Flash Cards for Quantum/Nuclear Monte Carlo

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Parameters in the Code

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

f2b(s,s',ij) $? = \langle ss'|\,\mathcal{O}^p_{ij}\,|s_i s_j\rangle$

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.

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 $P(\mathbf{R})$.