Telluride Summer School AFQMC Exercises

July 15, 2017

Basic AFQMC Pseudocode

1. Construct One-Body Hamiltonian, K
2. Construct One-Body Propagator by Exponentiating One-Body Hamiltonian, $e^{-\Delta\tau K}$
3. Repeatedly Propagate:
    a. By One-Body Propagator, $e^{-\Delta\tau K/2}$
    b. Use HS Transformation to Transform Two-Body Propagator into One-Body Propagator, $e^{-\Delta\tau V}$
    c. By One-Body Propagator, $e^{-\Delta\tau K/2}$
    d. Measure Observables

Hubbard Hamiltonian

$$\hat{H}_{Hubbard} = -t \sum_{\langle i\, j\rangle,\sigma} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \hat{c}^{\dagger}_{j\sigma} \hat{c}_{i\sigma} \right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

One-Body Two-Body

Consists of One-Body Kinetic Terms and Two-Body Potential Terms

Propagation

$$|\Psi_G\rangle = \lim_{n\to\infty}\left(e^{-\Delta\tau\hat{H}}\right)^n |\Psi_{Trial}\rangle$$

$$\begin{aligned}|\Psi^{(n+1)}\rangle &= e^{-\Delta\tau\hat{H}}|\Psi^{(n)}\rangle \\ &\approx e^{-\Delta\tau\hat{K}/2}e^{-\Delta\tau\hat{V}}e^{-\Delta\tau\hat{K}/2}|\Psi^{(n)}\rangle\end{aligned}$$

Propagation Consists of Multiplying the Wave Function by Exponentials of the One and Two-Body Terms

HS Transformation

$$e^{y^2/2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-1/2(x^2 \pm 2xy)} dx$$

$$e^{-\Delta\tau\hat{V}} = \prod_i e^{-\Delta\tau U(\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow})/2} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx_i e^{-x_i^2/2} e^{x_i\sqrt{\Delta\tau U}(\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow})}$$

An HS Transformation Must Be Performed In Order to Rewrite the Two-Body Potential Propagator In Terms of One-Body Propagators

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