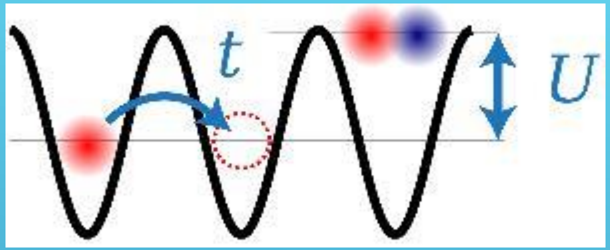
Solving The Hubbard Model Using Python and Monte Carlo Methods

- Translate Fortran code of existing Hubbard Model to Python
- Learn how to use Monte Carlo (MC) method to solve the Schrödinger equation for a simple harmonic oscillator
- Using Python write a program to solve the Schrödinger equation for a simple harmonic oscillator using MC method
- Generalize the MC Python program to apply to any Hamiltonian
- Use generalized MC python program to solve Hubbard Hamiltonian

One Band Hubbard Model PBC

$$H = -t\sum_{j}^{L}\left(c_{j\uparrow}^{\dagger}c_{(j+1)\uparrow} + c_{(j+1)\downarrow}^{\dagger}c_{j\downarrow}\right) + U\sum_{j}^{L} n_{j\uparrow}n_{j\downarrow}$$



$$t_{j,j+1} = \int \varphi_j^*(r)\left[-\frac{1}{2}\nabla^2 + V(r)\right]\varphi_{j+1}(r)d^3r$$

$$U_{jj} = \int \varphi_j^*(r)\varphi_i^*(r')\frac{1}{|r-r'|}\varphi_j(r)\varphi_j(r')d^3rd^3r'$$

$|0\rangle$ No electron on site j

$c_{j\uparrow}^{\dagger}|0\rangle$ Spin up electron on site j

$c_{j\downarrow}^{\dagger}|0\rangle$ Spin down electron on site j

$c_{j\uparrow}^{\dagger}c_{j\downarrow}^{\dagger}|0\rangle$ Spin up and down on electron on site j

$c_{2\uparrow}^{\dagger}c_{1\downarrow}^{\dagger}c_{3\downarrow}^{\dagger}|0\rangle$ All electron states can be expressed in terms of the vacuum state and creation/annihilation operators

$$c_{2\uparrow}^{\dagger}c_{1\downarrow}^{\dagger}c_{3\downarrow}^{\dagger}c_{3\uparrow}^{\dagger}|0\rangle = |\updownarrow\uparrow\downarrow 0\rangle = |\downarrow 0 \downarrow 0\rangle_{\downarrow}|\uparrow\uparrow 0\ 0\rangle_{\uparrow} = |1010\rangle_{\downarrow}|1100\rangle_{\uparrow}$$