

Flash Cards for Quantum/Nuclear Monte Carlo

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Parameters in the Code

hspot(???) ???

sxzupdate(sxznew(out),detrat(out),sxzold,i,opi,sp)

vnpsi2(w,dopot) This subroutine ...???

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

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

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

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

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

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

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

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

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

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

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

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

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 $P(\mathbf{R})$), E_V 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 $P(\mathbf{R})$.