

Flash Cards for Quantum/Nuclear Monte Carlo

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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 $P(\mathbf{R})$), $E_V = \langle E_L \rangle$ 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 $P(\mathbf{R})$.

Parameters in the Code