

# 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)** ???

**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)

**szxupdate(szxnew(out),detrat(out),sxzold,i,opi,sp)** Here the outputted detratt is simply di(i).

**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)** =  $\sum_k S_{ik} \langle k | \mathcal{O}_j | s_j \rangle$

**sigma(3,3,npair)** I think the 3 is x,y,z.

**sigtau(3,3,3,3,npair)** I think the 3 is x,y,z.

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

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

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

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

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

$$\mathbf{sxzi}(\mathbf{s}, \mathbf{n}, \mathbf{m}) = \sum_k S_{mk}'^{-1} S_{kn}'(s)$$

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

$$\mathbf{tau}(\mathbf{3}, \mathbf{3}, \mathbf{npair}) \text{ I think the 3 is x,y,z.}$$

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

## 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  $P(\mathbf{R})$ ),  $\mathbf{x2} + E_L$  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  $P(\mathbf{R})$ .