Hubbard

December 31, 2018

1 Free spinless fermions

Spinless free fermions on a lattice can be written as

$$H_0 = -t\sum_{\langle ij\rangle}(c_i^\dagger c_j + h.c.), \tag{1}$$

where $\{c_i^\dagger, c_j\} = \delta_{i,j}$. In the first place, let us consider the simplest lattice, namely a one dimensional bipartite ring with L (even) sites. With periodic boundary condition (PBC), by a discrete Fourier transformation

$$c_j = \frac{1}{\sqrt{L}}\sum_k e^{\mathrm{i}kj}c_k, \tag{2}$$

with the quantization condition imposed by the boundary condition. Then the Hamiltonian becomes

$$H_0 = -t\sum_k(2\cos k)c_k^\dagger c_k. \tag{3}$$

suppose there are $N, (N \leq L)$ fermions in the system.

1.1 Ground state

The ground state is simply the one in which the lowest N orbitals are occupied. Different boundary conditions also impose different quantization conditions of k, for examples,

- **Periodic boundary condition** (PBC). $kL = 2n\pi, n \in Z$. If N is even, there is a **two-fold ground state degeneracy**. Otherwise not.
- **Anti-periodic boundary condition** (APBC). $kL = (2n+1)\pi, n \in Z$. If N is odd, there is a two-fold ground state degeneracy. Otherwise not.

For two pieces of free fermions $\sigma = \uparrow, \downarrow$, they have no interactions and can be treated separately as $H_0 = -t\sum_k(2\cos k)c_k^\dagger c_k - t\sum_{k'}(2\cos k')c_{k'}^\dagger c_{k'}$.

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Ground state energy of free electrons: -12.94427190999916
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1.2 Lieb-Wu solution

The exact solution for 1D half-filed Hubbard model is

$$E_0(N/2, N/2) = -4N \int_0^\infty \frac{J_0(\omega) J_1(\omega)}{\omega \left(1 + e^{\omega U/2}\right)} d\omega \tag{4}$$

where $J_{0,1}$ are the Bessel function of first and second order. It is only valid in the thermodynamic limit as $L \to \infty$.

```
/Users/wayne/Library/Python/3.7/lib/python/site-packages/ipykernel_launcher.py:10: IntegrationW
  If increasing the limit yields no improvement it is advised to analyze
  the integrand in order to determine the difficulties.  If the position of a
  local difficulty can be determined (singularity, discontinuity) one will
  probably gain from splitting up the interval and calling the integrator
  on the subranges.  Perhaps a special-purpose integrator should be used.
  # Remove the CWD from sys.path while we load stuff.
```

```
Out[107]: (-12.732361117393589, 0.017693385239684126)
```

2 Electron interaction

When the simplest on-site interaction is turned on such as

$$H_1 = U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{5}$$

we have the Hamiltonian of Hubbard model $H = H_0 + H_1$.