Flash Cards for Quantum/Nuclear Monte Carlo

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Parameters in the Code

g2bval(d2b,sxz,fij) Given sxz this computes the d2b terms.

hspot(???) ???

op2val(d2b,sp,spx) Makes tz, sz, and stz, and makes tau, sigma, and sigtau.

opmult(sp) This multiplies sp(s,i) by the 15 operators in this order 1-3 sx,sy,sz, 4-6 tx,ty,tz, 7-9 sx*(tx,ty,tz), 10-12 sy*(tx,ty,tz), 13-15 sz*(tx,ty,tz). This outputs opmult(s,kop,i)

sxzupdate(sxznew(out),detrat(out),sxzold,i,opi,sp) Here the outputted detrat is simply di(i).

vnpsi2(w,dopot) This subroutine returns the wave function, and the potential if dopot=.true.

cvs(2) $=\sum_{\alpha=1}^{3}\sum_{ss'=1}^{4}$ d2b(s,s',ij) $\langle ss'|\, v2(i,j)\tau_{\alpha i}\tau_{\alpha j}\,|s_i s_j\rangle$

cvs(3) $=\sum_{\alpha=1}^{3}\sum_{ss'=1}^{4}$ d2b(s,s',ij) $\langle ss'|\, v3(i,j)\sigma_{\alpha i}\sigma_{\alpha j}\,|s_i s_j\rangle$

cvs(4) $=\sum_{\alpha=1}^{3}\sum_{\gamma=1}^{3}\sum_{ss'=1}^{4}$ d2b(s,s',ij) $\langle ss'|\, v4(i,j)\sigma_{\alpha i}\tau_{\gamma i}\sigma_{\alpha j}\tau_{\gamma j}\,|s_i s_j\rangle$

cvs(5) $=\sum_{\alpha=1}^{3}\sum_{\beta=1}^{3}\sum_{ss'=1}^{4}$ d2b(s,s',ij) $\langle ss'|\, v5(\alpha,i,\beta,j)\sigma_{\alpha i}\sigma_{\beta j}\,|s_i s_j\rangle$

cvs(6) $=\sum_{\alpha=1}^{3}\sum_{\beta=1}^{3}\sum_{\gamma=1}^{3}\sum_{ss'=1}^{4}$ d2b(s,s',ij) $\langle ss'|\, v6(\alpha,i,\beta,j)\sigma_{\alpha i}\tau_{\gamma i}\sigma_{\beta j}\tau_{\gamma j}\,|s_i s_j\rangle$

d15(kop) =di(i)= $\sum_k S^{-1}_{ik}\langle k|\,\mathcal{O}_i\,|\mathbf{r},s_i\rangle = (S'/S)_{ii}$ for a specific kop (1 of 15)

d2b(s,s',ij) $= \frac{\langle\Phi|R,s_1,\ldots,s_{i-1},s,s_{i+1},\ldots,s_{j-1},s',s_{j+1},\ldots,s_A\rangle}{\langle\Phi|RS\rangle}$

d2bip(s,s',s",s"',ij,kl) $= \frac{\langle\Phi|R,s_1,\ldots,s,\ldots,s',\ldots,s'',\ldots,s''',\ldots,s_A\rangle}{\langle\Phi|R,S\rangle}$ OR

di(m) $= \sum_k S^{-1}_{mk} \langle k| \mathcal{O}_i |\mathbf{r_i}, s_i\rangle = \sum_s \text{opi(s, m)} \langle s|s_i\rangle$

f2b(s,s',ij) $= \sum_{kop=1}^{15} f^{kop}_{ij} \langle ss'| \mathcal{O}^{kop}_{ij} |s_i s_j\rangle$

fst(3,3,ij) $= f$ in front of specific operator

opi(s,m) $= \sum_k S^{-1}_{mk} \langle k| \mathcal{O}_i |\mathbf{r_i}, s\rangle = \sum_{s'} \text{sxz(s', i, m)} \langle s'| \mathcal{O}_i |s\rangle$

ph(i,4,j,idet) $= \sum_k S_{ik} \langle k| \mathcal{O}_j |s_j\rangle$

sigma(α,β,ij) $\sum_{ss'=1}^{4}$ d2b(s,s',ij) $\langle ss'| \sigma_{\alpha i}\sigma_{\beta j} |s_i s_j\rangle$

sigtau(α,β,γ,γ,ij) $\sum_{ss'=1}^{4}$ d2b(s,s',ij) $\langle ss'| \sigma_{\alpha i}\tau_{\gamma i}\sigma_{\beta j}\tau_{\gamma j} |s_i s_j\rangle$

sp(s,i) $= \langle s|s_i\rangle$

spx(s,15,i) $= \langle s| \mathcal{O}^p_i |s_i\rangle$, where p goes over the 15 cartesian coordinates.

stz(s,s') =spx(s,$\sigma_\alpha\tau_\gamma$,i)*spx(s',$\sigma_\beta\tau_\gamma$,j)= $\langle s, s'| \sigma_{\alpha i}\tau_{\gamma i}\sigma_{\beta j}\tau_{\gamma j} |s_i s_j\rangle$

sx15(s,15,i,j) $= \sum_k S^{-1}_{jk} \langle k| \sum_{kop=1}^{15} \mathcal{O}_{kop} |\mathbf{r}, s\rangle =$ opmult(sxz0), where sx15(:,kop,:,k) = opi(s,k)

sxz(s,i,j) $= \sum_k S^{-1}_{jk} \langle k|\mathbf{r}_i, s\rangle$

sxzi(s,i,j,iop) $= \sum_k S'^{-1}_{jk} S'_{ki}(s) = \sum_k S'^{-1}_{jk} \langle k| \mathcal{O}^{iop}_i |\mathbf{r}_i, s\rangle$

sxzj(s,i,j) $= \sum_k S''^{-1}_{jk} S''_{ki}(s) = \sum_k S'^{-1}_{jk} \langle k| \mathcal{O}^{iopjop}_{ij} |\mathbf{r}_i, s\rangle$, each *iop* and *jop* is looped over and added to d2b using call g2bval(d2b,sxzj,fij).

sz(s,s') =spx(s,σ_α,i)*spx(s',σ_β,j)= $\langle s, s'| \sigma_{\alpha i}\sigma_{\beta j} |s_i s_j\rangle$

tau(α,α,ij) $\sum_{ss'=1}^{4}$ d2b(s,s',ij) $\langle ss'| \tau_{\alpha i}\tau_{\alpha j} |s_i s_j\rangle$

tz(s,s') =spx(s,τ_α,i)*spx(s',τ_α,j)= $\langle s, s'| \tau_{\alpha i}\tau_{\alpha j} |s_i s_j\rangle$

Variational Monte Carlo

Steps for Metropolis Algorithm:

1. Start with some random walker configuration $\mathbf{R}$
2. Propose a move to a new walker $\mathbf{R}'$ from the distribution $T(\mathbf{R}' \leftarrow \mathbf{R})$
3. The probability of accepting the move is given by

$$A(\mathbf{R}' \leftarrow \mathbf{R}) = \min\left(1, \frac{T(\mathbf{R}' \leftarrow \mathbf{R})P(\mathbf{R}')}{T(\mathbf{R}' \leftarrow \mathbf{R})P(\mathbf{R})}\right).$$

   The move is accepted if $U[0,1] < A(\mathbf{R}' \leftarrow \mathbf{R})$.

4. Repeat from step 2.

Variational Energy (In terms of $E_L(\mathbf{R})$ and $P(\mathbf{R})$), x2 + E_L and P:

$$E_V = \frac{\int \Psi^*(\mathbf{R})\hat{H}\Psi(\mathbf{R})d\mathbf{R}}{\int \Psi^*(\mathbf{R})\Psi(\mathbf{R})d\mathbf{R}} = \int P(\mathbf{R})E_L(\mathbf{R})d\mathbf{R}$$

$$P(\mathbf{R}) = |\Psi_T(\mathbf{R})|^2 / \int |\Psi_T(\mathbf{R})|^2 d\mathbf{R}$$

$$E_L(\mathbf{R}) = \Psi_T^{-1}(\mathbf{R})\hat{H}\Psi_T(\mathbf{R})$$

Sampled Variational Energy:

$$E_V \approx \frac{1}{N}\sum_{n=1}^{N} E_L(\mathbf{R}_n)$$

where $\mathbf{R}_n$ are drawn from $P(\mathbf{R})$.

General Physics

Atomic Shell Model

- **Shells** are areas in which an electron can "orbit" a nucleus. They correspond to the principle quantum numbers (n=1,2,3,4,...) where n=1 is the closest shell.
- The number of allowed electrons is controlled by the spin statistics the other allowed quantum numbers being l=0,1,...,n-1 and ml=-l,...,l. The number allowed for each shell is all the possible times two since ms=-1/2,1/2.
- **Subshells** are given by the l quantum numbers where l=1,2,3,4 are s,p,d,f,g.
- List of how many each shell can hold

Nuclear Shell Model
The nuclear shell model is similar to the atomic shell model except that n=1,2,3,4,... and l=0,1,2,3,... independently from n. So you can have states like 1g

Shell name	Subshell name	Subshell max electrons	Shell max electrons
K	1s	2	**2**
L	2s	2	2 + 6 = **8**
	2p	6	
M	3s	2	2 + 6 + 10 = **18**
	3p	6	
	3d	10	
N	4s	2	2 + 6 + + 10 + 14 = **32**
	4p	6	
	4d	10	
	4f	14	

Definitions

Pedagogical: Of or relating to teachers or education.
Coherence length: It sounds like it's something like the length over which correlations/interactions can happen.
Cluster decomposition: If a system is cluster decomposable it means that the expectation value of a product of operators (each operating in seperate regions) is equal to the product the their individual expectation values.