Learning features of superconductor using Tight Binding model

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Abstract

First I get a numerical image of the Hofstader's Butterfly, then I will learn two different method to get high spectral resolution while maintaining the minimum calculation time.First by dividing the brillouin zone to magnetic cells, in that way we get number of 1D problem instead of one 2D problem. The second method base on using the "Almost anti symmetric" gauge instead the "Landau" gauge. This way we will receive the same spectral resolution as in the first method with lattice smaller from the lattice we use in the first method. Finally, I use this method to learn about "S-wave" superconductor.

Hofstader Butterfly

Hofstadter's butterfly is a mathematical object describing the theorized behavior of electrons in a constant magnetic field in 2D system.

In this part I will get numerically the Hofstader Butterfly using three different methods.

I will write the Hamiltonian in the location basis and diagonalize it and get the energies of the system using matlab.

The Hofstader butterfly is the spectrum of the energy as a function of the magnetic field.

The Tight-Binding Hamiltonian in second quantization for 2D system with qXq sites is:

$$H = \sum_{m=0,n=0}^{m=q-1,n=q-1} -t_x \cdot c^{\dagger}_{m+1,n} c_{m,n} - t_y \cdot c^{\dagger}_{m,n+1} c_{m,n} + h.c.$$

When $x = ma, y = na$, and 'a' is the lattice constant. For simplify, in all the calculation I made: I set a to be a=1.

Landau gauge

The 2D system is in the X-Y direction and the magnetic field in Z direction. According to Landau gauge we can choose the magnetic potential to be $\vec{A} = (0, B \cdot x, 0)$.

In this gauge

$$t_x = t, t_y = t \cdot e^{\frac{ie}{\hbar}\int A \cdot dl} = t \cdot e^{2\pi i m \cdot \frac{\Phi}{\Phi_0}} = te^{2\pi i m \cdot \frac{p}{q}}$$

Φ is the magnetic flux in one cell , p is an integer and $t = \frac{\hbar}{2ma^2} \equiv 1$.

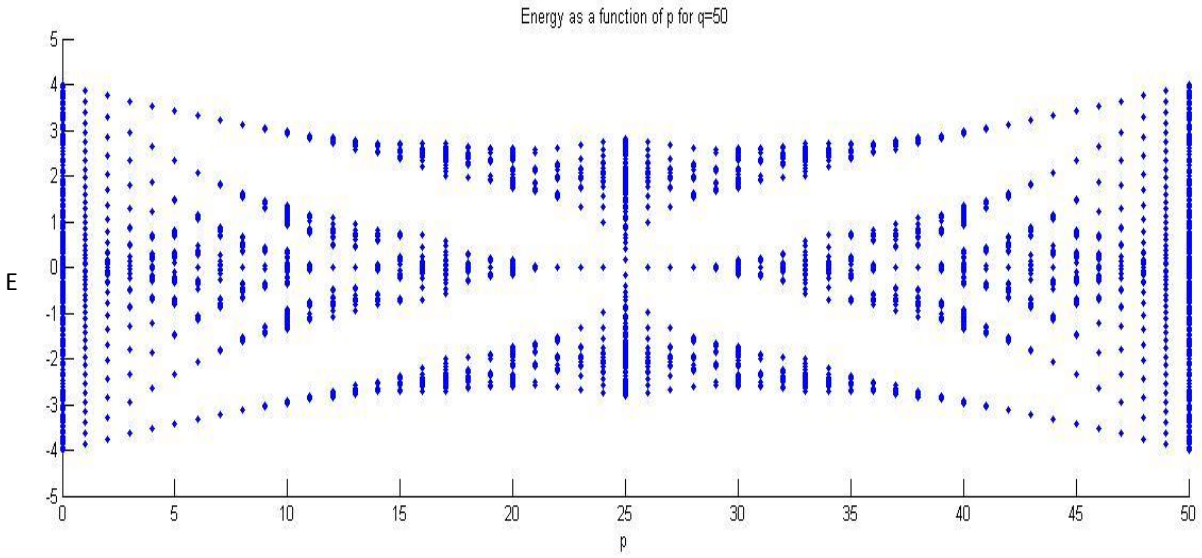
The strength of the magnetic field determined by p and the flux over the entire lattice is

$$\Phi = 2\pi pq$$

For specific p there are q energies, the Hamiltonian is periodic in p:

$H(p = q) = H(p = 0)$ Therefore, to get the entire energy spectrum of the system we should find energies as function of p, when $0 \leq p \leq q - 1$.

The spectrum obtained by this method is:



In this method the calculation takes too long and the resolution was not so good.

To improve the resolution and reducing the computation time I tried two different methods.

First method: dividing the brillouin zone to magnetic cells

Start with the Hamiltonian

$$H = \sum_{m=0,n=0}^{m=q-1,n=q-1} -t_x \cdot c^{\dagger}_{m+1,n} c_{m,n} - t_y \cdot c^{\dagger}_{m,n+1} c_{m,n} e^{2\pi i \Phi m} + h.c.$$

Then use Fourier-Transform:

$$c_{m,n} = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} dk_x \int_{-\pi}^{\pi} dk_y \, | e^{i(k_x m + k_y n)} c_{k_x,k_y}$$

$$-\pi \le k_x, k_y \le \pi \ , c_{k_x+2\pi n, k_y+2\pi n} = c_{k_x,k_y}$$

$$H = -\int_{-\pi}^{\pi} \frac{dk_x}{2\pi} \int_{-\pi}^{\pi} \frac{dk_y}{2\pi} [t_x \cos(k_x)\, c^{\dagger}_{k_x,k_y} c_{k_x,k_y} + t_y e^{-ik_y} c^{\dagger}_{k_x+2\pi\Phi,k_y} c_{k_x,k_y} + h.c.]$$

To diagonalize this Hamiltonian we need to find a momentum space that does not mix$\left(k_x, k_y\right)$ and $(k_x + 2\pi\Phi, k_y)$, if we demand $\Phi = \frac{p}{q}$ where p and q are relatively prime, the Hamiltonian can broke to q sectors when the brillouin zone is q time smaller in the x direction.

Now the Hamiltonian is:

$$H = \frac{1}{(2\pi)^2} \int_{-\frac{\pi}{q}}^{\frac{\pi}{q}} dk_x^0 \int_{-\pi}^{\pi} dk_y \, \widehat{H}_{k_x^0,k_y} \, , k_x = k_x^0 + 2\pi\Phi n$$

$$\widehat{H}_{k_x^0,k_y} = \sum_{n=0}^{q-1} -2t_x \cos(k_x^0 + 2\pi\,\Phi n) c^{\dagger}_{k_x^0+2\pi\Phi n,k_y} c_{k_x^0+2\pi\Phi n,k_y}$$
$$- t_y (e^{-ik_y} c^{\dagger}_{k_x^0+2\pi\Phi(n+1),k_y} c_{k_x^0+2\pi\Phi n,k_y}$$
$$+ \underbrace{e^{ik_y} c^{\dagger}_{k_x^0+2\pi\Phi(n-1),k_y} c_{k_x^0+2\pi\Phi n,k_y}}_{h.c.})$$

The Schrodinger equation:

$$\widehat{H}_{k_x^0,k_y} \left|\psi\right> = \mathrm{E}_{k_x^0,k_y} \left|\psi\right>$$

$$|\psi>=\sum_{n=0}^{q-1} a_n c^{\dagger}_{k_x^0+2\pi\Phi n,k_y}|0>$$

The eigenstate equation is:

$$-2t_x\cos(k_x^0+2\pi\Phi n)\,a_n - t_y\left(e^{-ik_y}a_{n-1}+e^{ik_y}a_{n+1}\right)=\mathrm{E}_{\mathrm{k}_x^0,k_y}a_n$$

To simplify the equation I use the transformation: $a_n = b_n e^{-ik_y n}$ and then we get the equation:

$$-2t_x\cos(k_x^0+2\pi\Phi n)\,b_n - t_y(b_{n-1}+b_{n+1})=\mathrm{E}_{\mathrm{k}_x^0,k_y}b_n$$

With boundary condition: $b_{n+q}=e^{ik_y q}b_n$

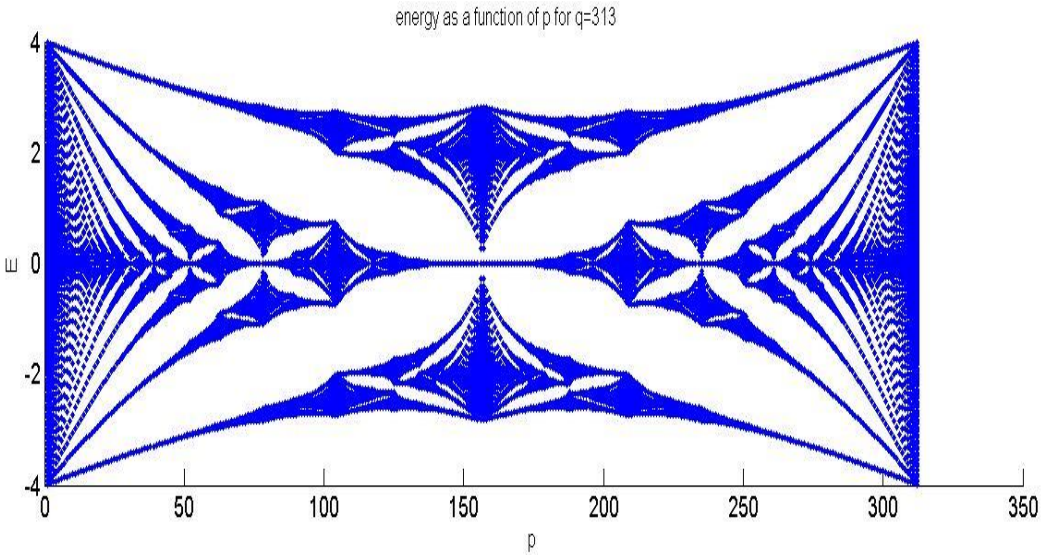
The Hamiltonian is now qXq matrix (q^2 smaller than before).

In matrix display:

$$H=\begin{pmatrix} v_1 & -t_y & 0 & & 0 & 0 & -t_y e^{-iqk_y} \\ -t_y & v_2 & -t_y & \cdots & 0 & 0 & 0 \\ 0 & -t_y & v_3 & & 0 & 0 & 0 \\ & \vdots & & \ddots & & \vdots & \\ 0 & & 0 & 0 & v_{q-2} & -t_y & 0 \\ 0 & & 0 & 0 & \cdots -t_y & v_{q-1} & -t_y \\ -t_y e^{iqk_y} & & 0 & 0 & 0 & -t_y & v_q \end{pmatrix}$$

$$v_n=-2t_x\cos(k_x^0+2\pi\Phi n)$$

The Hamiltonian is smaller than in the last calculation so I can make the computation on bigger lattice and get better resolution:



Second method: using the "Almost Anti-Symmetric" gauge instead "Landau" gauge

The Hamiltonian for lattice with qX(q+1) sites is:

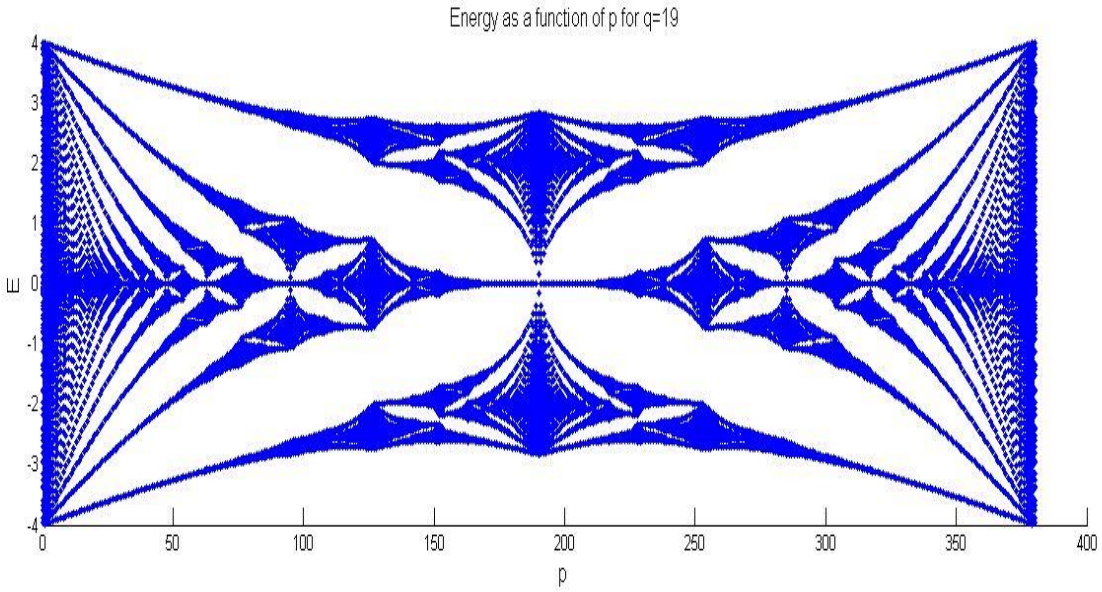
$$H = \sum_{m=0,n=0}^{m=q-1,n=q-1} -t_x \cdot c^{\dagger}_{m+1,n} c_{m,n} - t_y \cdot c^{\dagger}_{m,n+1} c_{m,n} + h.c.$$

$$t_x = te^{2\pi i n \cdot \frac{p}{q}}, t_y = te^{2\pi i m \cdot \frac{p}{(q+1)}}$$

In this gauge I we can use lattice smaller than the previous calculation and get the same spectral resolution because in this case $0 \leq p \leq q \cdot (q+1)$ instead of $0 \leq p \leq q$ in the previous calculation.

Another advantage of using this gauge is the fact that the flux over the lattice can be controlled more precisely because it's depend only on p: $\Phi = 2\pi p$.

Now the Hamiltonian matrix is q(q+1)Xq(q+1) so we have q(q+1) energies for each value of p and the energy spectrum is:



s-wave superconductor

s-wave superconductor had an isotropic gap and it's Hamiltonian is:

$$H = \sum_{k} \left(\psi_{k\uparrow}^{\dagger}, \psi_{k\downarrow}\right) \cdot \left[-t\left(\cos(k_x) + \cos\left(k_y\right)\right) - (\mu - 2t) \cdot \sigma_1 + \Delta \cdot \sigma_3\right] \cdot \begin{pmatrix} \psi_{k\uparrow} \\ \psi_{k\downarrow}^{\dagger} \end{pmatrix}$$

I want to get numerically the energies of the system, so I prefer to write the Hamiltonian in the location basis.

$$H(x,y) = FT\left(H\left(\vec{k}\right)\right)$$

$$\psi_{k,\sigma} = \sum_{m=0,n=0}^{m=q,n=q-1} e^{i(k_x m + k_y n)}\, \psi_{m,n,\sigma}$$

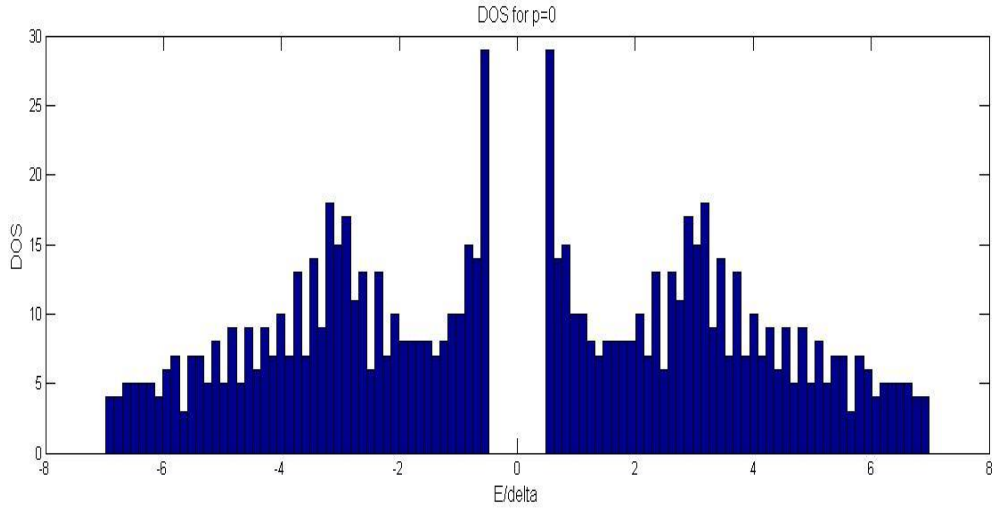
$$H(x,y) = \sum_{m,n} \left(\sum_{m',n'} e^{-i\left(k_x m' + k_y n'\right)} \psi_{m',n',\uparrow}^{\dagger}, \sum_{m',n'} e^{i\left(k_x m' + k_y n'\right)} \psi_{m\prime,n\prime,\downarrow} \right) \cdot$$

$$\begin{pmatrix} -t\left(\delta_{m'+1,m''}\delta_{n',n''} + \delta_{m',m''}\delta_{n'+1,n''}\right) - (\mu - 2t)\delta_{m',m''}\delta_{n',n''} & \Delta\delta_{m',m''}\delta_{n',n''} \\ \Delta\delta_{m',m''}\delta_{n',n''} & t\left(\delta_{m'+1,m''}\delta_{n',n''} + \delta_{m',m''}\delta_{n'+1,n''}\right) + (\mu - 2t)\delta_{m',m''}\delta_{n',n''} \end{pmatrix}$$

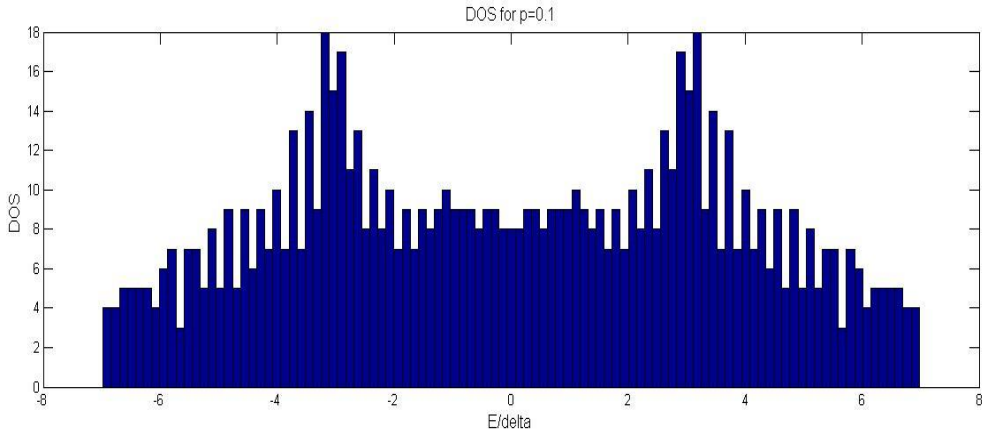
$$\cdot \begin{pmatrix} \sum_{m'',n''} e^{i\left(k_x m'' + k_y n''\right)} \psi_{m'',n'',\uparrow} \\ \sum_{m'',n''} e^{-i\left(k_x m'' + k_y n''\right)} \psi_{m'',n'',\downarrow}^{\dagger} \end{pmatrix}$$

$$= \sum_{m,n} [-t(\psi_{m+1,n,\uparrow}^{\dagger}\, \psi_{m,n,\uparrow} + \psi_{m,n+1,\uparrow}^{\dagger} \psi_{m,n,\uparrow}) + \Delta \psi_{m,n,\uparrow}^{\dagger} \psi_{m,n,\downarrow}^{\dagger}$$
$$+ t^{*}\left(\psi_{m,n,\downarrow} \psi_{m+1,n,\downarrow}^{\dagger} + \psi_{m,n,\downarrow} \psi_{m,n+1,\downarrow}^{\dagger}\right)] + h.c. - (\mu - 2t^{*}) \psi_{m,n,\uparrow}^{\dagger} \psi_{m,n,\uparrow}$$
$$+ (\mu - 2t) \psi_{m,n,,\downarrow} \psi_{m,n,,\downarrow}^{\dagger}$$

Using the "Almost Anti-Symmetric" gauge I can write the Hamiltonian matrix at the location basis as a function of the magnetic field ($B_x \sim \frac{p}{q+1}$, $B_y \sim \frac{p}{q}$) and find the density of states of the superconductor with and without magnetic field.



In this case there is not magnetic field in the system and we see the energy gap in the graph so the computation indicates on superconducting state.



When we apply a magnetic field (in our case it's could be small field because the lattice is small to reduce the calculation time) the energy gap is broken and the sample in normal phase (not superconductor).

Electrons distribution in the lattice without magnetic field

In this part I will find the electron distribution in the s-wave superconductor when the lattice had an edge.

I diagonalize the Hamiltonian and found the energies of the system, any energy had an eigenstate that satisfy the equation $H|\varphi>=E|\varphi>$.

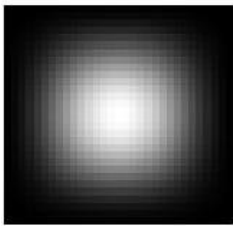
Each element of the eigenstate represent site in the lattice in that way:

$$|\varphi>=(\varphi_{1,1},\varphi_{1,2}\dots,\varphi_{1,q},\varphi_{2,1}\dots\varphi_{2,q}\dots\dots,\varphi_{q+1,q})$$

$|\varphi_{i,j}|$^2 is the probability of electron to be in the site i,j.

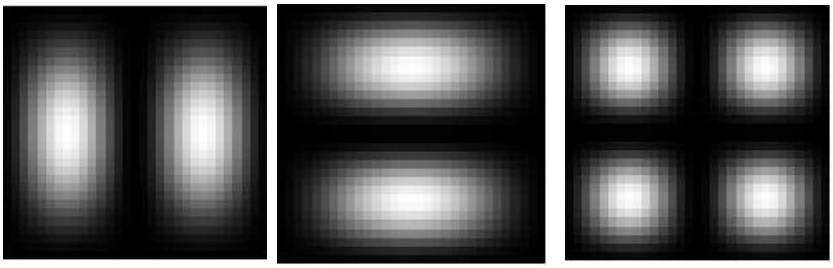
The square absolute value of each element of the eigenstate is the probability of electron to be in the site that the element represents.

The electrons distribution in the fundamental mode:

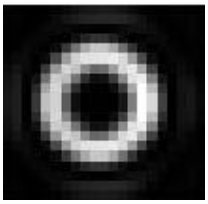


The electrons prefer to settle in the center of the lattice.

The first three excited states:



When I put a vortex in the center of the lattice:



The electrons will settle around the vortex.

BCS ground state in the energy basis

The Hamiltonian:

$$H = \sum_k \left(\psi^\dagger_{k\uparrow}, \psi_{k\downarrow}\right) \cdot \left[-t\left(\cos(k_x) + \cos\left(k_y\right)\right) - (\mu - 2t) \cdot \sigma_1 + \Delta \cdot \sigma_3\right] \cdot \begin{pmatrix} \psi_{k\uparrow} \\ \psi^\dagger_{k\downarrow} \end{pmatrix}$$

In K space: $|gs> = \prod_k \left(u_k + v_k \psi^\dagger_{k\uparrow} \psi^\dagger_{-k\downarrow}\right) |0>$

After diagonalization we get:

$$\psi^\dagger_\epsilon(k) = \alpha \sum_{k(\epsilon)} (u_k \psi^\dagger_{k\uparrow} + v_k \psi_{k\downarrow}) \ , \alpha \ is \ a \ normalizing \ constant$$

$$\psi_\epsilon(k) = \alpha \sum_{k(\epsilon)} (u_k \psi_{-k\uparrow} + v_k \psi^\dagger_{-k\downarrow})$$

$$\left\{\psi^\dagger_\epsilon, \psi_\epsilon\right\} = \alpha^2 \sum_{k(\epsilon)} u_k^2 + v_k^2 \ = 1$$

When k satisfy relation:

$$\epsilon = \sqrt{\left(t\left(\cos(k_x) + \cos\left(k_y\right)\right) - (\mu - 2t)\right)^2 + \Delta^2}$$

$$|\Phi> = \prod_\epsilon \psi_\epsilon \psi^\dagger_\epsilon |0> = \prod_\epsilon \sum_{k'(\epsilon)} (u_{k'} \psi_{-k'\uparrow} + v_{k'} \psi^\dagger_{-k'\downarrow}) \sum_{k(\epsilon)} (u_k \psi^\dagger_{k\uparrow} + v_k \psi_{k\downarrow}) =$$

$$= \prod_\epsilon \sum_{k(\epsilon)} (-u_k v_k \psi^\dagger_{k\uparrow} \psi^\dagger_{-k\downarrow} + u_k^2) \ |0>$$

$$< \Phi|\Phi> = < 0| \prod_\epsilon \psi^\dagger_\epsilon \psi_\epsilon \prod_{\epsilon'} \psi_{\epsilon'} \psi^\dagger_{\epsilon'} |0> =$$

$$< 0| \prod_{\epsilon'} \sum_{k'(\epsilon)} (-u_{k'} v_{k'} \psi_{-k'\downarrow} \psi_{k'\uparrow} + u^2_{k'}) \prod_\epsilon \sum_{k(\epsilon)} (-u_k v_k \psi^\dagger_{k\uparrow} \psi^\dagger_{-k\downarrow}$$

$$+ u_k^2)|0> = \ < 0| \prod_\epsilon \sum_{k(\epsilon)} (u_k^4 + v_k^2 u_k^2)|0> \ =$$

$$= \prod_\epsilon \sum_{k(\epsilon)} u_k^2 (v_k^2 + u_k^2) \ = \prod_\epsilon u_k^2$$

So the normalized gs in energy basis is:

$$|gs> = A^{-1} \prod_\epsilon \psi_\epsilon \psi^\dagger_\epsilon |0> \ , A = \prod_\epsilon \sum_{k(\epsilon)} u_k^2$$

References

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