

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

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

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.

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

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

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

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

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

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

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

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

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

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

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 $P(\mathbf{R})$.

General Physics

Atomic Shell Model

- **Shells** are areas in which an electron can "orbit" a nucleus. They correspond to the principle quantum numbers ($n=1,2,3,4,\dots$) where $n=1$ is the closest shell.
- The number of allowed electrons is controlled by the spin statistics the other allowed quantum numbers being $l=0,1,\dots,n-1$ and $ml=-l,\dots,l$. 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

| Shell name | Subshell name | Subshell max electrons | Shell max electrons |
|------------|---------------|------------------------|---------------------------------|
| K | 1s | 2 | 2 |
| L | 2s | 2 | $2 + 6 = \mathbf{8}$ |
| | 2p | 6 | |
| M | 3s | 2 | $2 + 6 + 10 = \mathbf{18}$ |
| | 3p | 6 | |
| | 3d | 10 | |
| N | 4s | 2 | $2 + 6 + 10 + 14 = \mathbf{32}$ |
| | 4p | 6 | |
| | 4d | 10 | |
| | 4f | 14 | |

Nuclear Shell Model

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

Definitions

Pedagogical: Of or relating to teachers or education.