Notes on 1D Quantum Chains

Moayad M. Ekhwan

October 22, 2020

Useful Definitions & Relations

Pauli Spin Operator Relations

$$\sigma_i^x = \sigma_i^+ + \sigma_i^-; \quad \sigma_i^y = -i(\sigma_i^+ - \sigma_i^-); \quad \sigma_i^z = 2\sigma_i^+\sigma_i^- - 1 \tag{1}$$

(1D) Jordan-Wigner Transformation

$$\sigma_i^- = \prod_{j=1}^{i-1}(-\sigma_j^z)c_i; \qquad \sigma_i^+ = c_i^\dagger \prod_{j=1}^{i-1}(-\sigma_j^z) \tag{2}$$

Nearest Neighbor Relations

$$\sigma_i^+\sigma_{i+1}^+ = c_i^\dagger c_{i+1}^\dagger; \quad \sigma_i^+\sigma_{i+1}^- = c_i^\dagger c_{i+1}; \quad \sigma_i^-\sigma_{i+1}^+ = -c_i c_{i+1}^\dagger; \quad \sigma_i^-\sigma_{i+1}^- = -c_i c_{i+1} \tag{3}$$

(Discrete) Fourier Transformation

$$c_i = \frac{1}{\sqrt{N}}\sum_q^N c_q e^{-iqR_i}; \qquad c_i^\dagger = \frac{1}{\sqrt{N}}\sum_q^N c_q^\dagger e^{iqR_i} \tag{4}$$

Fourier Relations

$$\begin{gathered}\sum_i c_i^\dagger c_i = \sum_q c_q^\dagger c_q; \quad \sum_i c_i c_{i+1}^\dagger = \sum_q e^{iq}\, c_q c_q^\dagger; \quad \sum_i c_i^\dagger c_{i+1} = \sum_q e^{-iq}\, c_q^\dagger c_q \\ \sum_i c_i c_{i+1} = \sum_q e^{iq}\, c_q c_{-q}; \quad \sum_i c_i^\dagger c_{i+1}^\dagger = \sum_q e^{-iq}\, c_q^\dagger c_{-q}^\dagger\end{gathered} \tag{5}$$

1 Exact Solutions Using Jordan-Wigner

1.1 General Procedure

0. Express spin operators in terms of creation and annihilation spin operators using (1).

+ If there is a quartic term in the creation/annihilation operators, try a canonical transformation to get it to quadratic form. For example, a rotation is used later in Section 1.2.

1. Apply the Jordan-Wigner Transformation.

2. Transform to momentum space.

+ If H cannot be put directly in Bogoliubov form then try summing over positive modes $q > 0$.

3. Diagonalize the Bogoliubov hamiltonian by a similarity transformation.

1.2 Example 1: Transverse Ising Chain

$$H = -\sum_i \sigma_i^x + \bar{\lambda}\sigma_i^z \sigma_{i+1}^z \tag{6}$$

Here $\bar{\lambda} = J/\Gamma$ is a proportionality factor where J is the nearest neighbor interaction and Γ is the applied external transverse magnetic field strength.

Rotation

we rotate the system by $\pi/2$ counterclockwise around the y-axis:

$$\begin{aligned} \sigma^x &\to \sigma^z \\ \sigma^y &\to \sigma^y \\ \sigma^z &\to -\sigma^x \end{aligned} \qquad \begin{pmatrix} \sigma^z \\ \sigma^y \\ -\sigma^x \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \begin{pmatrix} \sigma^x \\ \sigma^y \\ \sigma^z \end{pmatrix} \tag{7}$$

This eliminates the quartic term resulting from $\sigma_i^z \sigma_{i+1}^z$.

$$H = -\sum_i (\sigma_i^z - \bar{\lambda}\sigma_i^x \sigma_{i+1}^x) \tag{8}$$

1.2.1 Jordan-Wigner Transformation

$$H = N - \sum_i [2\sigma_i^+ \sigma_i^- - \bar{\lambda}(\sigma_i^+ + \sigma_i^-)(\sigma_{i+1}^+ + \sigma_{i+1}^-)] \tag{9}$$

Using (1). Next we apply the Jordan-Wigner Transformation (2). For the first term, the Pauli strings cancel each other ($\prod_{j=1}^{i-1}(-\sigma_j^z)^2 = \mathbb{1}$). Now using the nearest neighbor relations (3), with $N = \sum_i 1$:

$$H = N - \sum_i [2c_i^\dagger c_i + \bar{\lambda}(c_i^\dagger c_{i+1}^\dagger + c_i^\dagger c_{i+1} - c_i c_{i+1}^\dagger - c_i c_{i+1})] \tag{10}$$

Steps: Computing $\sigma_i^- \sigma_{i+1}^+$

$$\sigma_i^- \sigma_{i+1}^+ = \prod_{j=1}^{i-1}(-\sigma_j^z) c_i c_{i+1}^\dagger \prod_{j=1}^{i}(-\sigma_j^z)$$

The left string commutes with c_i and the right string commutes with $c_{i+1}^\dagger$:

$$\begin{aligned} &= c_i \prod_{j=1}^{i-1}(-\sigma_j^z) \prod_{j=1}^{i}(-\sigma_j^z) c_{i+1}^\dagger = -c_i \sigma_i^z c_{i+1}^\dagger \\ &= -c_i(2\sigma_i^+\sigma_i^- - 1)c_{i+1}^\dagger = -c_i(2c_i^\dagger c_i - 1)c_{i+1}^\dagger \\ &= -2c_i c_i^\dagger c_i c_{i+1}^\dagger + c_i c_{i+1}^\dagger = 2(\cancel{c_i c_i c_i^\dagger} - c_i)c_{i+1}^\dagger + c_i c_{i+1}^\dagger \\ &= -2c_i c_{i+1}^\dagger + c_i c_{i+1}^\dagger = -c_i c_{i+1}^\dagger \end{aligned}$$

1.2.2 Fourier Transformation

Now using (4) one can find (5):

$$H = N - \sum_q \left[2(1 + \bar{\lambda}\cos q)c_q^\dagger c_q + \bar{\lambda}(e^{-iq} c_q^\dagger c_{-q}^\dagger - e^{iq} c_q c_{-q})\right] \tag{11}$$

Steps: Transforming Quadratic Terms to Momentum Space

$$c_i^\dagger c_i = \sum_i \frac{1}{N} \sum_{qq'} c_q^\dagger c_{q'} e^{ij(q-q')} = \frac{1}{N} \sum_{qq'} c_q^\dagger c_{q'} \delta_{qq'} = \sum_q c_q^\dagger c_q$$

$$c_i c_{i+1}^\dagger = \sum_i \frac{1}{N} \sum_{qq'} c_q c_{q'}^\dagger e^{ij(q-q')} e^{iq'} = \frac{1}{N} \sum_{qq'} c_q c_{q'}^\dagger \delta_{qq'} e^{iq'} = \sum_q e^{iq}\, c_q c_q^\dagger$$

$$c_i^\dagger c_{i+1} = -(c_i c_{i+1}^\dagger)^\dagger = \sum_q -e^{-iq}\,(c_q c_q^\dagger)^\dagger = \sum_q e^{-iq}\, c_q^\dagger c_q$$

$$c_i^\dagger c_{i+1} - c_i c_{i+1}^\dagger = \sum_q e^{-iq}\, c_q^\dagger c_q - e^{iq}\, c_q c_q^\dagger = \sum_q c_q^\dagger c_q (e^{-iq} + e^{iq}) - \cancel{e^{iq}} = \sum_q 2\cos q\, c_q^\dagger c_q$$

$$c_i c_{j+1} = \frac{1}{N} \sum_{qq'} c_q c_{q'} e^{-ij(q+q')} e^{-iq'} = \frac{1}{N} \sum_{qq'} c_q c_{q'} \delta_{-qq'} e^{-iq'} = \sum_q e^{iq}\, c_q c_{-q}$$

$$c_i^\dagger j c_{j+1}^\dagger = -(c_i c_{j+1})^\dagger = \sum_q -e^{-iq} (c_q c_{-q})^\dagger = \sum_q e^{-iq}\, c_q^\dagger c_{-q}^\dagger$$

1.2.3 Sum Over Positive Modes

This does not mean we neglect the sum over negative value, but we make it up symbolically so the values are included over a positive sum.

$$H = -2 \sum_{q>0} \left[(1 + \bar{\lambda} \cos q)(c_q^\dagger c_q - c_{-q} c_{-q}^\dagger) + i\bar{\lambda} \sin q\, (c_q^\dagger c_{-q}^\dagger - c_{-q} c_q) \right] \tag{12}$$

This step is might not be needed, (as in this case,) but it gives a neater expression here.

Steps: Sum Over Positive Modes

$$H = N - \left\{ \sum_{q<0} (\cdots) + \sum_{q>0} (\cdots) \right\}$$

$$\sum_{q<0} \left[2(1 + \bar{\lambda} \cos q) c_q^\dagger c_q + \bar{\lambda}(e^{-iq}\, c_q^\dagger c_{-q}^\dagger - e^{iq}\, c_q c_{-q}) \right]$$

$$= \sum_{q>0} \left[2(1 + \bar{\lambda} \cos q) c_{-q}^\dagger c_{-q} + \bar{\lambda}(e^{iq}\, c_{-q}^\dagger c_q^\dagger - e^{-iq}\, c_{-q} c_q) \right]$$

$$= \sum_{q>0} \left[2(1 + \bar{\lambda} \cos q)(1 - c_{-q} c_{-q}^\dagger) - \bar{\lambda}(e^{-iq}\, c_{-q} c_q + e^{iq}\, c_q^\dagger c_{-q}^\dagger) \right]$$

$$= \sum_{q>0} 2(1 + \cancel{\bar{\lambda} \cos q}) + \sum_{q>0} \left[-2(1 + \bar{\lambda} \cos q) c_{-q} c_{-q}^\dagger - \bar{\lambda}(e^{iq}\, c_q^\dagger c_{-q}^\dagger + e^{-iq}\, c_{-q} c_q) \right]$$

$$= N + \sum_{q>0} \left[-2(1 + \bar{\lambda} \cos q) c_{-q} c_{-q}^\dagger - \bar{\lambda}(e^{iq}\, c_q^\dagger c_{-q}^\dagger + e^{-iq}\, c_{-q} c_q) \right]$$

$$\implies H = -\sum_{q>0} \left[2(1 + \bar{\lambda} \cos q)(c_q^\dagger c_q - c_{-q} c_{-q}^\dagger) + \bar{\lambda}(e^{-iq} c_q^\dagger c_{-q}^\dagger - e^{iq}\, c_q c_{-q} + e^{iq}\, c_q^\dagger c_{-q}^\dagger - e^{-iq}\, c_{-q} c_q) \right]$$

$$= -\sum_{q>0} \left[2(1 + \bar{\lambda} \cos q)(c_q^\dagger c_q - c_{-q} c_{-q}^\dagger) + \bar{\lambda}(e^{-iq} c_q^\dagger c_{-q}^\dagger + e^{iq}\, c_q c_{-q} - e^{iq}\, c_q^\dagger c_{-q}^\dagger - e^{-iq}\, c_{-q} c_q) \right]$$

$$= -\sum_{q>0} \left[2(1 + \bar{\lambda} \cos q)(c_q^\dagger c_q - c_{-q} c_{-q}^\dagger) + \bar{\lambda}(e^{-iq} - e^{iq})(c_q^\dagger c_{-q}^\dagger - c_{-q} c_q) \right]$$

$$= -2 \sum_{q>0} \left[(1 + \bar{\lambda} \cos q)(c_q^\dagger c_q - c_{-q} c_{-q}^\dagger) - \bar{\lambda} i \sin q (c_q^\dagger c_{-q}^\dagger - c_{-q} c_q) \right]$$

1.2.4 Bogoliubov Hamiltonian

$$H = -2\sum_{q>0} \begin{pmatrix} c_q^\dagger & c_{-q} \end{pmatrix} \begin{pmatrix} 1+\bar\lambda\cos q & -i\bar\lambda\sin q \\ i\bar\lambda\sin q & -(1+\bar\lambda\cos q) \end{pmatrix} \begin{pmatrix} c_q \\ c_{-q}^\dagger \end{pmatrix} \tag{13}$$

Now the hamiltonian is diagonalized using a canonical similarity transformation with $U^\dagger U = 1$:

$$\vec{c}^\dagger H\vec{c} = (\vec{c}^\dagger U^\dagger)(UHU^\dagger)(U\vec{c}) = \vec{\eta}^\dagger D\vec{\eta} \tag{14}$$

Steps: Diagonalization

$$\begin{pmatrix} \alpha & -i\beta \\ i\beta & -\alpha \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \omega_\pm \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \to \begin{vmatrix} \alpha-\omega & -i\beta \\ i\beta & -(\alpha+\omega) \end{vmatrix} = \omega^2-\alpha^2-\beta^2 = 0 \to \omega_\pm = \pm\sqrt{\alpha^2+\beta^2}$$

$$\alpha c_1 - i\beta c_2 = \omega_\pm c_1 \to (\alpha+\omega_\mp)c_1 = i\beta c_2 \to \mathbf{v}_1 = \frac{1}{\sqrt{(\alpha+\omega)^2+\beta^2}}\begin{pmatrix} i\beta \\ \alpha+\omega_\mp \end{pmatrix}$$

$$i\beta c_1 - \alpha c_2 = \omega_\pm c_2 \to i\beta c_1 = (\alpha+\omega_\pm)c_2 \to \mathbf{v}_2 = \frac{1}{\sqrt{(\alpha+\omega)^2+\beta^2}}\begin{pmatrix} \alpha+\omega_\pm \\ i\beta \end{pmatrix}$$

For convenience, the unitary matrix is (arbitrarily) defined with positive-valued ω_q:

$$D = \mathrm{diag}(\omega_q, -\omega_q); \quad U = \frac{1}{\sqrt{(\alpha+\omega)^2+\beta^2}}\begin{pmatrix} \alpha+\omega_q & i\beta \\ i\beta & \alpha+\omega_q \end{pmatrix} \tag{15}$$

Using (15) with $\alpha = 1+\bar\lambda\cos q$ and $\beta = \bar\lambda\sin q$, thus $\omega_q = \sqrt{1+2\bar\lambda\cos q+\bar\lambda^2}$:

$$U = \begin{pmatrix} u_q & iv_q \\ iv_q & u_q \end{pmatrix}; \quad u_q = \frac{1+\bar\lambda\cos q+\omega_q}{\sqrt{2\omega_q(1+\bar\lambda\cos q+\omega_q)}}; \quad v_q = \frac{\bar\lambda\sin q}{\sqrt{2\omega_q(1+\bar\lambda\cos q+\omega_q)}}$$

1.2.5 Diagonalized Hamiltonian

$$H = 2\sum_q \omega_q\eta_q^\dagger\eta_q + E_0; \qquad E_0 = -\sum_q \omega_q \tag{16}$$

Steps: Diagonalized Hamiltonian

$$\begin{aligned} H &= -2\begin{pmatrix} \eta_q^\dagger & \eta_{-q} \end{pmatrix} \mathrm{diag}(\omega_q, -\omega_q) \begin{pmatrix} \eta_q & \eta_{-q}^\dagger \end{pmatrix}^T = 2\sum_{q>0}\omega_q(\eta_q^\dagger\eta_q - \eta_{-q}\eta_{-q}^\dagger) \\ &= 2\sum_{q>0}\omega_q(\eta_q^\dagger\eta_q - 1 + \eta_{-q}^\dagger\eta_{-q}) = 2\sum_q \omega_q\eta_q^\dagger\eta_q - \sum_q\omega_q \end{aligned}$$

1.3 Example 2: XY Model

$$H = \sum_i (1+\gamma)\sigma_i^x\sigma_{i+1}^x + (1-\gamma)\sigma_i^y\sigma_{i+1}^y \tag{17}$$

Here γ is the anisotropy parameter. The system is isotropic (independent of orientation) for $\gamma = 0$. The limiting anisotropic case $\gamma = \pm 1$ reduces to the Ising case (but without the transverse field).

Steps: Rewriting The Hamiltonian in S^+ and S^-

Using (1):

$$(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y) + \gamma(\sigma_i^x\sigma_{i+1}^x - \sigma_i^y\sigma_{i+1}^y)$$
$$= (\sigma_i^+ + \sigma_i^-)(\sigma_{i+1}^+ + \sigma_{i+1}^-) - (\sigma_i^+ - \sigma_i^-)(\sigma_{i+1}^+ - \sigma_{i+1}^-) + \gamma((\sigma_i^+ + \sigma_i^-)(\sigma_{i+1}^+ + \sigma_{i+1}^-) + (\sigma_i^+ - \sigma_i^-)(\sigma_{i+1}^+ - \sigma_{i+1}^-))$$
$$(\sigma_i^+ + \sigma_i^-)(\sigma_{i+1}^+ + \sigma_{i+1}^-) = \sigma_i^+\sigma_{i+1}^+ + \sigma_i^+\sigma_{i+1}^- + \sigma_i^-\sigma_{i+1}^+ + \sigma_i^-\sigma_{i+1}^-$$
$$(\sigma_i^+ - \sigma_i^-)(\sigma_{i+1}^+ - \sigma_{i+1}^-) = \sigma_i^+\sigma_{i+1}^+ - \sigma_i^+\sigma_{i+1}^- - \sigma_i^-\sigma_{i+1}^+ + \sigma_i^-\sigma_{i+1}^-$$
$$\boxed{H = 2\sum_i \left[(\sigma_i^+\sigma_{i+1}^- + \sigma_i^-\sigma_{i+1}^+) + \gamma(\sigma_i^+\sigma_{i+1}^+ + \sigma_i^-\sigma_{i+1}^-)\right]}$$

1.3.1 Jordan-Wigner Transformation

Using the nearest neighbor relations (3) on the boxed equation:

$$H = 2\sum_i \left[(c_i^\dagger c_{i+1} - c_i c_{i+1}^\dagger) + \gamma(c_i^\dagger c_{i+1}^\dagger - c_i c_{i+1})\right] \tag{18}$$

1.3.2 Fourier Transformation

Using the fourier relations in (5) into equation (18):

$$H = \sum_q \left[4\cos q\, c_q^\dagger c_q + 2\gamma(e^{-iq}\, c_q^\dagger c_{-q}^\dagger - e^{iq}\, c_q c_{-q})\right] \tag{19}$$

Steps: Fourier Transform

$$\sum_i c_i^\dagger c_{i+1} - c_i c_{i+1}^\dagger = \sum_q e^{-iq}\, c_q^\dagger c_q - e^{iq}\, c_q c_q^\dagger = \sum_q (e^{-iq} + e^{iq}) c_q^\dagger c_q = \sum_q 2\cos q\, c_q^\dagger c_q$$

1.3.3 Sum Over Positive Modes

$$H = 4\sum_{q>0} \left[\cos q\,(c_q^\dagger c_q - c_{-q}c_{-q}^\dagger) + \gamma i \sin q\,(c_{-q}c_q - c_q^\dagger c_{-q}^\dagger)\right] \tag{20}$$

Arranging $(c_q^\dagger, c_{-q})$ to the left and $(c_q, c_{-q}^\dagger)$ to the right to obtain the Bogoliubov form more easily.

Steps: Sum Over Positive Modes

$$\sum_{q<0} \left[4\cos q\, c_q^\dagger c_q + 2\gamma(e^{-iq}\, c_q^\dagger c_{-q}^\dagger - e^{iq}\, c_q c_{-q})\right] = \sum_{q>0} \left[4\cos q\, c_{-q}^\dagger c_{-q} + 2\gamma(e^{iq}\, c_{-q}^\dagger c_q^\dagger - e^{-iq}\, c_{-q} c_q)\right]$$
$$= \sum_{q>0} \left[\cancel{4\cos q} - 4\cos q\, c_{-q}c_{-q}^\dagger - 2\gamma(e^{-iq}\, c_{-q}c_q + e^{iq}\, c_q^\dagger c_{-q}^\dagger)\right]$$

Then: $$H = \sum_{q>0} \left[4\cos q(c_q^\dagger c_q - c_{-q}c_{-q}^\dagger) + 2\gamma(e^{-iq}\, c_q^\dagger c_{-q}^\dagger - e^{iq}\, c_q c_{-q} - e^{-iq}\, c_{-q}c_q - e^{iq}\, c_q^\dagger c_{-q}^\dagger)\right]$$
$$= \sum_{q>0} \left[4\cos q(c_q^\dagger c_q - c_{-q}c_{-q}^\dagger) + 2\gamma(e^{-iq}\, c_q^\dagger c_{-q}^\dagger + e^{iq}\, c_q c_{-q} - e^{-iq}\, c_{-q}c_q - e^{iq}\, c_q^\dagger c_{-q}^\dagger)\right]$$
$$= \sum_{q>0} \left[4\cos q(c_q^\dagger c_q - c_{-q}c_{-q}^\dagger) + 2\gamma(e^{-iq} - e^{iq})(c_q^\dagger c_{-q}^\dagger - c_{-q}c_q)\right]$$
$$= 4\sum_{q>0} \left[\cos q(c_q^\dagger c_q - c_{-q}c_{-q}^\dagger) + \gamma i \sin q\,(c_{-q}c_q - c_q^\dagger c_{-q}^\dagger)\right]$$

Note that $[c_q^\dagger, c_{-q}^\dagger] = [c_q, c_{-q}] = 0$ but $\{c_q^\dagger, c_q\} = 1$ and $\sum_{q>0}\cos q = 0$.

1.3.4 Bogoliubov Hamiltonian

$$H = 4 \sum_{q>0} \begin{pmatrix} c_q^\dagger & c_{-q} \end{pmatrix} \begin{pmatrix} \cos q & -i\gamma \sin q \\ i\gamma \sin q & -\cos q \end{pmatrix} \begin{pmatrix} c_q \\ c_{-q}^\dagger \end{pmatrix} \tag{21}$$

Note that the matrix has the same form or symmetry as for the transverse Ising chain, so we could use our result from (15): $\alpha = \cos q$, $\beta = \gamma \sin q$, and $\omega_q = \sqrt{\cos^2 q + \gamma^2 \sin^2 q} = \sqrt{1 - (1-\gamma^2)\sin^2 q}$, so:

$$U = \begin{pmatrix} u_q & iv_q \\ iv_q & u_q \end{pmatrix}; \quad u_q = \sqrt{\frac{\cos q + \omega_q}{2\omega_q}}; \quad v_q = \frac{\gamma \sin q}{\sqrt{2\omega_q(\cos q + \omega_q)}}$$

Steps: Unitary Matrix Elements

$$u_q = \frac{\alpha+\omega}{\sqrt{(\alpha+\omega)^2+\beta^2}} = \frac{\alpha+\omega}{\sqrt{\omega^2+2\omega\alpha+(\alpha^2+\beta^2)}} \xrightarrow{\alpha^2+\beta^2=\omega^2} = \frac{\alpha+\omega}{\sqrt{2\omega(\alpha+\omega)}} = \sqrt{\frac{\alpha+\omega}{2\omega}}$$

1.3.5 Diagonalized Hamiltonian

$$H = 4\sum_q \omega_q \eta_q^\dagger \eta_q + E_0; \qquad E_0 = -2\sum_q \omega_q \tag{22}$$

If normalized pauli matrices were used instead, one would have: $H = \sum_q \omega_q \eta_q^\dagger \eta_q + E_0$; $E_0 = -\sum_q \omega_q/2$.

Steps: Diagonalized Hamiltonian

$$\begin{aligned} H &= 4\begin{pmatrix} \eta_q^\dagger & \eta_{-q} \end{pmatrix} \operatorname{diag}(\omega_q, -\omega_q) \begin{pmatrix} \eta_q & \eta_{-q}^\dagger \end{pmatrix}^T = 4\sum_{q>0} \omega_q(\eta_q^\dagger \eta_q - \eta_{-q}\eta_{-q}^\dagger) \\ &= 4\sum_{q>0} \omega_q(\eta_q^\dagger\eta_q - 1 + \eta_{-q}^\dagger \eta_{-q}) = 4\sum_q \omega_q \eta_q^\dagger \eta_q - 2\sum_q \omega_q \end{aligned}$$

What is Next?

Once the hamiltonian is diagonalized, many aspects of the system can be studied, of which the following are examined here:

1. **Elementary Excitations Spectrum** (Section 2) Sound can be decomposed to (collective) phonon excitations, (which do not belong to a specific position). Similarly, the excitations of our system in position basis may be decomposed to (collective) elementary excitation in momentum space. In effect what did by "Exact Diagonalization" is map positional excitations to elementary excitation by the Fourier-Bogoliubov transformation ($\mathbb{Z}_N \mapsto S^1$ or $\mathbb{R} \mapsto S^1$).
2. **Ground State Energy** (Section 3) Examining the ground state energy is a critical component to studying low-energy case of the system, which is often the considered case. In both examples we could study the ground state energy as a function of the parameter in question:
   - Relative coupling strength $\bar{\lambda}$ for transverse Ising chain 1.2
   - Anisotropy parameter γ for the XY model 1.3.
3. **Correlation Functions** (Section 4) Quantum phase transitions and order are two the most important features of an Ising model, such properties are investigated by computing correlation functions.

2 Elementary Excitations

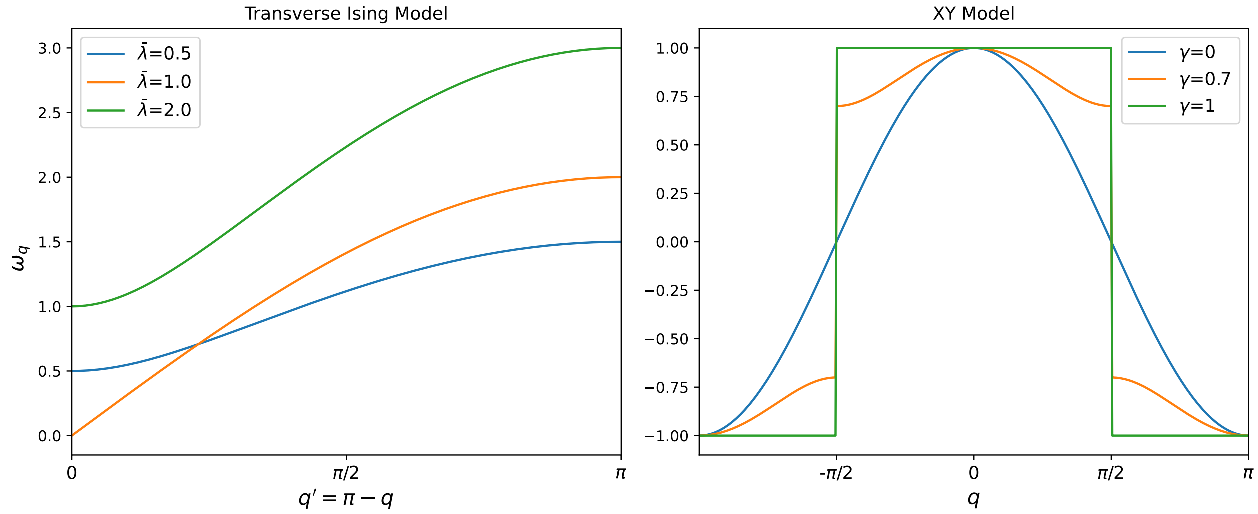

Figure 2.1 Elementary excitation energy for different parameter values as a function of q.

2.1 Transverse Ising Model

The lowest 'transition' energy, q at which the ground state and excitation energies are closest to each other, occurs at $q' = 0$. The system always has a gap at this mode ($q' = 0$) except for the critical value of $\bar{\lambda} = 1$ where $\omega = 0$ and the gap vanishes. The critical value at which the spectra 'overlap' give rise to degeneracy, because it costs no energy for excitation at $q' = 0$, also called a *Goldestone* mode. Consequently, degeneracy give rise to disorder, so the critical case is important in that aspect as well. This model was first solved by [1]. For a textbook-like treatment [2].

Particle-Hole Symmetry

Note: Because our eigenvalues were $\pm\omega$, our system possess the property that the energy of an excitation at q is equal (with a minus sign) to the corresponding ground state energy at q, (i.e. symmetric about the Fermi energy line,) this is property Particle-hole symmetry.

If we assume a hamiltonian with two different eigenvalues ($\omega_1, \omega_2; |\omega_1| \neq |\omega_2|$), then we would obtain a solution of this form:

$$H = \sum_q (\omega_{(1)q} - \omega_{(2)q})\eta_q^\dagger \eta_q - \sum_q \omega_{(2)q}$$

Meaning $\langle H \rangle_q$ is $\omega_{(2)q}$ at the ground-state and $\omega_{(1)q}$ for an excitation at q

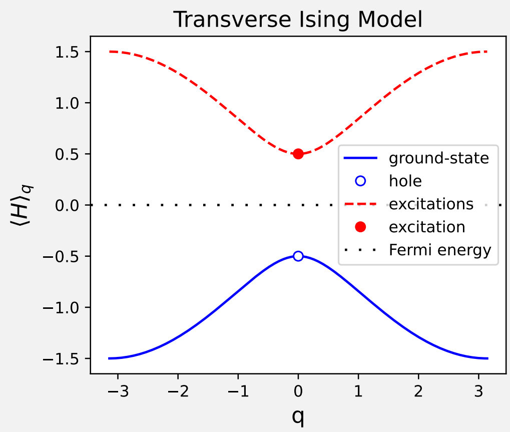

Figure 2.2 Expectation values of elementary excitations and ground states at positions q.

2.2 XY Model

There is a gap proportional to the anisotropy $|\gamma|$ but it vanishes in the isotropic case $\gamma = 0$.

Correction to Pfeuty [1] (Fig. 1) and Chakrabarti [2] (Fig. 2.2)

$\bar{\lambda} = 2$ is incorrectly denoted by $\bar{\lambda} = 1.5$ (**Figure 2.2**).

$$\omega(q' = 0, \bar{\lambda} = 3/2) = \sqrt{1 + 2\,(3/2)\cos(\pi) + (3/2)^2} = \sqrt{1 - 3 + 9/4} = 1/2 \neq 1$$
$$\omega(q' = 0, \bar{\lambda} = 2) = \sqrt{1 + 2\,(2)\cos(\pi) + 2^2} = \sqrt{1 - 4 + 4} = 1 \qquad (q' = \pi - q = 0 \to q = \pi)$$

3 Ground State Energy

For the ground state, we evaluate the integral in the continuum limit:

$$E_0 = -\sum_q \omega_q \to \frac{E_0}{N} = -\int_{-\pi}^{\pi} \frac{dq}{2\pi}\omega_q \tag{23}$$

3.1 Transverse Ising Chain

$$E_0/N = -\frac{1}{\pi}\int_0^{\pi} \sqrt{1 + 2\bar{\lambda}\cos q + \bar{\lambda}^2}\, dq = -\frac{2}{\pi}(1 + \bar{\lambda})\, \mathbf{E}\left(\sqrt{4\bar{\lambda}/(1 + \bar{\lambda})^2}\right) \tag{24}$$

where $\mathbf{E}(k) \equiv E(\pi/2, k)$ is the complete elliptic integral of the second kind.

Steps: Obtaining 2nd Kind The Elleptic Integral in Normal Form

Legendre normal form of The elliptic integral of the second kind $E(\phi, k)$:

$$E(\phi, k) = \int_0^{\phi} \sqrt{1 - k^2 \sin^2\phi}\, d\phi$$

We note we can use the half-angle identity, $1 - \cos q = 2\sin^2(q/2)$, so:

$$\begin{aligned}
E_0/N &= -\frac{1}{\pi}\int_0^{\pi} \sqrt{(1 + \bar{\lambda}^2) + 2\bar{\lambda}\cos q}\, dq \\
&= -\frac{1}{\pi}\int_0^{\pi} \sqrt{(1 + \bar{\lambda}^2)^2 - 2\bar{\lambda}(1 - 2\bar{\lambda}\cos q)}\, dq \\
&= -\frac{1}{\pi}(1 + \bar{\lambda}^2)\int_0^{\pi} \sqrt{1 - \frac{4\bar{\lambda}}{1 + \bar{\lambda}^2}\sin^2(q/2)}\, dq \\
&\qquad \phi = q/2,\ \ dq = 2d\phi\ \ (0, \pi) \to (0, \pi/2);\ \ k = \sqrt{4\bar{\lambda}/(1 + \bar{\lambda})^2} \\
&= -\frac{2}{\pi}(1 + \bar{\lambda}^2)\mathbf{E}\left(\sqrt{4\bar{\lambda}/(1 + \bar{\lambda})^2}\right)
\end{aligned}$$

3.2 XY Model

Here we take the normalized version of (16), noting the symmetry of the integral and that it is readily obtained in complete elleptic form of the second kind:

$$E_0/N = -\frac{1}{\pi}\int_0^{\pi/2} \sqrt{1 - (1 - \gamma^2)\sin^2 q}\, dq = -\mathbf{E}\left(\sqrt{1 - \gamma^2}\right)/\pi \tag{25}$$

$$\begin{aligned}
&\text{Isotropic case } (\gamma = 0): \quad && E_0/N = -1/\pi \qquad && \mathbf{E}(1) = \mathbf{E}'(0) = 1 \\
&\text{Ising case } (\gamma = \pm 1): \quad && E_0/N = -1/2 \qquad && \mathbf{E}(0) = \pi/2
\end{aligned}$$

where $k' \equiv \sqrt{1 - k^2}$ is the *complementary module* (whereas k is the *module*) and $\mathbf{E}'(k' = 0)$ gives the first term of the series with all others zero.

Further Definitions and Relations

Majorana Operators

$$A_i \equiv c_i^\dagger + c_i \qquad B_i \equiv c_i^\dagger - c_i \tag{26}$$

$$\sigma_i^z = 2c_i^\dagger c_i - 1 = c_i^\dagger c_i - c_i c_i^\dagger = c_i^{\dagger 2} + c_i^\dagger c_i - c_i c_i^\dagger + c_i^2 = (c_i^\dagger - c_i)(c_i^\dagger + c_i) = B_i A_i \tag{27}$$

$$B_i A_j = c_i^\dagger c_j^\dagger + c_i^\dagger c_j - c_i c_j^\dagger - c_i c_j = -c_j^\dagger c_i^\dagger - c_j c_i^\dagger + c_j^\dagger c_i + c_j c_i = -A_j B_i \tag{28}$$

$$\left(\prod_{1\le k<i} -\sigma_k^z\right)^2 = \prod_{1\le k<i}\left(-\sigma_k^z\right)^2 = \mathbb{1} \qquad \prod_{i\le k<j}\left(-\sigma_k^z\right) = \prod_{i\le k<j} A_k B_k \tag{29}$$

$$A_i^2 = c_i^{\dagger 2} + \left\{c_i^\dagger, c_i\right\} + c_i^2 = 1 \qquad B_i^2 = c_i^{\dagger 2} - \left\{c_i^\dagger, c_i\right\} + c_i^2 = -1 \tag{30}$$

Forier-Bogoliubov Transformation (Specific)

$$c_i = \frac{1}{\sqrt{N}}\sum_q e^{-iqR_i}\left(u_q\eta_q - iv_q\eta_{-q}^\dagger\right) \qquad c_i^\dagger = \frac{1}{\sqrt{N}}\sum_q e^{iqR_i}\left(u_q\eta_q^\dagger + iv_q\eta_{-q}\right) \tag{31}$$

Vacuum Expectation Values

$$\begin{aligned} \langle\eta_q^\dagger\eta_{q'}^\dagger\rangle &= \langle\eta_q\eta_{q'}\rangle = \langle\eta_q^\dagger\eta_{-q'}\rangle = 0 \\ \langle\eta_{-q}\eta_{q'}^\dagger\rangle &= \langle\delta_{-q,q'} - \eta_q^\dagger\eta_{-q'}\rangle = \delta_{-q,q'} \end{aligned} \tag{32}$$

4 Correlation Functions

In the case where no field is applied:

$$C_{ij}^x = \langle 0|\sigma_i^x\sigma_j^x|0\rangle\,; \quad C_{ij}^y = \langle 0|\sigma_i^y\sigma_j^y|0\rangle\,; \quad C_{ij}^z = \langle 0|\sigma_i^z\sigma_j^z|0\rangle \tag{33}$$

which can be expressed in terms Majorana operators A_i and B_i (26).

$$C_{ij}^x = \langle \Pi_{i\le k<j} B_k A_{k+1}\rangle\,; \quad C_{ij}^y = \langle \Pi_{i\le k<j} B_{k+1} A_k\rangle\,; \quad C_{ij}^z = \langle B_i A_i B_j A_j\rangle \tag{34}$$

If a transverse field is present (say in z-direction), then it is defined as (with $m^z = \langle 0|\sigma_i^z|0\rangle$):

$$C_{ij}^z = \langle 0|\sigma_i^z\sigma_j^z|0\rangle - m^{z2} = \langle B_i A_i B_j A_j\rangle - \langle B_i A_i\rangle^2 \tag{35}$$

Steps: Correlation functions in terms of A and B:

The expression for C_{ij}^z is obtained by using (27) directly. Meanwhile for C_{ij}^x and C_{ij}^y we need:

$$\begin{aligned} \sigma_i^x\sigma_j^x &= (\sigma_i^+ + \sigma_i^-)(\sigma_j^+ + \sigma_j^-) \\ \text{Using (2)} &= (c_i^\dagger + c_i)\prod_{1\le k<i}\left(-\sigma_k^z\right)\prod_{1\le k<j}\left(-\sigma_k^z\right)(c_j^\dagger + c_j) \\ \text{Using (29, (30))} &= (c_i^\dagger + c_i)\prod_{i\le k<j}\left(-\sigma_k^z\right)(c_j^\dagger + c_j) = A_i\prod_{i\le k<j}(A_k B_k)\,A_j \boxed{= \prod_{i\le k<j} B_k A_{k+1}} \\ \sigma_i^y\sigma_j^y &= -(\sigma_i^+ - \sigma_i^-)(\sigma_j^+ - \sigma_j^-) \\ \text{Using (2, 29)} &= -B_i\prod_{i\le k<j}(A_k B_k)\,B_j = -B_i A_i B_i\prod_{i<k<j}(A_k B_k)\,B_j \\ \text{Using (28, 30)} &= -A_i\prod_{i<k<j}(-B_k A_k)\,B_j \boxed{= \prod_{i\le k<j} B_{k+1} A_k} \end{aligned}$$

4.1 Wick's Theorem

For two operators $\hat{A}$ and $\hat{B}$, their (Wick) contraction is defined as:

$$\hat{A}^{\bullet}\hat{B}^{\bullet} \equiv \hat{A}\hat{B} - :\hat{A}\hat{B}:$$

where $:\hat{O}:$ is the normal order (usually defined with creation operators left of annihilation operators).

Wick's theorem states that any string (of creation and annihilation operators) can be decomposed into a sum of products of contractions and normal ordered strings (online proof [3], Wick's paper [4]):

$$\hat{A}\hat{B}\hat{C}\hat{D}\hat{E}\hat{F}\ldots = :\hat{A}\hat{B}\hat{C}\hat{D}\hat{E}\hat{F}\ldots: + \sum_{\text{singles}} \operatorname{sgn}(\sigma):\hat{A}^{\bullet}\hat{B}^{\bullet}\hat{C}\hat{D}\hat{E}\hat{F}\ldots: + \sum_{\text{doubles}} \operatorname{sgn}(\sigma):\hat{A}^{\bullet}\hat{B}^{\bullet\bullet}\hat{C}^{\bullet\bullet}\hat{D}^{\bullet}\hat{E}\hat{F}\ldots: + \ldots$$

where $\operatorname{sgn}(\sigma)$ is the sign of permutation parity $= (-1)^{N(\sigma)}$ for fermionic strings (σ denotes a permutation). The expression for bosonic strings can be obtained by replacing sgn with 1.

Wick's Theorem for Correlation Functions The first simplification occur when considering Wick's theorem for VEVs: all terms involving normal orders vanish, leaving only full contractions:

$$\langle 0|ABCDEF\ldots|0\rangle = \sum_{\sigma} \operatorname{sgn}(\sigma) \prod_{\text{all pairs}} \text{contraction pair}$$

For strings described in A and B operators, full contraction terms are products of the following elementary contractions: $\langle A_iA_j\rangle$, $\langle B_iB_j\rangle$, $\langle A_iB_j\rangle$, and $\langle B_iA_j\rangle$. The former two are equal to δ_{ij} and $-\delta_{ij}$ (shown in box), respectively (neither $\langle A_iA_i\rangle$ nor $\langle B_iB_i\rangle$ occur in C^x, C^y, C^z). Therefore, full contractions can be written in terms of $\langle B_iA_j\rangle$ (as $\langle B_iA_j\rangle = -\langle A_jB_i\rangle$ using (28)). From (40):

$$\langle B_iA_j\rangle = \delta_{ij} - \frac{2}{N}\sum_q \left(u_qv_q\sin qr - u_q^2\cos qr\right) \tag{36}$$

Noting that the contraction only depends on qr where $r \equiv R_j - R_i$ (i.e. $B_iA_j = A_{i+1}B_{j+1}$), the correlation functions can be expressed as the following determinants, with defining $G_r \equiv \langle B_iA_{i+r}\rangle$:

$$C_r^x = \begin{vmatrix} G_1 & G_2 & \ldots & G_r \\ G_0 & G_1 & \ldots & G_{r-1} \\ \ldots & \ldots & \ldots & \ldots \\ G_{2-r} & G_2 & \ldots & G_1 \end{vmatrix} \qquad C_r^y = \begin{vmatrix} G_{-1} & G_0 & \ldots & G_{r-2} \\ G_{-2} & G_{-1} & \ldots & G_{r-1} \\ \ldots & \ldots & \ldots & \ldots \\ G_{-r} & G_{1-r} & \ldots & G_{-1} \end{vmatrix} \qquad C_r^z = \begin{vmatrix} G_0 & G_r \\ G_{-r} & G_0 \end{vmatrix} \tag{37}$$

For the transverse field (35): $C_r^z = G_0^2 - G_rG_{-r} - G_0^2 = -G_rG_{-r}$

VEV of Elementary Contractions

$$\begin{aligned} \langle A_iA_j\rangle &= \langle c_i^\dagger c_j^\dagger + c_ic_j\rangle + \langle c_i^\dagger c_j + c_ic_j^\dagger\rangle \\ \langle B_iB_j\rangle &= \langle c_i^\dagger c_j^\dagger + c_ic_j\rangle - \langle c_i^\dagger c_j + c_ic_j^\dagger\rangle \\ \langle B_iA_j\rangle &= \langle c_i^\dagger c_j^\dagger - c_ic_j\rangle + \langle c_i^\dagger c_j - c_ic_j^\dagger\rangle \end{aligned} \tag{38}$$

Using (31):

$$\begin{aligned} c_i^\dagger c_j^\dagger &= \frac{1}{N}\sum_{qq'} \exp(i(qR_i + q'R_j)) \left(u_q\eta_q^\dagger + iv_q\eta_{-q}\right)\left(u_{q'}\eta_{q'}^\dagger + iv_{q'}\eta_{-q'}\right) \\ c_ic_j &= \frac{1}{N}\sum_{qq'} \exp(-i(qR_i + q'R_j)) \left(u_q\eta_q - iv_q\eta_{-q}^\dagger\right)\left(u_{q'}\eta_{q'} - iv_{q'}\eta_{-q'}^\dagger\right) \\ c_i^\dagger c_j &= \frac{1}{N}\sum_{qq'} \exp(i(qR_i - q'R_j)) \left(u_q\eta_q^\dagger + iv_q\eta_{-q}\right)\left(u_{q'}\eta_{q'} - iv_{q'}\eta_{-q'}^\dagger\right) \\ c_ic_j^\dagger &= \frac{1}{N}\sum_{qq'} \exp(-i(qR_i - q'R_j)) \left(u_q\eta_q - iv_q\eta_{-q}^\dagger\right)\left(u_{q'}\eta_{q'}^\dagger + iv_{q'}\eta_{-q'}\right) \end{aligned} \tag{39}$$

For the VEV using (32) in (39) with $r \equiv R_j - R_i$:

$$\langle c_i^\dagger c_j^\dagger \rangle = \frac{1}{N}\sum_q e^{-iqr}\, iu_q v_q \qquad \langle c_i c_j \rangle = \frac{1}{N}\sum_q e^{iqr}\, iu_q v_q$$
$$\langle c_i^\dagger c_j \rangle = \frac{1}{N}\sum_q e^{-iqr}\, v_q^2 \qquad \langle c_i c_j^\dagger \rangle = \frac{1}{N}\sum_q e^{iqr}\, u_q^2$$

Note that $c_i\,|0\rangle \neq 0$ because we are working in momentum basis! ($\eta_q\,|0\rangle = 0$). Now, exploiting the symmetries of $u_q = u_{-q}$, $v_{-q} = -v_q$:

$$\langle c_i^\dagger c_j^\dagger \rangle = \frac{1}{N}\sum_q u_q v_q \sin qr \qquad \langle c_i c_j \rangle = \frac{-1}{N}\sum_q u_q v_q \sin qr = -\langle c_i^\dagger c_j^\dagger \rangle$$
$$\langle c_i c_j^\dagger \rangle = \frac{1}{N}\sum_q u_q^2 \cos qr \qquad \langle c_i^\dagger c_j \rangle = \frac{1}{N}\sum_q v_q^2 \cos qr = \delta_{ij} - \langle c_i c_j^\dagger \rangle$$

where $\det U = u_q^2 + v_q^2 = 1$; $\Sigma_q \cos qr = N\delta_{ij}$ has been used.

$$\langle A_i A_j \rangle = \langle c_i^\dagger c_j + c_i c_j^\dagger \rangle = -\langle B_i B_j \rangle = \delta_{ij} \qquad \langle B_i A_j \rangle = \delta_{ij} + 2(\langle c_i^\dagger c_j^\dagger \rangle - \langle c_i c_j^\dagger \rangle) \tag{40}$$

Now considering the continuum limit:

$$G_r = \delta_{0,r} - 2\int_{-\pi}^{\pi} \frac{dq}{2\pi}\left(u_q v_q \sin qr - u_q^2 \cos qr\right)$$

where $uv = 1/2(\beta/\omega)$ and $u^2 = 1/2(\alpha/\omega + 1)$, from (15), with $\int_{-\pi}^{\pi} \frac{dq}{2\pi} \cos qr = \delta_{0,2}$:

$$G_r = \int_{-\pi}^{\pi} \frac{dq}{2\pi}\left(\frac{\alpha_q}{\omega_q}\cos qr - \frac{\beta_q}{\omega_q}\sin qr\right) \tag{41}$$

4.2 Transverse Ising Chain

$$\omega_q = \sqrt{1 + 2\bar\lambda\cos q + \bar\lambda^2} \quad \alpha_q = 1 + \bar\lambda\cos q \quad \beta_q = \bar\lambda \sin q$$

Using the trigonometric identity $\cos q \cos qr - \sin q \sin qr = \cos[q(1+r)]$:

$$G_r = \frac{1}{\pi}\int_0^{\pi} \frac{\cos qr \ + \ \bar\lambda\cos[q(r+1)]}{\sqrt{1+\bar\lambda^2 + 2\bar\lambda\cos q}}\, dq = I_r + \bar\lambda I_{r+1}; \qquad I_r = \frac{1}{\pi}\int_0^{\pi}\frac{\cos qr}{\omega_q}\, dq$$

At the limiting cases:

$$G_r(\bar\lambda = 0) = \frac{1}{\pi}\int_0^{\pi} \cos qr\, dq = \delta_{0,r}$$
$$G_r(\bar\lambda \to \infty) = \frac{1}{\pi}\int_0^{\pi} \cos q(r+1)\, dq = \delta_{-1,r}$$

At the critical value:

$$I_r = \frac{\sqrt{2}}{2\pi}\int_0^{\pi} \frac{\cos qr}{\sqrt{1+\cos q}}\, dq = -\int_{-1}^{1} \frac{T_n(x)}{\sqrt{1+x}}\, dx$$

4.3 XY Model

$$\omega_q = \sqrt{1-(1-\gamma^2)\sin^2 q} \quad \alpha_q = \cos q \quad \beta_q = \gamma \sin q$$

$$G_r = \frac{1}{\pi}\int_0^{\pi} \frac{(1-\gamma)\cos[q(r+1)] + (1+\gamma)\cos[q(r-1)]}{\sqrt{1-(1-\gamma^2)\sin^2 q}}\,dq = \begin{cases} (1-\gamma)I_{r+1} + (1+\gamma)I_{r-1}, & r \text{ odd} \\ 0, & r \text{ even} \end{cases}$$

with $I_r = \frac{2}{\pi}\int_0^{\pi/2} \cos(qr)/\omega_q \; dq$. For the limiting cases:

$$G_r(\gamma = \pm 1) = \frac{1}{r \pm 1} \qquad \left(I_r(\gamma = \pm 1) = \frac{2}{\pi}\int_0^{\pi/2} \cos qr \, dq\right)$$

An exact solution can be obtained for both models if the following definite integral is known:

$$\int_0^{\pi/2} \frac{\cos n\theta \, d\theta}{\sqrt{1-k^2\sin^2\theta}}$$

It is similar to a complete elliptic integral of the first kind.

References

[1] P. Pfeuty, “The one-dimensional ising model with a transverse field,” *ANNALS of Physics*, vol. 57, no. 1, pp. 79–90, 1970.

[2] B. K. Chakrabarti, A. Dutta, and P. Sen, *Quantum Ising phases and transitions in transverse Ising models*, vol. 41. Springer Science & Business Media, 2008.

[3] Wikipedia contributors, “Wick’s theorem — Wikipedia, the free encyclopedia.” `https://en.wikipedia.org/w/index.php?title=Wick%27s_theorem&oldid=1114331217`, 2022. [Online; accessed 22-October-2022].

[4] G.-C. Wick, “The evaluation of the collision matrix,” *Physical review*, vol. 80, no. 2, p. 268, 1950.