Quantum Mechanics 3 - Class Exercise 9

4.1.2022

Question 1

Diagonalize the general quadratic form of the Hamiltotnian,

$$\hat{H} = \sum_{i,j=1}^{N} \left[\hat{c}_i^\dagger A_{ij} \hat{c}_j + \frac{1}{2} \left(\hat{c}_i^\dagger B_{ij} \hat{c}_j^\dagger + \text{h.c.} \right) \right], \tag{1}$$

where $\hat{c}_i$, $\hat{c}_i^\dagger$ are fermionic annihilation and creation operators.

Solution

The Hermiticity of $\hat{H}$ requires that A be a Hermitian matrix, while the anti-commutation rules among the $\hat{c}_i$ require that B be an anti-symmetric matrix. By re-definning the phases of the $\hat{c}_i$ it is always possible to arrange A and B to be real. We wish to find a linear transformation of the form (with g_{ki}, h_{ki} real)

$$\hat{\eta}_k = \sum_{i=1}^{N} \left(g_{ki} \hat{c}_i + h_{ki} \hat{c}_i^\dagger \right) \tag{2}$$

$$\hat{\eta}_k^\dagger = \sum_{i=1}^{N} \left(g_{ki} \hat{c}_i^\dagger + h_{ki} \hat{c}_i \right), \tag{3}$$

so that

$$\hat{H} = \sum_{k=1}^{N} \Lambda_k \hat{\eta}_k^\dagger \hat{\eta}_k + E_0, \tag{4}$$

where E_0 is a constant. If $\hat{\eta}_k$ and $\hat{\eta}_k^\dagger$ are fermionic annihilation and creation operators, they must obey

$$\left\{ \hat{\eta}_k, \hat{\eta}_{k'}^\dagger \right\} = \delta_{kk'} \implies \sum_{i=1}^{N} \left(g_{ki} g_{k'i} + h_{ki} h_{k'i} \right) = \delta_{kk'} \tag{5}$$

$$\left\{ \hat{\eta}_k, \hat{\eta}_{k'} \right\} = 0 \implies \sum_{i=1}^{N} \left(g_{ki} h_{k'i} + g_{k'i} h_{ki} \right) = 0. \tag{6}$$

If the Hamiltonian can indeed have the diagonal form of Eq. (4), it implies that (**You will prove that in your HW!**)

$$\left[\hat{\eta}_k, \hat{H} \right] - \Lambda_k \hat{\eta}_k = 0. \tag{7}$$

From Eq. (7), it can be shown that the following relations hold (**You will prove that in your HW!**),

$$\sum_{j=1}^{N} \left(g_{kj}A_{ji} - h_{kj}B_{ji}\right) = \Lambda_k g_{ki} \tag{8}$$

$$\sum_{j=1}^{N} \left(g_{kj}B_{ji} - h_{kj}A_{ji}\right) = \Lambda_k h_{ki}. \tag{9}$$

If we define

$$g_k^{\mathrm{T}} \equiv \begin{bmatrix} g_{k1} & g_{k2} & \cdots & g_{kN} \end{bmatrix} \tag{10}$$

$$h_k^{\mathrm{T}} \equiv \begin{bmatrix} h_{k1} & h_{k2} & \cdots & h_{kN} \end{bmatrix} \tag{11}$$

we could write Eqs. (8)-(9) in matrix notation

$$g_k^{\mathrm{T}} A - h_k^{\mathrm{T}} B = \Lambda_k g_k^{\mathrm{T}} \tag{12}$$

$$g_k^{\mathrm{T}} B - h_k^{\mathrm{T}} A = \Lambda_k h_k^{\mathrm{T}}. \tag{13}$$

These equations can be simplified with

$$\phi_k^{\mathrm{T}} \equiv g_k^{\mathrm{T}} + h_k^{\mathrm{T}} \tag{14}$$

$$\psi_k^{\mathrm{T}} \equiv g_k^{\mathrm{T}} - h_k^{\mathrm{T}}. \tag{15}$$

Now, with these definitions, by either adding or subtracting Eqs. (12)-(13), we get

$$\phi_k^{\mathrm{T}} \left(A - B\right) = \Lambda_k \psi_k^{\mathrm{T}} \tag{16}$$

$$\psi_k^{\mathrm{T}} \left(A + B\right) = \Lambda_k \phi_k^{\mathrm{T}}, \tag{17}$$

and by plugging Eq. (16) into Eq. (17) (or vice versa) we end up with

$$\boxed{\phi_k^{\mathrm{T}} \left(A - B\right)\left(A + B\right) = \Lambda_k^2 \phi_k^{\mathrm{T}}} \tag{18}$$

$$\boxed{\psi_k^{\mathrm{T}} \left(A + B\right)\left(A - B\right) = \Lambda_k^2 \psi_k^{\mathrm{T}}}. \tag{19}$$

Therefore, we identify Λ_k^2 as the eigen-values of either $(A - B)(A + B)$ or $(A + B)(A - B)$.

Since A is symmetric and B is anti-symmetric, $(A + B)^{\mathrm{T}} = A - B$, so both $(A - B)(A + B)$ and $(A + B)(A - B)$ are symmetric and positive semi-definite. Therefore the eigen-energies Λ_k are real and the eigen-vectors ϕ_k^{T} and ψ_k^{T} can be chosen to be real and orthogonal. The orthogonality conditions imply

$$\sum_{i=1}^{N} \phi_{ki}\phi_{k'i} = \delta_{kk'} \implies \sum_{i=1}^{N} \left(g_{ki}g_{k'i} + h_{ki}h_{k'i}\right) + \sum_{i=1}^{N} \left(g_{ki}h_{k'i} + g_{k'i}h_{ki}\right) = \delta_{kk'} \tag{20}$$

$$\sum_{i=1}^{N} \psi_{ki}\psi_{k'i} = \delta_{kk'} \implies \sum_{i=1}^{N} \left(g_{ki}g_{k'i} + h_{ki}h_{k'i}\right) - \sum_{i=1}^{N} \left(g_{ki}h_{k'i} + g_{k'i}h_{ki}\right) = \delta_{kk'}, \tag{21}$$

or

$$\sum_{i=1}^{N}(g_{ki}g_{k'i}+h_{ki}h_{k'i})=\delta_{kk'} \tag{22}$$

$$\sum_{i=1}^{N}(g_{ki}h_{k'i}+g_{k'i}h_{ki})=0, \tag{23}$$

which are precisely the conditions we required for the anti-commutation relations of $\hat{\eta}_k$ and $\hat{\eta}_k^\dagger$, Eqs. (5)-(6).

The last thing we would like to find is E_0, the constant in the Hamiltonian of Eq. (4). One way to do so is comparing the Hamiltonians of Eq. (1) and Eq. (4). Fortunately, we could find it in a less tedious manner by comparing the trace of the Hamiltonians. On the one hand, from Eq. (1),

$$\mathrm{Tr}\hat{H}=2^{N-1}\sum_{i=1}^{N}A_{ii}. \tag{24}$$

On the other hand, from Eq. (4),

$$\mathrm{Tr}\hat{H}=2^{N-1}\sum_{k=1}^{N}\Lambda_k+2^N E_0. \tag{25}$$

By comparing these two expressions, we can extract the constant E_0,

$$\boxed{E_0=\frac{1}{2}\left(\sum_{i=1}^{N}A_{ii}-\sum_{k=1}^{N}\Lambda_k\right)}. \tag{26}$$

Here's a brief calculation in case you don't understand where the 2^{N-1} factor comes from in Eq. (25).

$$\begin{aligned}
\mathrm{Tr}\sum_{k=1}^{N}\Lambda_k\hat{\eta}_k^\dagger\hat{\eta}_k &= \mathrm{Tr}\sum_{k=1}^{N}\Lambda_k\hat{n}_k=\sum_{n_1,n_2\ldots,n_N=0}^{1}\langle n_1,n_2,\ldots,n_N|\sum_{k=1}^{N}\Lambda_k\hat{n}_k|n_1,n_2,\ldots,n_N\rangle \\
&= \sum_{k=1}^{N}\Lambda_k\sum_{n_1,n_2\ldots,n_N=0}^{1}\langle n_1,n_2,\ldots,n_N|\hat{n}_k|n_1,n_2,\ldots,n_N\rangle \\
&= \sum_{k=1}^{N}\Lambda_k\langle n_k=1|\hat{n}_k|n_k=1\rangle\sum_{\substack{n_1,n_2\ldots,n_N=0\\ \text{without } n_k}}^{1}1=2^{N-1}\sum_{k=1}^{N}\Lambda_k.
\end{aligned} \tag{27}$$

The anisotropic XY model[1]

The anisotropic XY Hamiltonian for a chain of N spins is (N is even)

$$\hat{H} = -\frac{J}{2} \sum_i \left[(1+\gamma)\, \hat{\sigma}_i^x \hat{\sigma}_{i+1}^x + (1-\gamma)\, \hat{\sigma}_i^y \hat{\sigma}_{i+1}^y \right], \tag{28}$$

where $\hat{\sigma}_i^{x,y}$ are the Pauli matrices and γ, J are constants. There are two reasonable conditions to take for the ends of the chain.

1. **Free ends**, in which case the range of the summation index is $1 \leq i \leq N-1$.
2. **Cyclic chain**, in which case $1 \leq i \leq N$, and we also have to demand $\hat{\sigma}_{N+1}^x \equiv \hat{\sigma}_1^x$, $\hat{\sigma}_{N+1}^y \equiv \hat{\sigma}_1^y$.

Clearly, if $\gamma = 0$, we have an isotropic chain in the XY plane. On the other hand, $\gamma = \pm 1$ corresponds to the Ising model. For example, in the limit where $\gamma = 1$ we have

$$\hat{H} = -J \sum_i \hat{\sigma}_i^x \hat{\sigma}_{i+1}^x. \tag{29}$$

We could diagonalize that Hamiltonian easily by rotating the system 90° around the y-axis[2]. Then the Hamiltonian is given by

$$\hat{H} = -J \sum_i \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z. \tag{30}$$

From here, it should be clear how the chain looks like in the ground state (see Fig. 1). If $J > 0$, the chain is ordered in the ground state and all the spins are pointing either ↑ or ↓. If $J < 0$, the system is in complete disorder as adjacent spins point to opposite directions. Either way, for very long chains, we can expect that the energy of the ground state is $E_0 = -N\,|J|$. Since every spin flip results a contribution of $2\,|J|$ to the total energy, we can expect that excited states come in energy quanta of $2\,|J|$.

[1]This model (and many of the results presented here) is based on the paper of Lieb, Schultz and Mattis (1961).
[2]Mathematically speaking, this is done by $\hat{H} \to \hat{U}\hat{H}\hat{U}^\dagger$ with $\hat{U} = \prod_i \exp\left(i\frac{\pi}{4}\hat{\sigma}_i^y\right)$.

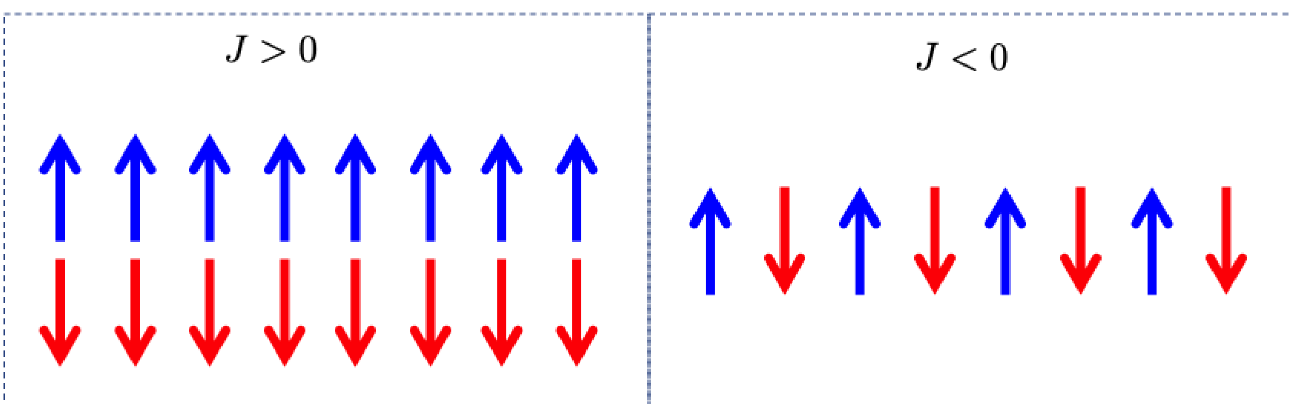

Figure 1: The ground state of the Ising chain.

Question 2

For the anisotropic XY Hamiltonian provided by Eq. (28),

1. Write the Hamiltonian in form of fermionic annihilation and creation operators.
2. Find the energy spectrum of the excited states.
3. Find the energy of the ground state.
4. Find the free energy of the system.

Solution to 1

Instead of using the Pauli matrices, we may write the Hamiltonian with raising/lowering operators

$$\hat{a}_i^\dagger \equiv \frac{\hat{\sigma}_i^x + i\hat{\sigma}_i^y}{2}, \qquad \hat{a}_i \equiv \frac{\hat{\sigma}_i^x - i\hat{\sigma}_i^y}{2} \tag{31}$$

$$\implies \hat{\sigma}_i^x = \hat{a}_i^\dagger + \hat{a}_i, \qquad \hat{\sigma}_i^y = -i\left(\hat{a}_i^\dagger - \hat{a}_i\right) \tag{32}$$

and then

$$\hat{H} = -J\sum_i \left[\hat{a}_i^\dagger \hat{a}_{i+1} + \gamma \hat{a}_i^\dagger \hat{a}_{i+1}^\dagger + \text{h.c.}\right]. \tag{33}$$

The operators $\hat{a}_i$ and $\hat{a}_i^\dagger$ partly resemble fermionic annihilation and creation operators because

$$\left\{\hat{a}_i, \hat{a}_i^\dagger\right\} = 1, \qquad \hat{a}_i^2 = \left(\hat{a}_i^\dagger\right)^2 = 0, \tag{34}$$

but they also resemble bosonic operators because

$$\left[\hat{a}_i, \hat{a}_j^\dagger\right] = \left[\hat{a}_i, \hat{a}_j\right] = \left[\hat{a}_i^\dagger, \hat{a}_j^\dagger\right] = 0, \qquad \text{for } i \neq j. \tag{35}$$

If we wish to write the Hamiltonian with true fermionic operators we would need to apply the *Jordan-Wigner transformation*. For that purpose, let us define the string operator[3]

$$\hat{K}_i \equiv \prod_{j=1}^{i-1}\left(1 - 2\hat{a}_j^\dagger \hat{a}_j\right), \qquad \hat{K}_1 \equiv 1. \tag{36}$$

The string operator is manifestly Hermitian, but it is also unitary. So $\hat{K}_i = \hat{K}_i^\dagger$ and $\hat{K}_i^2 = 1$ (**You will prove that in your HW!**). Now, the Jordan-Wigner transformation is given by

$$\hat{c}_i \equiv \hat{K}_i \hat{a}_i, \qquad \hat{c}_i^\dagger \equiv \hat{a}_i^\dagger \hat{K}_i. \tag{37}$$

Since $\hat{K}_i^2 = 1$ we can easily find the inverse transformation,

$$\hat{a}_i = \hat{K}_i \hat{c}_i, \qquad \hat{a}_i^\dagger = \hat{c}_i^\dagger \hat{K}_i. \tag{38}$$

[3]There are places in the literature where the string operator is defined as $\hat{K}_i \equiv \exp\left(i\pi \sum_{j=1}^{i-1} \hat{a}_j^\dagger \hat{a}_j\right)$. One can show that these two definitions are completely equivalent.

It turns out that $\hat{c}_i$ and $\hat{c}_i^\dagger$ are fermionic annihilation and creation operators (**You will prove that in your HW!**), i.e.

$$\left\{\hat{c}_i, \hat{c}_j^\dagger\right\} = \delta_{ij} \tag{39}$$

$$\{\hat{c}_i, \hat{c}_j\} = \left\{\hat{c}_i^\dagger, \hat{c}_j^\dagger\right\} = 0. \tag{40}$$

Note that

$$\hat{c}_i^\dagger \hat{c}_i = \hat{a}_i^\dagger \hat{K}_i \hat{K}_i \hat{a}_i = \hat{a}_i^\dagger \hat{a}_i. \tag{41}$$

Furthermore, for $1 \leq i \leq N-1$,

$$\hat{a}_i^\dagger \hat{a}_{i+1} = \hat{a}_i^\dagger \hat{K}_{i+1} \hat{c}_{i+1} = \hat{a}_i^\dagger \hat{K}_i \left(1 - 2\hat{a}_i^\dagger \hat{a}_i\right) \hat{c}_{i+1} = \hat{c}_i^\dagger \hat{K}_i \hat{K}_i \hat{c}_{i+1} - 2\hat{K}_i \left(\hat{a}_i^\dagger\right)^2 \hat{a}_i \hat{c}_{i+1} = c_i^\dagger c_{i+1} \tag{42}$$

$$\hat{a}_i^\dagger \hat{a}_{i+1}^\dagger = \hat{a}_i^\dagger \hat{K}_{i+1} \hat{c}_{i+1}^\dagger = \hat{a}_i^\dagger \hat{K}_i \left(1 - 2\hat{a}_i^\dagger \hat{a}_i\right) \hat{c}_{i+1}^\dagger = \hat{c}_i^\dagger \hat{K}_i \hat{K}_i \hat{c}_{i+1}^\dagger - 2\hat{K}_i \left(\hat{a}_i^\dagger\right)^2 \hat{a}_i \hat{c}_{i+1}^\dagger = c_i^\dagger \hat{c}_{i+1}^\dagger \tag{43}$$

and thus, for the case of free ends, the Hamiltonian is

$$\hat{H}_{\text{free}} = -J \sum_{i=1}^{N-1} \left[\hat{c}_i^\dagger \hat{c}_{i+1} + \gamma \hat{c}_i^\dagger \hat{c}_{i+1}^\dagger + \text{h.c.}\right]. \tag{44}$$

However, for the cyclic chain we also have

$$\hat{a}_N^\dagger \hat{a}_1 = -\hat{c}_N^\dagger \hat{c}_1 \hat{K}_{N+1} \neq \hat{c}_N^\dagger \hat{c}_1 \tag{45}$$

$$\hat{a}_N^\dagger \hat{a}_1^\dagger = -\hat{c}_N^\dagger \hat{c}_1^\dagger \hat{K}_{N+1} \neq \hat{c}_N^\dagger \hat{c}_1^\dagger. \tag{46}$$

Here's the proof for Eq. (45) (the proof for Eq. (46) is almost identical).

$$\begin{aligned}\hat{a}_N^\dagger \hat{a}_1 = {} & \hat{c}_N^\dagger \hat{K}_N \hat{a}_1 = \hat{c}_N^\dagger \prod_{j=1}^{N-1} \left[1 - 2\hat{a}_j^\dagger \hat{a}_j\right] \hat{a}_1 = \hat{c}_N^\dagger \prod_{j=1}^{N} \left[1 - 2\hat{a}_j^\dagger \hat{a}_j\right] \hat{a}_1 = \hat{c}_N^\dagger \left[1 - 2\hat{a}_1^\dagger \hat{a}_1\right] \hat{a}_1 \prod_{j=2}^{N} \left[1 - 2\hat{a}_j^\dagger \hat{a}_j\right] \\ = {} & -\hat{c}_N^\dagger \hat{a}_1 \left[1 - 2\hat{a}_1^\dagger \hat{a}_1\right] \prod_{j=2}^{N} \left[1 - 2\hat{a}_j^\dagger \hat{a}_j\right] + \hat{c}_N^\dagger \left\{1 - 2\hat{a}_1^\dagger \hat{a}_1, \hat{a}_1\right\} \prod_{j=2}^{N} \left[1 - 2\hat{a}_j^\dagger \hat{a}_j\right]. \end{aligned} \tag{47}$$

The anti-commutator vanishes,

$$\left\{1 - 2\hat{a}_1^\dagger \hat{a}_1, \hat{a}_1\right\} = 2\hat{a}_1 - 2\hat{a}_1 \hat{a}_1^\dagger \hat{a}_1 = 2\hat{a}_1 - 2\left\{\hat{a}_1, \hat{a}_1^\dagger\right\} \hat{a}_1 = 2\hat{a}_1 - 2\hat{a}_1 = 0, \tag{48}$$

and thus

$$\hat{a}_N^\dagger \hat{a}_1 = -\hat{c}_N^\dagger \hat{a}_1 \left[1 - 2\hat{a}_1^\dagger \hat{a}_1\right] \prod_{j=2}^{N} \left[1 - 2\hat{a}_j^\dagger \hat{a}_j\right] = -\hat{c}_N^\dagger \hat{K}_1 \hat{c}_1 \prod_{j=1}^{N} \left[1 - 2\hat{a}_j^\dagger \hat{a}_j\right] = -\hat{c}_N^\dagger \hat{c}_1 \hat{K}_{N+1}. \tag{49}$$

Therefore, the Hamiltonian of the cyclic chain is

$$\hat{H}_{\text{cyclic}} = -J \sum_{i=1}^{N} \left(\hat{c}_i^\dagger \hat{c}_{i+1} + \gamma \hat{c}_i^\dagger \hat{c}_{i+1}^\dagger + \text{h.c.}\right) - J\left(\hat{c}_N^\dagger \hat{c}_1 + \gamma \hat{c}_N^\dagger \hat{c}_1^\dagger + \text{h.c.}\right)\left(\hat{K}_{N+1} + 1\right). \tag{50}$$

We shall neglect the second term in the Hamiltonian as it gives $\mathcal{O}\left(N^{-1}\right)$ corrections[4].

$$\boxed{\hat{H}_{\text{cyclic}} = -J\sum_{i=1}^{N}\left(\hat{c}_i^{\dagger}\hat{c}_{i+1} + \gamma\hat{c}_i^{\dagger}\hat{c}_{i+1}^{\dagger} + \text{h.c.}\right).} \tag{51}$$

Solution to 2

Fortunately, this Hamiltonian has the quadratic form in terms of the $\hat{c}_i$ (as in Eq. (1)). Hence, we know that the energies of the elementary excitations, Λ_k, are the eigen-values solutions for

$$\phi_k^{\mathrm{T}}\left(A-B\right)\left(A+B\right) = \Lambda_k^2\phi_k^{\mathrm{T}}. \tag{52}$$

In our problem, the matrices A and B are

$$A = -J\begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 1 & \ddots & 0 & 0 \\ 0 & 1 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 & 1 & 0 \\ 0 & 0 & \ddots & 1 & 0 & 1 \\ 1 & 0 & \cdots & 0 & 1 & 0 \end{bmatrix}, \qquad B = -J\gamma\begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & -1 \\ -1 & 0 & 1 & \ddots & 0 & 0 \\ 0 & -1 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 & 1 & 0 \\ 0 & 0 & \ddots & -1 & 0 & 1 \\ 1 & 0 & \cdots & 0 & -1 & 0 \end{bmatrix} \tag{53}$$

$$\Longrightarrow \left(A-B\right)\left(A+B\right) =$$

$$J^2\begin{bmatrix} 2\left(1+\gamma^2\right) & 0 & 1-\gamma^2 & 0 & \cdots & 0 & 1-\gamma^2 & 0 \\ 0 & 2\left(1+\gamma^2\right) & 0 & 1-\gamma^2 & 0 & \cdots & 0 & 1-\gamma^2 \\ 1-\gamma^2 & 0 & 2\left(1+\gamma^2\right) & \ddots & \ddots & \ddots & \vdots & 0 \\ 0 & 1-\gamma^2 & \ddots & \ddots & \ddots & \ddots & 0 & \vdots \\ \vdots & 0 & \ddots & \ddots & \ddots & \ddots & 1-\gamma^2 & 0 \\ 0 & \vdots & \ddots & \ddots & \ddots & 2\left(1+\gamma^2\right) & 0 & 1-\gamma^2 \\ 1-\gamma^2 & 0 & \cdots & 0 & 1-\gamma^2 & 0 & 2\left(1+\gamma^2\right) & 0 \\ 0 & 1-\gamma^2 & 0 & \cdots & 0 & 1-\gamma^2 & 0 & 2\left(1+\gamma^2\right) \end{bmatrix} \tag{54}$$

For the above matrix, the eigen-values turns out to be

$$\boxed{\Lambda_k^2 = 4J^2\left[1-\left(1-\gamma^2\right)\sin^2\left(k\right)\right]}, \tag{55}$$

where

$$k \equiv \frac{2\pi}{N}m, \qquad m = -\frac{N}{2},\cdots,-1,0,1,\cdots,\frac{N}{2}-1. \tag{56}$$

Note that the sign of Λ_k is arbitrary. If we assign a minus sign to Λ_k, this choice corresponds to particles with negative energy (and no ground state). Instead, we shall take the positive solutions, corresponding to the picture of particles and holes. Interestingly, as $\Lambda_k \propto |J|$, the energy spectrum of the spin chain does not depend on the sign of J.

[4] Plus, $\hat{K}_{N+1} = \prod_{j=1}^{N}\left[1-2\hat{c}_j^{\dagger}\hat{c}_j\right] = \prod_{j=1}^{N}\left[1-2\hat{n}_j\right]$. Since n_j can be either 0 or 1, this means that for half of the Fock space, for states with an odd number of particles, $\hat{K}_{N+1}+1=0$.

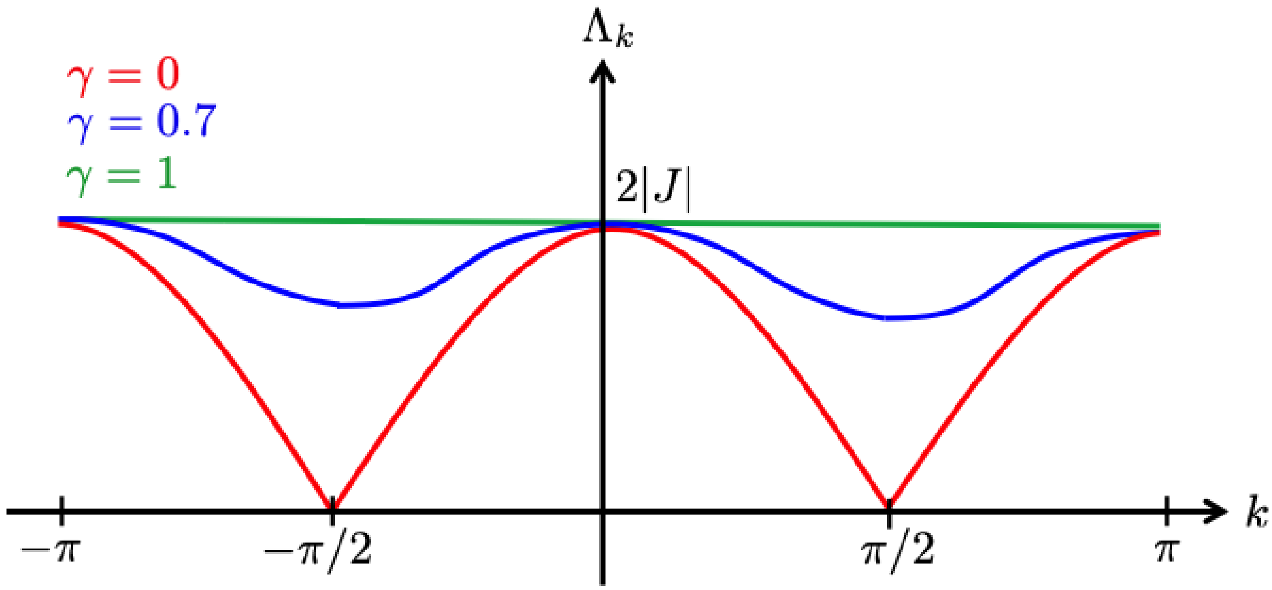

Figure 2: The energy of the elementary excitations in the XY model for three different degree of anisotropy.

Solution to 3

According to Eq. (26), the ground state energy is given by

$$E_0 = \frac{1}{2}\left(\sum_{i=1}^{N} A_{ii} - \sum_{k=1}^{N} \Lambda_k\right) = -\frac{1}{2}\sum_{k=1}^{N} \Lambda_k = -\frac{1}{2}\sum_{k=1}^{N} \frac{\Delta k}{2\pi/N}\Lambda_k. \tag{57}$$

For $N \to \infty$, the average energy of each spin is

$$\boxed{E_0/N \to -\frac{1}{4\pi}\int_{-\pi}^{\pi} dk \Lambda_k = -\frac{|J|}{2\pi}\int_{-\pi}^{\pi} dk \sqrt{1-(1-\gamma^2)\sin^2(k)} = -\frac{2|J|}{\pi}\mathcal{E}\left(\sqrt{1-\gamma^2}\right)}, \tag{58}$$

where $\mathcal{E}(x)$ is the complete elliptic integral of the second kind,

$$\mathcal{E}(x) \equiv \frac{1}{4}\int_{-\pi}^{\pi} dk \sqrt{1-x^2\sin^2(k)} = \int_0^{\pi/2} dk \sqrt{1-x^2\sin^2(k)}. \tag{59}$$

E_0/N goes smoothly between the limiting cases

$$E_0/N = \begin{cases} -\frac{2|J|}{\pi} & \gamma = 0 \text{ (isotropic)} \\ -|J| & \gamma = \pm 1 \text{ (Ising)} \end{cases}. \tag{60}$$

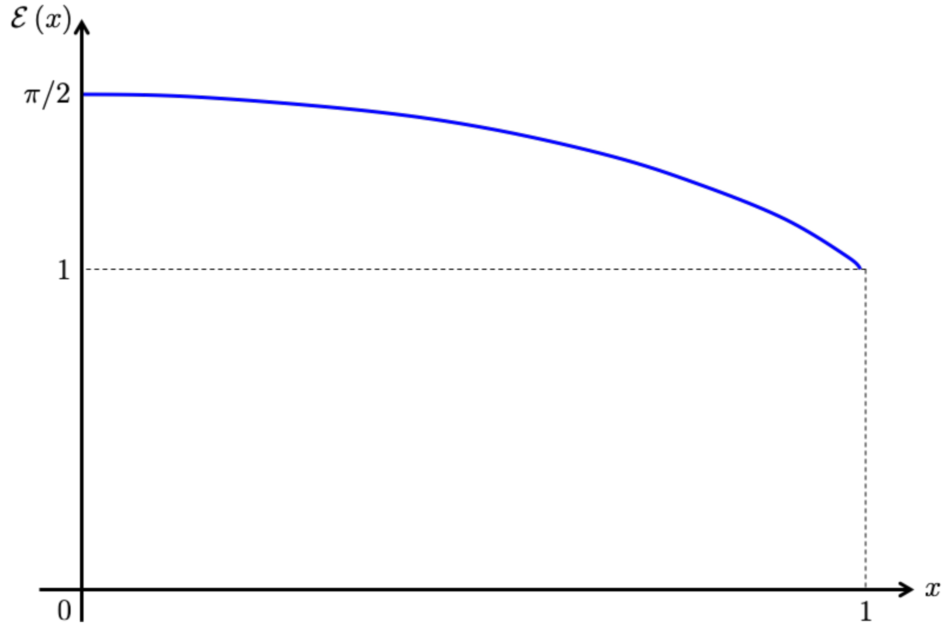

Figure 3: Graphical representation of the complete elliptic integral of the second kind.

Solution to 4

In a previous tutorial we found that the partition function for fermions is given by

$$Z = \det\left(\mathbb{I} + e^{-\beta\Lambda}\right). \tag{61}$$

This partition function however corresponds to a system with $E_0 = 0$. In the case of non-vanishing ground-state energy, the expression is slightly modified,

$$\begin{aligned} Z &= e^{-\beta E_0}\det\left(\mathbb{I} + e^{-\beta\Lambda}\right) = e^{-\beta E_0}\det\left[\left(e^{-\beta\Lambda/2}\left(e^{+\beta\Lambda/2} + e^{-\beta\Lambda/2}\right)\right)\right] = e^{-\beta E_0}\det\left[2e^{-\beta\Lambda/2}\cosh\left(\frac{\beta\Lambda}{2}\right)\right] \\ &= e^{-\beta E_0}\det\left[e^{-\beta\Lambda/2}\right]\det\left[2\cosh\left(\frac{\beta\Lambda}{2}\right)\right] = e^{-\beta E_0}\exp\left(-\frac{\beta}{2}\sum_{k=1}^{N}\Lambda_k\right)\det\left[2\cosh\left(\frac{\beta\Lambda}{2}\right)\right] \\ &= e^{-\beta E_0}e^{\beta E_0}\det\left[2\cosh\left(\frac{\beta\Lambda}{2}\right)\right] = \det\left[2\cosh\left(\frac{\beta\Lambda}{2}\right)\right]. \end{aligned} \tag{62}$$

The Helmholtz free energy can be computed from the partition function,

$$F = -\frac{1}{\beta}\ln Z = -\frac{1}{\beta}\ln\left[\det\left[2\cosh\left(\frac{\beta\Lambda}{2}\right)\right]\right] = -\frac{1}{\beta}\mathrm{Tr}\left[\ln\left[2\cosh\left(\frac{\beta\Lambda}{2}\right)\right]\right] \tag{63}$$

$$= -k_BT\sum_k \ln\left(2\cosh\left(\beta\Lambda_k/2\right)\right) = -Nk_BT\sum_k\frac{\Delta k}{2\pi}\ln\left(2\cosh\left(\beta\Lambda_k/2\right)\right) \tag{64}$$

$$\rightarrow -\frac{Nk_BT}{2\pi}\int_{-\pi}^{\pi}dk\ln\left(2\cosh\left(\beta\Lambda_k/2\right)\right) = -\frac{2Nk_BT}{\pi}\int_0^{\pi/2}dk\ln\left(2\cosh\left(\beta\Lambda_k/2\right)\right). \tag{65}$$

And in the Ising limit ($\gamma = \pm 1$) we find

$$\boxed{F_{\text{Ising}} = -Nk_BT\ln\left(2\cosh\left(\beta J\right)\right)}. \tag{66}$$

This is the same classical expression you saw in your thermodynamics course.