Analytics

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1 Ferromagnetic Calculation

Apply the variational method.

The Hamiltonian is:

$$H = -t\sum_i \left(c_i^\dagger c_{i+1} + \text{h.c.}\right) - \mu \sum_i c_i^\dagger c_i + \Delta \sum_i \left(c_i \sigma^z_{i,i+1} c_{i+1} + \text{h.c.}\right) - J\sum_i \sigma^z_{i,i+1}\sigma^z_{i+1,i+2} - h\sum_i \sigma^x_{i,i+1} \tag{1}$$

The trial wavefunction is:

$$|\Psi\rangle = |\Phi_s\rangle \otimes |\Phi_f\rangle \tag{2}$$

$$|\Phi_s\rangle = \bigotimes_{j=1}^{N} \left(\cos(\theta/2)|\uparrow\rangle_j + e^{-i\phi}\sin(\theta/2)|\downarrow\rangle_j\right) \tag{3}$$

$$|\Phi_f\rangle = \prod_k \left(u_k + v_k c_k^\dagger c_{-k}^\dagger\right)|0\rangle \tag{4}$$

The wavefunction must be normalized:

$$1 = \langle \Phi_f | \Phi_f\rangle = \prod_k \left(|u_k|^2 + |v_k|^2\right) \tag{5}$$

1.1 Variational energy

We wish to evaluate:

$$\langle\Psi| H |\Psi\rangle \tag{6}$$

We will split the Hamiltonian into 5 parts, and evaluate these separately:

$$\langle\Psi| H |\Psi\rangle = \langle\Psi| H_t |\Psi\rangle + \langle\Psi| H_\mu |\Psi\rangle + \langle\Psi| H_\Delta |\Psi\rangle + \langle\Psi| H_J |\Psi\rangle + \langle\Psi| H_h |\Psi\rangle \tag{7}$$

Some terms only $|\Psi_f\rangle$ or $|\Psi_s\rangle$, so simplify

$$\langle\Psi| H |\Psi\rangle = \langle\Psi_f| H_t |\Psi_f\rangle + \langle\Psi_f| H_\mu |\Psi_f\rangle + \langle\Psi| H_\Delta |\Psi\rangle + \langle\Psi_s| H_J |\Psi_s\rangle + \langle\Psi_s| H_h |\Psi_s\rangle \tag{8}$$

The first expectation value is:

$$\langle\Psi_s| H_h |\Psi_s\rangle, \quad H_h = -h\sum_i \sigma^x_{i,i+1} \tag{9}$$

The action of $\sigma^x_{i,i+1}$ is that

$$\sigma^x_{i,i+1}|\uparrow\rangle_j = |\downarrow\rangle_j \tag{10}$$
$$\sigma^x_{i,i+1}|\downarrow\rangle_j = |\uparrow\rangle_j \tag{11}$$

Hence

$$\begin{aligned}
\langle\Psi_s|\, H_h \,|\Psi_s\rangle &= \langle\Psi_s| - h\sum_i \sigma^x_{i,i+1}\,|\Psi_s\rangle && (12)\\
&= -h\sum_i \langle\Psi_s|\,\sigma^x_{i,i+1}\,|\Psi_s\rangle && (13)\\
&= -h\sum_i \langle\Psi_s|\,\sigma^x_{i,i+1}\left(\bigotimes_{j=1}^{N}\big(\cos(\theta/2)|\uparrow\rangle_j + e^{-i\phi}\sin(\theta/2)|\downarrow\rangle_j\big)\right) && (14)\\
&= -h\sum_i \langle\Psi_s|\begin{bmatrix}\cos(\theta/2)\\ e^{-i\phi}\sin(\theta/2)\end{bmatrix}_1 \otimes\dots\begin{bmatrix}e^{-i\phi}\sin(\theta/2)\\ \cos(\theta/2)\end{bmatrix}_i \otimes\dots\begin{bmatrix}\cos(\theta/2)\\ e^{-i\phi}\sin(\theta/2)\end{bmatrix}_N && (15)\\
&= -h\sum_i \Big(\begin{bmatrix}\cos(\theta/2) & e^{i\phi}\sin(\theta/2)\end{bmatrix}_1 \otimes\dots\begin{bmatrix}\cos(\theta/2) & e^{i\phi}\sin(\theta/2)\end{bmatrix}_N\Big) && (16)\\
&\left(\begin{bmatrix}\cos(\theta/2)\\ e^{i\phi}\sin(\theta/2)\end{bmatrix}_1 \otimes\dots\begin{bmatrix}e^{-i\phi}\sin(\theta/2)\\ \cos(\theta/2)\end{bmatrix}_i \otimes\dots\begin{bmatrix}\cos(\theta/2)\\ e^{-i\phi}\sin(\theta/2)\end{bmatrix}_N\right) && (17)\\
&= -h\sum_i \cos(\theta/2)\sin(\theta/2)e^{-i\phi} + \cos(\theta/2)\sin(\theta/2)e^{i\phi} && (18)\\
&= -2hN\cos(\theta/2)\sin(\theta/2)\left(\frac{e^{-i\phi}+e^{i\phi}}{2}\right) && (19)\\
&= \boxed{-hN\sin(\theta)\cos(\phi)} && (20)
\end{aligned}$$

The next expectation value is:

$$\langle\Psi_s|\, H_J \,|\Psi_s\rangle\,, \quad H_J = -J\sum_i \sigma^z_{i,i+1}\sigma^z_{i+1,i+2} \tag{21}$$

The action of $\sigma^z_{i,i+1}$ is that

$$\sigma^z_{i,i+1}|\uparrow\rangle_j = |\uparrow\rangle_j \tag{22}$$
$$\sigma^z_{i,i+1}|\downarrow\rangle_j = -|\downarrow\rangle_j \tag{23}$$

$$\langle\Psi_s| H_J |\Psi_s\rangle = \langle\Psi_s| - J\sum_i \sigma^z_{i,i+1}\sigma^z_{i+1,i+2} |\Psi_s\rangle \tag{24}$$

$$= -J\sum_i \langle\Psi_s| \sigma^z_{i,i+1}\sigma^z_{i+1,i+2} |\Psi_s\rangle \tag{25}$$

$$= -J\sum_i \langle\Psi_s| \sigma^z_{i,i+1}\sigma^z_{i+1,i+2} \left(\bigotimes_{j=1}^{N} \left(\cos(\theta/2)|\uparrow\rangle_j + e^{-i\phi}\sin(\theta/2)|\downarrow\rangle_j\right)\right) \tag{26}$$

$$= -J\sum_i \langle\Psi_s| \begin{bmatrix}\cos(\theta/2)\\ e^{-i\phi}\sin(\theta/2)\end{bmatrix}_1 \otimes \dots \begin{bmatrix}\cos(\theta/2)\\ -e^{-i\phi}\sin(\theta/2)\end{bmatrix}_i \otimes \begin{bmatrix}\cos(\theta/2)\\ -e^{-i\phi}\sin(\theta/2)\end{bmatrix}_{i+1} \tag{27}$$

$$\otimes \dots \begin{bmatrix}\cos(\theta/2)\\ e^{-i\phi}\sin(\theta/2)\end{bmatrix}_N \tag{28}$$

$$= -J\sum_i \left(\begin{bmatrix}\cos(\theta/2) & e^{i\phi}\sin(\theta/2)\end{bmatrix}_1 \otimes \dots \begin{bmatrix}\cos(\theta/2) & e^{i\phi}\sin(\theta/2)\end{bmatrix}_N\right) \tag{29}$$

$$\begin{bmatrix}\cos(\theta/2)\\ e^{-i\phi}\sin(\theta/2)\end{bmatrix}_1 \otimes \dots \begin{bmatrix}\cos(\theta/2)\\ -e^{-i\phi}\sin(\theta/2)\end{bmatrix}_i \otimes \begin{bmatrix}\cos(\theta/2)\\ -e^{-i\phi}\sin(\theta/2)\end{bmatrix}_{i+1} \otimes \dots \begin{bmatrix}\cos(\theta/2)\\ e^{-i\phi}\sin(\theta/2)\end{bmatrix}_N \tag{30}$$

$$= -J\sum_i (\cos^2(\theta/2) - \sin^2(\theta/2))_i(\cos^2(\theta/2) - \sin^2(\theta/2))_{i+1} \tag{31}$$

$$= \boxed{-JN\cos^2(\theta)} \tag{32}$$

The third expectation value is:

$$\langle\Psi_f| H_t |\Psi_f\rangle, \quad -t\sum_i \left(c_i^\dagger c_{i+1} + \text{h.c.}\right) \tag{33}$$

Let us simplify this Hamiltonian first, which is written in position space. We need to transform this to momentum space:

$$H_t = -t\left(\sum_x c_x^\dagger c_{x+1} + h.c.\right) \tag{34}$$

The fourier transform is:

$$c_x = \frac{1}{\sqrt{N}}\sum_k e^{ixk}c_k \tag{35}$$

$$c_x^\dagger = \frac{1}{\sqrt{N}}\sum_k e^{-ixk}c_k^\dagger \tag{36}$$

So we just plug it in:

$$H_t = -t\left(\sum_x \frac{1}{N}\left(\sum_k e^{-ixk}c_k^\dagger\right)\sum_{k'}\left(e^{i(x+1)k'}c_{k'}\right) + h.c.\right) \tag{37}$$

$$= -t\left(\sum_x \frac{1}{N}\left(\sum_k\sum_{k'} e^{ix(k'-k)}e^{ik'}c_k^\dagger c_{k'}\right) + h.c.\right) \tag{38}$$

$$= -t\left(\left(\sum_k\sum_{k'} \delta(k'-k)e^{ik'}c_k^\dagger c_{k'}\right) + h.c.\right) \tag{39}$$

$$= -t\left(\left(\sum_k e^{ik}c_k^\dagger c_k\right) + h.c.\right) \tag{40}$$

$$= -t\left(\sum_k e^{ik}c_k^\dagger c_k + \sum_k e^{-ik}c_k^\dagger c_k\right) \tag{41}$$

$$= -t\left(\sum_k \left(e^{ik}+e^{-ik}\right)c_k^\dagger c_k\right) \tag{42}$$

$$= -2t\left(\sum_k \cos(k)c_k^\dagger c_k\right) \tag{43}$$

Now we can calculate the expectation:

$$\langle\Psi_f| H_t |\Psi_f\rangle = -2t\left(\sum_k \langle\Psi_f|\cos(k)c_k^\dagger c_k|\Psi_f\rangle\right) \tag{44}$$

$$= -2t\left(\sum_k \langle\Psi_f|\cos(k)c_k^\dagger c_k\left(u_k + iv_k c_k^\dagger c_{-k}^\dagger\right)\prod_{q\neq k}\left(u_q + iv_q c_q^\dagger c_{-q}^\dagger\right)|0\rangle\right) \tag{45}$$

$$= -2t\left(\sum_k \langle\psi|\left(v_k c_{-k}c_k\right)\cos(k)c_k^\dagger c_k\left(v_k c_k^\dagger c_{-k}^\dagger\right)|\psi\rangle\right) \tag{46}$$

$$= \boxed{-2t\sum_k v_k^2\cos(k)} \tag{47}$$

Where

$$|\psi\rangle = \prod_{q\neq k}\left(u_q + iv_q c_q^\dagger c_{-q}^\dagger\right)|0\rangle \tag{48}$$

The fourth term is the μ term:

$$\langle\Psi_f| H_\mu |\Psi_f\rangle, \quad -\mu\sum_i c_i^\dagger c_i \tag{49}$$

Begin by simplifying:

$$H_\mu = -\mu \sum_i c_i^\dagger c_i \tag{50}$$

$$= -\mu \sum_x \left(\frac{1}{N} \sum_k e^{-ixk} c_k^\dagger \sum_{k'} e^{ixk'} c_{k'} \right) \tag{51}$$

$$= -\mu \sum_x \frac{1}{N} \sum_k \sum_{k'} e^{ix\left(k'-k\right)} c_k^\dagger c_{k'} \tag{52}$$

$$= -\mu \sum_k \sum_{k'} \delta\left(k'-k\right) \quad c_k^\dagger c_{k'} \tag{53}$$

$$= -\mu \sum_k c_k^\dagger c_k \tag{54}$$

By comparison with the previous result, the expected value is

$$\boxed{\langle \Psi_f | \, H_\mu \, | \Psi_f \rangle = -\mu N \sum_k v_k^2} \tag{55}$$

The last term is the superconducting term:

$$\langle \Psi \, | H_\Delta | \, \Psi \rangle \,, \quad H_\Delta = -\Delta \sum_i \left(c_i \sigma^z_{i,i+1} c_{i+1} + \text{h.c.} \right) \tag{56}$$

It is clear H_Δ contains a spin and a fermion term. We calculate them separately and multiply at the end:

$$\left\langle \Psi_s \left| \sigma^z_{i,i+1} \right| \Psi_s \right\rangle = \cos(\theta) \tag{57}$$

The fermion part yields:

$$\langle \Psi_f \, | c_i c_{i+1} + \text{h.c.} | \, \Psi_f \rangle \tag{58}$$

$$\sum_i c_i c_{i+1} + \text{h.c.} = \sum_i \frac{1}{N} \sum_k e^{ixk} c_k \sum_{k'} e^{i(x+1)k'} c_{k'} + h.c. \tag{59}$$

$$= \sum_i \frac{1}{N} \sum_{k,k'} e^{ix(k+k')} e^{ik'} c_k c_{k'} + h.c. \tag{60}$$

$$= \sum_{k,k'} \delta(k+k') e^{ik'} c_k c_{k'} + h.c. \tag{61}$$

$$= \sum_k e^{-ik} c_k c_{-k} + h.c. \tag{62}$$

$$= \sum_k e^{-ik} c_k c_{-k} + e^{ik} c_{-k}^\dagger c_k^\dagger \tag{63}$$

As before, defining:

$$|\psi\rangle = \prod_{q \neq k} \left(u_q + i v_q c_q^\dagger c_{-q}^\dagger \right) |0\rangle \tag{64}$$

Now we can evaluate:

$$\langle \Psi_f \, | c_i c_{i+1} + \text{h.c.} | \, \Psi_f \rangle = \sum_k \langle \psi | \left(u_k - i v_k c_{-k} c_k \right) \left(e^{-ik} c_k c_{-k} + e^{ik} c_{-k}^\dagger c_k^\dagger \right) \left(u_k + i v_k c_k^\dagger c_{-k}^\dagger \right) |\psi\rangle \tag{65}$$

$$
\begin{aligned}
&(u_k - iv_k c_{-k}c_k)\left(e^{-ik}c_kc_{-k} + e^{ik}c^\dagger_{-k}c^\dagger_k\right)\left(u_k + iv_kc^\dagger_kc^\dagger_{-k}\right) && (66)\\
&= (u_k - iv_kc_{-k}c_k)\left(\left(e^{-ik}\cancel{c_kc_{-k}} + e^{ik}c^\dagger_{-k}c^\dagger_k\right)u_k + \left(e^{-ik}c_kc_{-k} + \cancel{e^{ik}c^\dagger_{-k}c^\dagger_k}\right)iv_kc^\dagger_kc^\dagger_{-k}\right) && (67)\\
&= (u_k - iv_kc_{-k}c_k)\left(\left(e^{ik}c^\dagger_{-k}c^\dagger_k\right)u_k + \left(e^{-ik}c_kc_{-k}\right)iv_kc^\dagger_kc^\dagger_{-k}\right) && (68)\\
&= (u_k - iv_kc_{-k}c_k)\left(e^{ik}c^\dagger_{-k}c^\dagger_ku_k - e^{-ik}iv_k\right) && (69)\\
&= \left(u_ke^{ik}c^\dagger_{-k}c^\dagger_ku_k - u_ke^{-ik}iv_k - iv_kc_{-k}c_ke^{ik}c^\dagger_{-k}c^\dagger_ku_k + iv_kc_{-k}c_ke^{-ik}iv_k\right) && (70)\\
&= \left(\cancel{u_ke^{ik}c^\dagger_{-k}c^\dagger_ku_k} - u_ke^{-ik}iv_k + iv_ke^{ik}u_k + \cancel{iv_kc_{-k}c_ke^{-ik}iv_k}\right) && (71)\\
&= \left(-u_ke^{-ik}iv_k + iv_ke^{ik}u_k\right) && (72)\\
&= \left(iu_kv_k\left(e^{ik} - e^{-ik}\right)\right) && (73)\\
&= \left(-2u_kv_k\frac{(e^{ik} - e^{-ik})}{2i}\right) = (-2u_kv_k\sin(k)) && (74)
\end{aligned}
$$

So the final expectation value is:

$$
\boxed{\langle\Psi\left|H_\Delta\right|\Psi\rangle = \left\langle\Psi_s\left|\sigma^z_{i,i+1}\right|\Psi_s\right\rangle\langle\Psi_f\left|c_ic_{i+1} + \text{h.c.}\right|\Psi_f\rangle = -\Delta\sum_k(2u_kv_k\sin(k))\cos(\theta)} \quad (75)
$$

The entire expression is:

$$
\boxed{
\begin{aligned}
\langle\Psi|H|\Psi\rangle &= -hN\sin(\theta)\cos(\phi) - JN\cos^2(\theta) && (76)\\
&- 2t\sum_k v_k^2\cos(k) - \mu N\sum_k v_k^2 - 2\Delta\sum_k u_kv_k\cos(\theta)\sin(k) && (77)
\end{aligned}
}
$$

1.2 Minimization

We would like to minimize

$$
\begin{aligned}
E_{var} = \langle\Psi|H|\Psi\rangle &= -hN\sin(\theta)\cos(\phi) - JN\cos^2(\theta) && (78)\\
&- 2t\sum_k v_k^2\cos(k) - \mu N\sum_k v_k^2 - 2\Delta\sum_k u_kv_k\cos(\theta)\sin(k) && (79)
\end{aligned}
$$

Making the substitutions and taking the derivative,

$$
u_k = \cos\alpha_k \quad v_k = \sin\alpha_k \quad (80)
$$

we obtain

$$
\begin{aligned}
\frac{\partial E_{var}}{\partial\alpha(k)} &= -2\Delta\sum_k\left(\cos(\theta)\sin(k)\cos^2(\alpha(k)) - \cos(\theta)\sin(k)\sin^2(\alpha(k))\right) && (81)\\
&- N\mu\sum_k 2\sin(\alpha(k))\cos(\alpha(k)) - 2t\sum_k 2\cos(k)\sin(\alpha(k))\cos(\alpha(k)) && (82)
\end{aligned}
$$

This can be rewritten as

$$\frac{\partial E_{var}}{\partial \alpha(k)} = -2\Delta \sum_k (\cos(\theta)\sin(k)\cos(2\alpha(k))) \tag{83}$$

$$- N\mu \sum_k \sin(2\alpha(k)) - 2t \sum_k \cos(k)\sin(2\alpha(k)) \tag{84}$$

And this allows us to rearrange and solve; since the entire expression is linear in k, each term in the summation must be minimal:

$$0 = \frac{\partial E_{var}}{\partial \alpha(k)} \implies \quad E_{k_{var}} \text{ minimal} \tag{85}$$

$$\implies 2\Delta\cos(\theta)\sin(k)\cos(2\alpha(k)) = (-N\mu - 2t\cos(k))\sin(2\alpha(k)) \tag{86}$$

$$\implies \frac{2\Delta\cos(\theta)\sin(k)}{-N\mu - 2t\cos(k)} = \tan(2\alpha(k)) \tag{87}$$

$$\implies \alpha(k) = \frac{1}{2}\arctan\left(\frac{2\Delta\cos(\theta)\sin(k)}{-N\mu - 2t\cos(k)}\right) \tag{88}$$

Now we need to solve for v_k^2 and $v_k u_k$:
Defining

$$\epsilon_k := -2t\cos(k) \tag{89}$$

$$\xi_k := \epsilon_k - N\mu \tag{90}$$

$$\Delta_k := 2\Delta\cos(\theta)\sin(k) \tag{91}$$

$$\tan(2\alpha(k)) = \frac{\Delta_k}{\xi_k} \implies \cos(2\alpha(k)) = \frac{\xi_k}{\sqrt{\xi_k^2 + \Delta_k^2}}, \quad \sin(2\alpha(k)) = \frac{\Delta_k}{\sqrt{\xi_k^2 + \Delta_k^2}} \tag{92}$$

After some trig identities and plugging in the definition,

$$u_k v_k = \cos(\alpha(k))\sin(\alpha(k)) = \frac{1}{2}\sin(2\alpha(k)) = \frac{1}{2}\frac{\Delta_k}{\sqrt{\xi_k^2 + \Delta_k^2}} \tag{93}$$

$$v_k^2 = \sin^2(\alpha(k)) = \frac{1}{2}(1 - \cos(2\alpha_k)) = \frac{1}{2}\left(1 - \frac{\xi_k}{\sqrt{\xi_k^2 + \Delta_k^2}}\right) \tag{94}$$

Now we are able to integrate these equations in Mathematica.

1.3 Integration

$$\sum_k \to N\int_{-\pi}^{\pi} \frac{dk}{2\pi} \tag{95}$$

After substituting $\alpha(k)$, we take the thermodynamic limit and evaluate the integrals using Mathematica:

$$E_{var} = -hN\sin(\theta)\cos(\phi) - JN\cos^2(\theta) \tag{96}$$

$$- \frac{tN}{\pi}\int_{-\pi}^{\pi} v_k^2\cos(k)dk - \frac{\mu N^2}{2\pi}\int_{-\pi}^{\pi} v_k^2 dk - \frac{\Delta N}{\pi}\int_{-\pi}^{\pi} u_k v_k\cos(\theta)\sin(k)dk \tag{97}$$

Calculating the ground energy density:

$$\frac{E_{var}}{N} = -h\sin(\theta)\cos(\phi) - J\cos^2(\theta) \tag{98}$$

$$-\frac{t}{\pi}\int_{-\pi}^{\pi} v_k^2\cos(k)dk - \frac{\mu N}{2\pi}\int_{-\pi}^{\pi} v_k^2 dk - \frac{\Delta}{\pi}\int_{-\pi}^{\pi} u_k v_k\cos(\theta)\sin(k)dk \tag{99}$$

We solve the integrals in the case $\mu = 0$. The μ integral vanishes, and we are left with the t and Δ integrals.

Mathematica is able to evaluate this integral:

The t integral is:

$$\begin{aligned}&-\frac{t}{\pi}\int_{-\pi}^{\pi} v_k^2\cos(k)dk\\ &= \frac{\Delta t\cos(\theta)\left(\Delta\cos(\theta)K\left(1-\frac{\Delta^2\cos^2(\theta)}{t^2}\right)+tK\left(1-\frac{t^2\sec^2(\theta)}{\Delta^2}\right)-tE\left(1-\frac{t^2\sec^2(\theta)}{\Delta^2}\right)\right)-t^3E\left(1-\frac{\Delta^2\cos^2(\theta)}{t^2}\right)}{\pi\left(t^2-\Delta^2\cos^2(\theta)\right)}\end{aligned} \tag{100}$$

The Δ integral is:

$$-\frac{\Delta}{\pi}\int_{-\pi}^{\pi} u_k v_k\cos(\theta)\sin(k)dk \tag{101}$$

$$= \frac{\Delta\cos(\theta)\left(t^2K\left(1-\frac{t^2\sec^2(\theta)}{\Delta^2}\right)-\Delta\cos(\theta)\left(-tK\left(1-\frac{\Delta^2\cos^2(\theta)}{t^2}\right)+tE\left(1-\frac{\Delta^2\cos^2(\theta)}{t^2}\right)+\Delta\cos(\theta)E\left(1-\frac{t^2\sec^2(\theta)}{\Delta^2}\right)\right)\right)}{\pi\left(\Delta^2\cos^2(\theta)-t^2\right)}$$

Combining the two gives:

$$-\frac{t}{\pi}\int_{-\pi}^{\pi} v_k^2\cos(k)dk - \frac{\Delta}{\pi}\int_{-\pi}^{\pi} u_k v_k\cos(\theta)\sin(k)dk = -\frac{tE\left(1-\frac{\Delta^2\cos^2(\theta)}{t^2}\right)+\Delta\cos(\theta)E\left(1-\frac{t^2\sec^2(\theta)}{\Delta^2}\right)}{\pi} \tag{102}$$

So, the final expression is:

$$\frac{E_{var}}{N} = -h\sin(\theta)\cos(\phi) - J\cos^2(\theta) - \left(\frac{tE\left(1-\frac{\Delta^2\cos^2(\theta)}{t^2}\right)+\Delta\cos(\theta)E\left(1-\frac{t^2\sec^2(\theta)}{\Delta^2}\right)}{\pi}\right) \tag{103}$$

Which simplifies to: [Add proof of Elliptic E equivalence]

$$\boxed{\frac{E_{var}}{N} = -J\cos^2(\theta) - h\sin(\theta)\cos(\phi) - \frac{2t}{\pi}E\left(1-\frac{\Delta^2\cos^2(\theta)}{t^2}\right)} \tag{104}$$

1.4 Minimization 2

To minimize ϕ, we observe that only the h-term depends on ϕ. Taking the derivative we see that $\cos(\phi)$ is minimized at $0, \pi$. Since $\cos(\theta)$ is maximal at 0, the minimal value of $\phi = 0$.

To minimize the expression, simply write E_{var}/N as a function of $\cos(\theta)$ minimize with respect to $\cos(\theta)$.

2 Anti-ferromagnetic Calculation

[Add j+2 terms]

First we relabel the indices. We have the mapping

$$j \to j_A, \quad j+1 \to j_B \tag{105}$$

Defining

$$\psi_j := \begin{bmatrix} c_{j_A} \\ c_{j_B} \\ c^\dagger_{j_A} \\ c^\dagger_{j_B} \end{bmatrix} \quad \psi^\dagger_j := \begin{bmatrix} c^\dagger_{j_A} & c^\dagger_{j_B} & c_{j_A} & c_{j_B} \end{bmatrix} \tag{106}$$

$$\begin{aligned} H_t &= -t\sum_j c^\dagger_j c_{j+1} + \text{h.c.} && (107)\\ &= -t\sum_j c^\dagger_{j_A} c_{j_B} + c^\dagger_{j_B} c_{j_A} && (108)\\ &= -\frac{t}{2}\sum_j \left(c^\dagger_{j_A} c_{j_B} - c_{j_B} c^\dagger_{j_A}\right) + \left(c^\dagger_{j_B} c_{j_A} - c_{j_A} c^\dagger_{j_B}\right) && (109)\\ &= \frac{1}{2}\sum_j \begin{bmatrix} c^\dagger_{j_A} & c^\dagger_{j_B} & c_{j_A} & c_{j_B} \end{bmatrix} \begin{bmatrix} 0 & -t & 0 & 0 \\ -t & 0 & 0 & 0 \\ 0 & 0 & 0 & t \\ 0 & 0 & t & 0 \end{bmatrix} \begin{bmatrix} c_{j_A} \\ c_{j_B} \\ c^\dagger_{j_A} \\ c^\dagger_{j_B} \end{bmatrix} && (110)\\ &= \frac{1}{2}\sum_j \psi^\dagger_j \mathcal{H}_{tj} \psi_j && (111) \end{aligned}$$

The fermion part of the Δ term is also rewritten similarly:

$$\begin{aligned} H_\Delta &= \Delta\sum_j \left(c_j c_{j+1} + \text{h.c.}\right) && (112)\\ &= \Delta\sum_j \left(c_{j_A} c_{j_B} + c^\dagger_{j_B} c^\dagger_{j_A}\right) && (113)\\ &= \frac{\Delta}{2}\sum_j \left(c_{j_A} c_{j_B} - c_{j_B} c_{j_A}\right) + \left(c^\dagger_{j_B} c^\dagger_{j_A} - c^\dagger_{j_A} c^\dagger_{j_B}\right) && (114)\\ &= \frac{1}{2}\sum_j \begin{bmatrix} c^\dagger_{j_A} & c^\dagger_{j_B} & c_{j_A} & c_{j_B} \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & -\Delta \\ 0 & 0 & \Delta & 0 \\ 0 & \Delta & 0 & 0 \\ -\Delta & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} c_{j_A} \\ c_{j_B} \\ c^\dagger_{j_A} \\ c^\dagger_{j_B} \end{bmatrix} && (115)\\ &= \frac{1}{2}\sum_j \psi^\dagger_j \mathcal{H}_{\Delta j} \psi_j && (116) \end{aligned}$$

$$\mathcal{H}_j = \mathcal{H}_{\Delta j} + \mathcal{H}_{tj} = \begin{bmatrix} 0 & -t & 0 & -\Delta \\ -t & 0 & \Delta & 0 \\ 0 & \Delta & 0 & t \\ -\Delta & 0 & t & 0 \end{bmatrix} \tag{117}$$

2.1 Diagonalization in Momentum Space

Since

$$H_t = -t\left(\sum_x c_x^\dagger c_{x+1} + h.c.\right) = -2t\sum_k \cos(k) c_k^\dagger c_k \tag{118}$$

$$H_\Delta = -\Delta \sum_i \left(c_i \sigma^z_{i,i+1} c_{i+1} + \text{h.c.}\right) = -\Delta \sum_k e^{-ik} c_k c_{-k} + e^{ik} c_{-k}^\dagger c_k^\dagger \tag{119}$$

We see that

$$t \to \epsilon_k := -2t\cos(k) \tag{120}$$

$$\Delta \to \Delta_k := 2\Delta\cos(\theta)\sin(k) \tag{121}$$

[Missing j+2, j terms but next equation is correct]

$$\mathcal{H}_k = \begin{pmatrix} 0 & -t\left(1+e^{2ik}\right) & 0 & -\Delta\cos(\theta)\left(1+e^{2ik}\right) \\ -t\left(1+e^{-2ik}\right) & 0 & \Delta\cos(\theta)\left(1+e^{-2ik}\right) & 0 \\ 0 & \Delta\cos(\theta)\left(1+e^{2ik}\right) & 0 & t\left(1+e^{2ik}\right) \\ -\Delta\cos(\theta)\left(1+e^{-2ik}\right) & 0 & t\left(1+e^{-2ik}\right) & 0 \end{pmatrix} \tag{122}$$

After diagonalization, we find the following four eigenvalues:

$$\{2(t-\Delta\cos(\theta))\cos(k), 2(\Delta\cos(\theta)-t)\cos(k), -2(\Delta\cos(\theta)+t)\cos(k), 2(\Delta\cos(\theta)+t)\cos(k)\} \tag{123}$$

Then, converting the summations into integrals once more we obtain:

$$\sum_k \to N\int_{-\pi/2}^{\pi/2}\frac{dk}{2\pi} \tag{124}$$

$$\{(t-\Delta\cos(\theta))/\pi, (\Delta\cos(\theta)-t)/\pi, -(\Delta\cos(\theta)+t)/\pi, (\Delta\cos(\theta)+t)/\pi\} \tag{125}$$

Notice that if we set $\Delta = 0$, we immediately recover

$$-\frac{2t}{\pi} \tag{126}$$

for the fermion term, for both the ferromagnetic and the antiferromagnetic calculation. Hence

$$\boxed{\frac{E_{var}}{N} = -J\cos^2(\theta) - h\sin(\theta)\cos(\phi) - \frac{(t+\Delta\cos(\theta))}{\pi} + -\frac{|t-\Delta\cos(\theta)|}{\pi}} \tag{127}$$