beta^* \alpha_i|$
  where $\beta_i = \alpha_i$ determined from trial state

- For each sample new $R'$ from
  $\exp[-(R'_i - R_i)^2/(\frac{4\hbar^2}{2m_i} \Delta \tau)]$

- Calculate new amplitudes
  $\alpha'_j = \exp[-V \delta \tau]_{ji} \alpha_i$
  and $\beta_j$ from trial state at $R'$

- Form new weight $|\sum \beta^* \alpha_i|$ sample
  configurations proportional to weights

- Measure observables & repeat
Real work (insight) in:

Good trial state or source:

\[ |\Psi^i_T\rangle = S \prod_{i<j} F_{ij} |\Phi^i_T\rangle \]

Nuclear Physics: Fij spin/isospin dependent; |\Phi^i_T\rangle shell-model `like'

Improved propagator exp [ - H t ]

\[ \exp[-H\Delta\tau] \approx S \prod \frac{\exp[-H_{ij}\Delta\tau]}{\exp[-H_{ij}^0\Delta\tau]} \exp[-T\delta\tau] \]
Fixed Node

For fermions in a spin-independent potential, do not allow diffusion across surfaces where the trial function is zero.

Variational upper bound, can optimize the fixed-node surface.

Optimize at variational level, or try to optimize by including parameters as diffusing elements in random walk.

Test results by relaxing nodal constraint.
Electron Gas

Transient Estimation

Cold Atoms

Ceperley and Alder, PRL 1980
Light Nuclear Spectra

Argonne $v_{18}$
With Illinois-2
GFMC Calculations

$^{4}\text{He}$  $^{6}\text{He}$  $^{6}\text{Li}$  $^{7}\text{Li}$  $^{8}\text{He}$

$^{8}\text{Be}$  $^{9}\text{Be}$  $^{10}\text{Be}$  $^{10}\text{B}$  $^{12}\text{C}$

$^{12}\text{C}$ IL2 result is preliminary.
Weakly Bound Helium Isotopes

To what extent is the alpha core changed in He isotopes?
Convergence vs. Imaginary Time

Energy

Charge Radius

Note: long correlations in imaginary time (low-E modes)
Helium Charge Radii

Norterhauser, et al, PRL 2009
Hamiltonian for Cold Atoms

\[ H = \sum_{i=1,n_l} \frac{-\hbar^2}{2m_l} \nabla_i^2 + \sum_{j=1,n_h} \frac{-\hbar^2}{2m_h} \nabla_j^2 + \sum_{i,j} V(r_{ij}) \]

\[ v(r) = -\frac{2}{m} \frac{\mu^2}{\cosh^2(\mu r)} \]

strength, \( \mu \leftrightarrow \) scattering length & effective range

for cold atoms want \( \mu \Rightarrow \infty \), range \( \Rightarrow 0 \)

for heavy-light compare at same reduced mass
Gap and Effective Mass

\[ |\psi_{BCS}\rangle = \prod_{k} (u_k + v_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger) |0\rangle, \]

\[ \Psi_0 = \Psi_{BCS} = \prod_{k} \left[ v_k / u_k \right] a_{\uparrow}^\dagger(k) a_{\downarrow}^\dagger(-k) |0\rangle \]

particle projected BCS state

Add a particle of momentum \( k \)

\[ \Psi_1(k') = a_{\uparrow}^\dagger(k') \Psi_{BCS} = a_{\uparrow}^\dagger(k') \prod_{k} \left[ v_k / u_k \right] a_{\uparrow}^\dagger(k) a_{\downarrow}^\dagger(-k) |0\rangle \]

`Easy’ to add excitation with different quantum numbers
Superfluid at Equal Mass, $T=0$

BCS (Mean-Field) Theory: Strongly-paired Superfluid
gap of same order as Fermi Energy

\[ \xi \sim 0.40(0.01) = E / E_{FG} \]
\[ \Delta = 0.5 \ (0.05) \ E_F \]

Quasiparticle Dispersion
**Experiments at Unitarity:**

**Cloud Size and Sound Velocity**

**Cloud Size vs E (B):**

\[ \xi = 0.39(02) \]

**Energy vs. Entropy:**

\[ \xi = 0.41(02) \]

**Sound Propagation**

Joseph, et al., PRL 2007

\[ \frac{c_0}{v_f} = \frac{\xi^{1/4}}{\sqrt(5)} \]

scaling verified as \( \rho \) varied by 30!

\[ \xi = 0.435(15) \]

Luo and Thomas, JLTP, 2009
Normal State at Large $P$

One particle in a sea of non-interacting fermions

Binding $\sim 0.6$ $E_F$

Effective mass $\sim 1$

Calculate systems with total momentum $k$, extract $E(k)$

$k=0$ gives binding, curvature gives effective mass
Unequal Masses

We concentrate on $M_h/M_l = 6.5$ approximate $K/Li$ ratio

BCS Equations unchanged for constant reduced mass

Individual Quasiparticle Excitation Energies:

$$E_{h(l)}(k) = \frac{\xi_{h(l)}(k) - \xi_{l(h)}(k)}{2} + \sqrt{\left(\frac{\xi_h(k) + \xi_l(k)}{2}\right)^2 + \Delta^2(k)},$$

$\xi$ Unchanged

Average Quasiparticle Energy Unchanged
Heavy-Light Fermions at Unitarity

$M/m = 6.5$

Understand structure for $N_h >> N_l$

Gezerlis, Gandolfi, Schmidt, JC, PRL 2009
Larger Mass Ratios

For 2H, 1L get collapse and Efimov States at $M/m > 13.6$

Nishida, Son, Tan 2008

For $M/m = 8.62 - 13.6$ can get weakly interacting gas of dimers and trimers
In a gas of light particles, heavy particles are attractive at moderate distances.

Three and four heavy centers at fixed pair distances approximately equal to sum of pair interactions.
Binding of One Heavy or One Light

\[ B(H) = 0.36 \, E_F(L) \]

effective mass \( \sim 1.0 \)

\[ B(L) = 2.3 \, E_F(H) \]

effective mass \( \sim 1.3 \)

Agreement w/ previous calculations

Efimov Physics in Few-Body Heavy Light Systems

2 Heavy Fermions - 1 Light
Collapse at $M/m = 13.6$
Efimov, NPA 210, 157

Assume nodes independent of light particle

- $N_h = 2$: $r_{12} \cdot \hat{z}$
- $N_h = 3$: $r_{12} \times r_{13} \cdot \hat{z}$
- $N_h = 4$: $r_{12} \times r_{13} \cdot r_{1,234}$

Nodes when ‘volume’ goes to zero

Collapse: 
- $2H \ 1L \ M/m = 13.6$
- $3H \ 1L \ M/m \sim 10.5$
- $4H \ 1L \ M/m \sim 9.5$

Gandolfi & JC, 2010
Low Energy Scattering: Explicit States

Enforce Logarithmic Derivative at \( \mathbf{R} \)

\[
\Psi_{n+1}(\mathbf{R}') = \int_{|\mathbf{r}|<R_0} d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r} G(\mathbf{R}', \mathbf{R}; \Delta \tau) \\
\times \left[ \Psi_n(\mathbf{R}) + \frac{G(\mathbf{R}', \mathbf{R}_e; \Delta \tau)}{G(\mathbf{R}', \mathbf{R}; \Delta \tau)} \left( \frac{r_e}{r} \right)^3 \Psi_n(\mathbf{R}_e) \right].
\]

Multiple Solutions at same \( E \) for multi-channel scattering.

Also useful for

Asymptotic constants

Viviani talk, Nollett, ...

Nollett, et al, PRL 2007
Shorter-Range Correlations required for Parity Violation

**PV Interaction: Pion exchange plus short-range**

- Analogous to optical rotation in an "handed" medium.
- Transversely-polarized neutrons corkscrew due to the NN weak interaction
- **PV Spin Angle** is independent of incident neutron energy in cold neutron regime, $d\phi_{PV}/dx \sim 10^{-6}$ rad/m based on dimensional analysis
- $d\phi_{PC}/dx$ (due to B field) can be much larger than $d\phi_{PV}/dx$, and is $\nu_n$ dependent

\[ f(0) = f_{PC} + f_{PV} (\mathbf{\sigma} \cdot \mathbf{k}) \]

\[ \frac{1}{\sqrt{2}} \left( e^{-i(\phi_{PC} + \phi_{PV})} |z\rangle + e^{-i(\phi_{PC} - \phi_{PV})} |-z\rangle \right) \]

\[ \phi_{PV} = \varphi_+ - \varphi_- = 2\pi l \rho f_{PV} \]

\[ \phi_{PV}(n, ^4\text{He}) = - \left( 0.97 f_\pi + 0.22 h_0^0 - 0.22 h_0^1 + 0.32 h_\rho^0 - 0.11 h_\rho^1 - 0.02 h_\rho^1 \right) \text{rad/m} \]

\[ \phi_{PV}(n, ^4\text{He}) = (1.2 \lambda_s^{nn} + 0.6 \lambda_s^{np} + 1.3 \lambda_t - 2.7 \rho_1) m_n \]

Also: np→dγ, ...

---


For complicated case (multi-particle breakup), we can enforce simple (unphysical) boundary conditions. (for example $^{11}\text{Li}$).

What information does this contain about the S-matrix?
Static Response

\[ V_{ext}(r) = 2v_q \cos(q \cdot r) \]

\[ n_q = \chi(q)v_q + C_3v_q^3 \]

\[ E_v = E_0 + \chi(q)v_q^2 + C_4v_q^4 \]

Liquid He-4
Moroni, et al PRL 1992
Neutron Drops in an External Well (HO)

\[ \omega = 10 \text{ MeV} \]

\[ \omega = 5 \text{ MeV} \]

Preliminary

Implies significantly more repulsive isovector gradient terms

Carlson, Pieper, Gandolfi, preliminary
Neutron Drop Densities

\[ N \text{UTRON DROPS - SINGLETUBIOTIN} \]

\[ 8,14n \text{ (5 & 10 MeV) H.O. Well+AV8'+UIX - Ratio extrp } \rho_n \text{ - 12 May 2009} \]

\[ \rho_n \text{ (fm}^{-3}\text{)} \]

\[ r \text{ (fm)} \]

\[ 8n, 5 \text{ MeV} \]
\[ 8n, 10 \text{ MeV} \]
\[ 14n, 5 \text{ MeV} \]
\[ 14n, 10 \text{ MeV} \]

\[ 0.00 \quad 0.001 \quad 0.004 \quad 0.010 \quad 0.040 \quad 0.100 \quad 0.400 \]

\[ 0.00 \quad 0.001 \quad 0.004 \quad 0.010 \quad 0.040 \]

\[ 0 \quad 1 \quad 2 \quad 3 \quad 4 \quad 5 \quad 6 \quad 8 \]

\[ 0.0 \quad 0.5 \quad 1.0 \quad 1.5 \text{ (meV)} \]
Dynamic Response

Inclusive Scattering at Higher Energy
- Imaginary Time Response

Linear Response

\[ S(k, \omega) = \sum_f \langle 0 | \rho^\dagger(k) | f \rangle \langle f | \rho(k) | 0 \rangle \delta(E_f - E_0 - \omega) \]

for example for electron scattering longitudinal response

\[ \rho(k) = \sum_i \exp(i k \cdot r) \left[ 1 + \tau_z(i) \right]/2 \]

Can really only calculate imaginary time response

\[ E(k, \tau) = \int d\omega \ S(k, \tau) \exp[-\omega \tau] \]

\[ E(k, \tau) = \langle 0 | \rho^\dagger(k) \exp[-H \tau] \rho(k) | 0 \rangle \]
Transverse response shows importance of 2-body currents
Maximum Entropy Techniques used to reconstruct $S(k,w)$
Would be very interesting to do neutrino scattering on $^{12}$C
Major Challenges

More complete scattering (more channels), breakup
Bigger Nuclei / Nuclear - Neutron Matter
More General Interactions
Improved/ More Response Calculations