Outline

- Coupled Harmonic Oscillator Code
- Sampling function
- VMC Walk
- VMC Averages
- DMC Walk
- DMC Averages
- History
- Effective Mass
- Response

Coupled Harmonic Oscillators

Same example as last time with code:

$$H = -\tfrac{\hbar^2}{2m}\nabla^2 \ + \begin{bmatrix} r^2 & z \\ z & 1+r^2 \end{bmatrix}$$

The code is general to *ndim dimensions* and *npart particles*, both set in params.f90. In general the Hamiltonian is

$$H = -\frac{\hbar^2}{2m}\nabla^2 \ + \sum_i |i\rangle \omega_{0,i} + \omega_i r_i^2 \ \langle i| \ + \sum_{i \neq j} |i\rangle \ |\gamma_{i,j} \sum_k {x_k}^{|i-j|} \langle j|$$

where the parameters $\omega_i, \omega_{0,i}$, and $\gamma_{i,j}$ are input. Other Hamiltonians can easily be input in 'wavefunction.f90'.

Wave function

The general form of the wave function is

$$|\Psi_i\rangle \;=\; \sum_i \beta_i \sum_k x_k^{i-1} \; \exp[-\alpha_i \sum_{k=1,N} \mathbf{r}_k^2] |i\rangle$$

where the parameters β_i and α_i are also inputs.

This can be changed in 'wavefunction.f90', note check of numerical derivatives is available.

Sampling function

In general the overlap of the propagated wave function Ψ_T (called 'psi' in the program) with the trial wave function Ψ_T (called 'psit' in the program) may not be positive or even real. We define a 'normal'

overlap function and a positive definite function used for sampline in both VMC and DMC in code 'spinops.f90'.

```
      complex(kind=r8) function cov(psil,psir)
      complex(kind=r8),dimension (nchan) :: psil,psir
      cov=dble(sum( conjg(psil(:))*psir(:)))
      return
      end function
      real(kind=r8) function acov(psil,psir)
!        a positive real function used for sampling dmc or
      complex(kind=r8),dimension (nchan) :: psil,psir
      acov=abs(dble(sum( conjg(psil(:))*psir(:))))+ &
    &                 0.01*sum(abs(conjg(psil(:))*psir(:))
      return
      end function
```

VMC observables

The random walk is taken with probabilities drawn from the function $G(\Psi_T, \Psi(\tau)$ calculabed from 'acov (psit, psil)'.

The expectation values are

$$\langle O \rangle \;=\; \frac{\frac{\langle \Psi_T | \mathcal{O} | \ominus(\tau) \rangle}{G(\Psi_T, \Psi(\tau)\rangle}}{\frac{\langle \Psi_T | 1 | \Psi(\tau) \rangle}{G(\Psi_T, \Psi(\tau)\rangle}} \qquad (1)$$

See 'operators.f90'. I have added expecation values for $\langle x^2 \rangle$ and $\langle r^2 \rangle$.

Diffusion Monte Carlo

The DMC calculation starts from the configurations generated by VMC. The code reads in a flag iread to either (0 - generate new configs randomly) or (1 - read in configurations from the file 'conin'). The codes (both VMC and DMC) write out the configurations to the file 'conout'. At the beginning of the DMC, the VMC and DMC

wave functions are equal. For each step the code computes two possible new steps:

$$\begin{aligned} \mathbf{R}_+ &= \mathbf{R}_0 + \delta\mathbf{R} \\ \mathbf{R}_- &= \mathbf{R}_0 - \delta\mathbf{R} \end{aligned}$$

where the (same) $\delta\mathbf{R}$ is chosen from the free-particle gaussian. It then calculates the new $\Psi(\tau + \delta\tau)$ for each of these possible choices:

$$\begin{aligned} \Psi_+(\tau + \delta\tau) &= \exp[E_t \delta\tau][1 - V(:,:)(\delta\tau) + V(:,:)^2(\delta\tau)^2/2]\Psi(\tau) \\ \Psi_+(\tau + \delta\tau) &= \exp[E_t \delta\tau][1 - V(:,:)(\delta\tau) + V(:,:)^2(\delta\tau)^2/2]\Psi(\tau) \end{aligned} \tag{2}$$

These are the same except the potentials are the average of those at the original point and the $(+/-)$ point, respectively.

DMC step

Here *w*2 and *w*3 are the two new possible walkers.

```
            w2%sfunc=acov(w2%psit,w2%psi)
            w3%sfunc=acov(w3%psit,w3%psi)
            w2%weight= (w2%sfunc/w1%sfunc)*w1%weight
            w3%weight= (w3%sfunc/w1%sfunc)*w1%weight
            weight= (w2%weight+w3%weight)/2
!           write(6,*) 'weight = ',weight
            prob= w2%weight/(w2%weight+w3%weight)
            if (ran(w2%irn).lt.prob ) then
!               choose step w2
                w2%weight=weight
            else
!               choose step w3
                w3%irn=w2%irn
                w3%weight=weight
                w2=w3
            endif
```

Can easily generalize to more choices, but it becomes inefficient at some point. Measurements are just like in VMC.

Keeping a History

I have added a history to the particle positions of each walker. This keeps track of the history of each path for each particle. For now I keep nhist= 100 points.
Each configuration has a flag istep (# of vmc steps) and itau (# of dmc steps). For each step we store the coordinates in place mod(flag,nhist)+1, looking 1 forward is equivalent to looking 99 steps back.

For now the mixed estimates of x2 and r2 (called x2old and r2old) are written out along with x2 and r2. This gives a 'true' estimate of x2 and r2 rather than the 'mixed estimate' that is also printed out.

Effective Mass

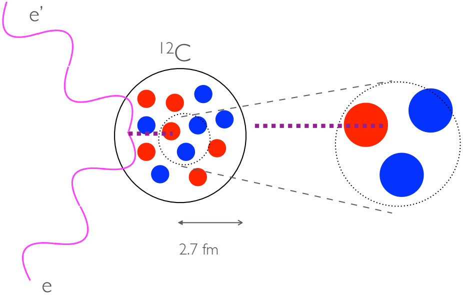
We could also keep track of how far each particle has defused over the last n steps. If we equate the average diffusion distance to a form relevant to free particles:

$$\exp[-r^2/(4\hbar^2\tau/2m)] \rightarrow \exp[-r^2/(4\hbar^2\tau/2m^\star)], \tag{3}$$

We can relate the average distance to the effective mass $m^\star$. For this problem the effective mass would be $\approx m$ for small τ, but eventually become larger because of the binding. The effective mass impacts the linear response functions of the system.

Response Functions

In many high-energy scattering experiments (neutron scattering, electron or neutrino scattering, the linear response of the system is measured.



The response function for an operator O is:

$$R^O(q,\omega) \;=\; \sum_f \langle \Psi_0 | O | f \rangle \langle f | O | \Psi_0 \rangle \delta(E_f - E_0 - \omega)$$

It depends on the energies of all final states in the system, but can be measured by the observing only the final state scattered particle.

Response

For operators O that only depend upon the particle coodinates, (and therefore commute with state-dependent operators), the imaginary time correlation response can be calculated.

$$\begin{aligned} R^O(q,\tau) &= \int d\omega Exp[-\omega\tau] R(q,\omega) \\ &= \sum_f \langle \Psi_0 | O | f \rangle \langle f | O | \Psi_0 \rangle \exp[-\omega_f \tau] \end{aligned}$$

This simple trick works for the density response, but for spin-dependent interactions, we hae to keep more information. This is particularly relevant for neutrino and electron scattering.