Flash Cards for Quantum/Nuclear Monte Carlo

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Parameters in the Code

hspot(???) ???

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 ...???

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

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

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

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

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

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.

sx15(s,15,i,j) $= \sum_k S^{-1}_{jk} \langle k| \sum_{kop=1}^{15} \mathcal{O}_{kop} |\mathbf{r}, s\rangle = \mathrm{opmult(sxz0)}$, 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,n,m) $= \sum_k S'^{-1}_{mk} S'_{kn}(s)$

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 $P(\mathbf{R})$.