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)

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

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

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

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.

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.

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

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

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

sxzj(s,i,j) $= \sum_k S''^{-1}_{jk} S''_{ki}(s) = \sum_k S'^{-1}_{jk}\langle k|\,\mathcal{O}_{ij}^{iopjop}\,|\mathbf{r}_i,s\rangle$, 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(3,3,npair) I think the 3 is x,y,z.

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:

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

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

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

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

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	

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