Many-body wave functions and sign problem

Stefano Gandolfi

Los Alamos National Laboratory (LANL)

Microscopic Theories of Nuclear Structure, Dynamics and
Electroweak Currents
June 12-30, 2017, ECT*, Trento, Italy

Let's consider a many-body general Hamiltonian describing a system of N particles.

$$H = -\frac{\hbar^2}{2m} \sum_i^N \nabla_i^2 + \sum_{i<j} v(r_{ij})$$

and we want to calculate the energy:

$$E_0 \leq E = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} = \frac{\int dr_1 \dots dr_N \, \Psi_T^*(r_1 \dots r_N) H \Psi_T(r_1 \dots r_N)}{\int dr_1 \dots dr_N \, \Psi_T^*(r_1 \dots r_N) \Psi_T(r_1 \dots r_N)}$$

where $\Psi_T(r_1 \dots r_N)$ is a variational wave function that depends on the coordinates (positions) of the particles, with variational parameters $\{\alpha\}$.

For a given form of $\Psi_T(r_1 \dots r_N)$ we want to find the best value(s) of α giving the lower energy, i.e. we need to study $E[\alpha]$. How do we solve the above integral?

Some definition:

- $r_i = (x_i, y_i, z_i, \dots)$ has coordinate(s) of particle i
- when used, $R = r_1 \dots r_N$ (and $dR = dr_1 \dots dr_N$)
- $\Psi(R) = \langle R | \Psi \rangle$

The many-body problem

A reasonable trial wave function for a homogeneous system (like, for example, a liquid) is:

$$|\Psi_T\rangle = \prod_{i<j} f(r_{ij})|\Phi\rangle \,,$$

where $|\Phi\rangle = 1$ for Bosons. The 'Jastrow' correlation $f(r_{ij})$ depends only upon the distance between the two particles. It keeps two particles from overlapping, and more or less at the right separation.
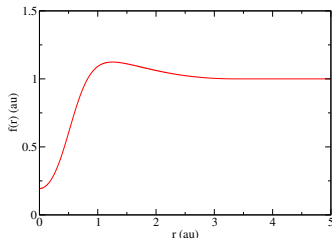
Note: the function $f(r)$ keep $H\Psi/\Psi$ finite even if the potential diverges (e.g. Coulomb).

For Fermions $|\Phi\rangle$ is a Slater determinant or a sum of Slater determinants.

A Slater determinant is an anti-symmetrized product of single particle states:

$$|\Phi\rangle = \mathcal{A} \prod_i [\phi_i(\mathbf{x_i})].$$

The square of the wave function is positive definite, so VMC works just like for Bosons.

Many Fermions wave function

- For unpolarized systems with two spin components (liquid 3He, electrons, cold atoms,...) we have the product of two determinants $|\Phi\rangle$, one for spin-up and one for spin-down particles (the interaction cannot change the spin of particles).
- These can be evaluated in the simulation as determinant
- The determinants have columns labeled by the state, and rows by the particle number
- The computer time is of order N^3 for a full evaluation.

$$|\Phi\rangle = \frac{1}{\sqrt{N}} \begin{vmatrix} \phi_1(r_1) & \phi_1(r_2) & \ldots & \phi_1(r_N) \\ \phi_2(r_1) & \phi_2(r_2) & \ldots & \phi_2(r_N) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_N(r_1) & \phi_N(r_2) & \ldots & \phi_N(r_N) \end{vmatrix}$$

Single particle orbitals

The single particle states depend upon the quantum numbers and the geometry of the system to study.

For homogeneous systems (N particles in a box of size L) a natural choice are plane waves (let's consider just one spin):

$$\phi_n(r) = \exp(i\,\vec{k_n} \cdot \vec{r})$$

where

$$k_1 = (0, 0, 0), \qquad k_2 = \frac{2\pi}{L}(1, 0, 0),$$
$$k_3 = \frac{2\pi}{L}(-1, 0, 0), \quad k_4 = \frac{2\pi}{L}(0, 1, 0),$$
$$\cdots$$

Single particle orbitals

For finite systems like nuclei, a good wave faction has typically good total angular momentum J, M (particles now have also spin s):

$$\Phi_{JM}(R, S) = \sum_n k_n \Big[\sum D\{\phi_\alpha(r, s)\} \Big]_{JM},$$

$$\phi_\alpha(r, s) = f_{nj}(r) \left[Y_{lm_l}(\hat{r}) \xi_{sm_s}(s) \right]_{jm_j},$$

where $[\ldots]_{JM}$ means a linear combination of Slater determinants coupled with Clebsch-Gordan coefficients to have the quantum numbers JM.

Similar functions ξ can be also added to account for the isospin.

More details will be given later in lectures 5 and 6.

Sign problem

For Fermionic wave function, Diffusion Monte Carlo methods suffer of the (in)famous sign problem.

We have seen that operators in DMC are calculated as

$$\langle O \rangle = \frac{\sum_i^M \omega_i \frac{\langle \Psi_T(x)|\hat{O}|W_i\rangle}{\langle \Psi_G(x)|W_i\rangle}}{\sum_i^M \omega_i \frac{\langle \Psi_T(x)|W_i\rangle}{\langle \Psi_G(x)|W_i\rangle}}$$

(Ψ_G is always positive as it is used to sample the configurations). Since the propagator G as introduced before is symmetric, the distribution of walkers will span over all the volume, and quickly the denominator above $\sum_i \Psi_T(W_i)/\Psi_G(W_i)$ will average to 0, and quickly increase the "signal" to "noise" ratio.

Fixed node approximation

Workaround: solve the problem in a restricted space where $\Psi > 0$. Kill a configuration if the wave function changes sign. In such a way, $\Psi(R, \tau)$ is always positive.

This is called **fixed node** (FN) approximation.

- The solution Ψ_{FN} is the ground state of an Hamiltonian with an infinite potential at the nodal surface
- Therefore Ψ_{FN} is an eigenstate of a different Hamiltonian H_{FN}
- Variational principle: $E_{FN} = \langle \Psi_{FN} | H | \Psi_{FN} \rangle \geq E_0$

Since the nodal surface determines the "quality" of the upperbound, a very careful optimization of the wave function is crucial!

For matter, plane waves can be improved by adding backflow, pairing, etc.
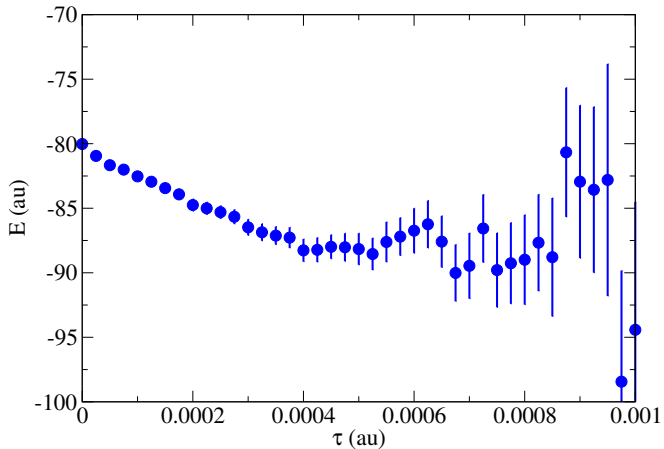
For finite systems by optimizing of the radial part of single particle states, or including low-lying excitations, etc.

There are other general possible improvements, like wave functions that include pairing, multi-determinant wave functions, etc...

Transient Estimation

The fixed-node energy can be improved by removing the fixed-node condition:

- Start with a FN simulation with an importance function Ψ_G that does not go to zero when Ψ_T does
- Allow walkers to pass through the surface where Ψ_T changes sign
- Keep calculating the numerator and denominator as before, and plot against the imaginary-time τ

Transient Estimation

Just an example:

... for now :-)