1 Quadratic Hamiltonians

1.1 Bosonic Models

The general noninteracting bosonic Hamiltonian is written

$$\hat{H} = \tfrac{1}{2}\Psi^\dagger_r\,\mathcal{H}_{rs}\Psi_s \quad , \tag{1}$$

where Ψ is a rank-$2N$ column vector whose Hermitian conjugate is the row vector

$$\Psi^\dagger = \Big(\psi^\dagger_1\,,\,\cdots\,,\,\psi^\dagger_N\,,\,\psi_1\,,\,\cdots\,,\,\psi_N\Big) \quad . \tag{2}$$

Since $\big[\psi_i\,,\,\psi^\dagger_j\big] = \delta_{ij}$, we have

$$\big[\Psi_r\,,\,\Psi^\dagger_s\big] = \varSigma_{rs} \quad , \quad \varSigma = \begin{pmatrix} \mathbb{I}_{N\times N} & 0 \\ 0 & -\mathbb{I}_{N\times N}\end{pmatrix} \quad , \tag{3}$$

with $\mathbb{I}$ the identity matrix. Note that the indices r and s run from 1 to $2N$, while i and j run from 1 to N. The matrix $\mathcal{H}$ is of the form

$$\mathcal{H} = \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \tag{4}$$

where $A = A^\dagger$ is Hermitian and $B = B^{\mathsf{t}}$ is symmetric.

The Hamiltonian is brought to diagonal form by a canonical transformation:

$$\begin{pmatrix} \psi \\ \psi^\dagger \end{pmatrix} = \overbrace{\begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}}^{\mathcal{S}} \begin{pmatrix} \phi \\ \phi^\dagger \end{pmatrix} \quad , \tag{5}$$

which is to say $\Psi = \mathcal{S}\,\Phi$, or in component form

$$\begin{aligned} \psi_i &= U_{ia}\,\phi_a + V^*_{ia}\,\phi^\dagger_a \\ \psi^\dagger_i &= V_{ia}\,\phi_a + U^*_{ia}\,\phi^\dagger_a \quad , \end{aligned} \tag{6}$$

where a, like i, runs from 1 to N. In order that the transformation be canonical, we must preserve the commutation relations, meaning $\big[\phi_a\,,\,\phi^\dagger_b\big] = \delta_{ab}$, *i.e.*

$$\big[\Phi_r\,,\,\Phi^\dagger_s\big] = \varSigma_{rs} \quad . \tag{7}$$

This then requires

$$\mathcal{S}\,\varSigma\,\mathcal{S}^\dagger = \mathcal{S}^\dagger\,\varSigma\,\mathcal{S} = \varSigma \quad , \tag{8}$$

which entails

$$U^\dagger U - V^\dagger V = \mathbb{I} \qquad\qquad U^{\mathsf{t}} V - V^{\mathsf{t}} U = 0 \tag{9}$$

$$U U^\dagger - V^* V^{\mathsf{t}} = \mathbb{I} \qquad\qquad U^* V^{\mathsf{t}} - V U^\dagger = 0 \quad . \tag{10}$$

Note that $\varSigma^2 = \mathcal{I}$, where $\mathcal{I} = \begin{pmatrix} \mathbb{I} & 0 \\ 0 & \mathbb{I} \end{pmatrix}$, hence

$$\mathcal{S}^{-1} = \varSigma\, \mathcal{S}^\dagger \varSigma = \begin{pmatrix} U^\dagger & -V^\dagger \\ -V^{\mathrm{t}} & U^{\mathrm{t}} \end{pmatrix} \quad . \tag{11}$$

Thus, the inverse relation between the Ψ and Φ operators is $\Phi = \mathcal{S}^{-1}\Psi = \varSigma\, \mathcal{S}^\dagger \varSigma\, \Psi$, or

$$\begin{aligned} \phi_a &= U^*_{ia}\, \psi_i - V^*_{ia}\, \psi^\dagger_i \\ \phi^\dagger_a &= -V_{ia}\, \psi_i + U_{ia}\, \psi^\dagger_i \quad , \end{aligned} \tag{12}$$

1.1.1 Bogoliubov equations

We are now in the position to demand

$$\mathcal{S}^\dagger \mathcal{H} \mathcal{S} = \mathcal{E} = \begin{pmatrix} E & 0 \\ 0 & E \end{pmatrix} \quad , \tag{13}$$

where E is a diagonal $N \times N$ matrix. Thus,

$$\mathcal{H}\, \mathcal{S} = \mathcal{S}^{\dagger -1} \mathcal{E} = \varSigma\, \mathcal{S}\, \varSigma\, \mathcal{E} \quad , \tag{14}$$

which is to say

$$\begin{pmatrix} A & B \\ B^* & A \end{pmatrix} \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} = \begin{pmatrix} U & -V^* \\ -V & U^* \end{pmatrix} \begin{pmatrix} E & 0 \\ 0 & E \end{pmatrix} \quad . \tag{15}$$

If the bosonic system is stable, each of the eigenvalues E_a is nonnegative. In component form, this yields the Bogoliubov equations,

$$\begin{aligned} A_{ij}\, U_{ja} + B_{ij}\, V_{ja} &= +U_{ia}\, E_a \\ B^*_{ij}\, U_{ja} + A^*_{ij}\, V_{ja} &= -V_{ia}\, E_a \quad , \end{aligned} \tag{16}$$

with no implied sum on a on either RHS. The Hamiltonian is then

$$\hat{H} = \sum_a E_a \left(\phi^\dagger_a \phi_a + \tfrac{1}{2} \right) \quad . \tag{17}$$

At temperature T, we have

$$\left\langle \phi^\dagger_a\, \phi_b \right\rangle = n(E_a)\, \delta_{ab} \quad , \tag{18}$$

where

$$n(E) = \frac{1}{\exp(E/k_{\mathrm{B}} T) - 1} \tag{19}$$

is the Bose distribution. The anomalous correlators all vanish, *e.g.* $\langle\phi_a\phi_b\rangle = 0$. The finite temperature two-point correlation functions are then

$$\langle\psi_i^\dagger\psi_j\rangle = \sum_a \Big\{ n_a\, U_{ia}^*\, U_{ja} + (1+n_a)\, V_{ia}\, V_{ja}^* \Big\} \tag{20}$$

$$\langle\psi_i\psi_j\rangle = \sum_a \Big\{ n_a\, V_{ia}^*\, U_{ja} + (1+n_a)\, U_{ia}\, V_{ja}^* \Big\} \quad , \tag{21}$$

where $n_a \equiv n(E_a)$.

1.1.2 Ground state

We have found

$$\Phi = \mathcal{S}^{-1}\Psi = \Sigma\, \mathcal{S}^\dagger\, \Sigma\, \Psi \quad , \tag{22}$$

hence

$$\begin{aligned} \phi_a &= U_{ai}^\dagger\, \psi_i - V_{ai}^\dagger\, \psi_i^\dagger \\ &= \psi_i\, U_{ia}^* - \psi_i^\dagger\, V_{ia}^* \quad . \end{aligned} \tag{23}$$

We assume the following Bogoliubov form for the ground state of $\hat{H}$:

$$|\,\mathrm{G}\,\rangle = C\, \exp\Big(\tfrac{1}{2} Q_{ij}\, \psi_i^\dagger\psi_j^\dagger\Big)\,|\,0\,\rangle \quad , \tag{24}$$

where C is a normalization constant, Q is a symmetric matrix, and $|\,0\,\rangle$ is the vacuum for the ψ bosons: $\psi_i|\,0\,\rangle = 0$. We now demand that $|\,\mathrm{G}\,\rangle$ be the vacuum for the ϕ bosons: $\phi_a|\,\mathrm{G}\,\rangle \equiv 0$. This means

$$\phi_a\, e^{\hat{Q}}\,|\,0\,\rangle = e^{\hat{Q}} \Big(e^{-\hat{Q}}\, \phi_a\, e^{\hat{Q}} \Big)\,|\,0\,\rangle \quad , \tag{25}$$

where

$$\hat{Q} \equiv \tfrac{1}{2} Q_{ij}\, \psi_i^\dagger\psi_j^\dagger \quad . \tag{26}$$

We now define

$$\psi_i(x) \equiv e^{-x\hat{Q}}\, \psi_i\, e^{x\hat{Q}} \tag{27}$$

and we find

$$\frac{d\psi_i(x)}{dx} = e^{-x\hat{Q}} \big[\psi_i\,,\,\hat{Q}\big] e^{x\hat{Q}} = Q_{ij}\, \psi_j^\dagger \quad , \tag{28}$$

and integrating[1] we obtain

$$\psi_i(x) \equiv e^{-x\hat{Q}}\, \psi_i\, e^{x\hat{Q}} = \psi_i(x) + x\, Q_{ij}\, \psi_j^\dagger \quad . \tag{29}$$

We may now write

$$e^{-\hat{Q}}\, \phi_a\, e^{\hat{Q}} = U_{ai}^\dagger\, \psi_i + \big(U_{ai}^\dagger\, Q_{ij} - V_{aj}^\dagger\big)\, \psi_j^\dagger \quad , \tag{30}$$

[1] Note that $e^{-x\hat{Q}}\, \psi_i^\dagger\, e^{x\hat{Q}} = \psi_i^\dagger$ since $\big[\psi_i^\dagger, \hat{Q}\big] = 0$.

and we demand that the coefficient of $\psi_j^\dagger$ vanish for all a, which yields

$$Q = \big(U^\dagger\big)^{-1} V^\dagger \quad , \tag{31}$$

or, equivalently, $Q^\dagger = VU^{-1}$. Note that $Q^{\rm t} = V^*(U^*)^{-1} = Q$ since $U^\dagger V^* = V^\dagger U^*$.

1.1.3 A final note on the boson problem

Note that $\mathcal{S}^\dagger \mathcal{H} \mathcal{S}$ has the same eigenvalues as $\mathcal{H}$ only if $\mathcal{S}^\dagger = \mathcal{S}^{-1}$, *i.e.* only if $\mathcal{S}$ is Hermitian. We have $\mathcal{S}^\dagger = \varSigma \mathcal{S}^{-1} \varSigma$ and therefore

$$\mathcal{S}^\dagger \mathcal{H}\, \mathcal{S} = \varSigma\, \mathcal{S}^{-1}\, \varSigma\, \mathcal{H}\, \mathcal{S} \quad . \tag{32}$$

Now

$$\varSigma\, \mathcal{H} = \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \quad . \tag{33}$$

Consider the characteristic polynomial $P(E) = \mathsf{det}(E - \varSigma \mathcal{H})$. Since $\mathsf{det}(M) = \mathsf{det}(M^{\rm t})$ for any matrix M, we consider

$$(\varSigma\, \mathcal{H})^{\rm t} = \begin{pmatrix} A^{\rm t} & -B^\dagger \\ B^{\rm t} & -A^\dagger \end{pmatrix} = \begin{pmatrix} A^* & -B^* \\ B & -A \end{pmatrix} = -\mathcal{J}^{-1} (\varSigma\, \mathcal{H})\, \mathcal{J} \quad , \tag{34}$$

where

$$\mathcal{J} = \begin{pmatrix} 0 & \mathbb{I} \\ -\mathbb{I} & 0 \end{pmatrix} \tag{35}$$

and $\mathcal{J}^{-1} = -\mathcal{J}$, *i.e.* $\mathcal{J}^2 = -\mathcal{I}$. But then we have

$$P(E) = \mathsf{det}(E - \varSigma\, \mathcal{H}) = \mathsf{det}(E + \mathcal{J}^{-1}\, \varSigma\, \mathcal{H}\, \mathcal{J}) = \mathsf{det}(E + \varSigma\, \mathcal{H}) = P(-E) \quad . \tag{36}$$

We conclude that the eigenvalues of $\varSigma\, \mathcal{H}$ come in $(+E, -E)$ pairs. To obtain the eigenenergies for the bosonic Hamiltonian $\hat{H}$, however, as per eqn. 32, we must multiply $\mathcal{S}^{-1} \varSigma\, \mathcal{H}\, \mathcal{S}$ on the left by Σ, which reverses the sign of the negative eigenvalues, resulting in a nonnegative definite spectrum of bosonic eigenoperators (for stable bosonic systems).

1.2 Fermionic Models

The general noninteracting fermionic Hamiltonian is written

$$\hat{H} = \tfrac{1}{2} \Psi_r^\dagger\, \mathcal{H}_{rs} \Psi_s \quad , \tag{37}$$

where once again Ψ is a rank-$2N$ column vector whose Hermitian conjugate is the row vector

$$\Psi^\dagger = \Big(\psi_1^\dagger \,, \, \cdots \,, \, \psi_N^\dagger \,, \, \psi_1 \,, \, \cdots \,, \, \psi_N \Big) \quad . \tag{38}$$

In contrast to the bosonic case, we now have $\{\, \psi_i \, , \, \psi_j^\dagger \,\} = \delta_{ij}$ with the anticommutator, hence

$$\big\{ \Psi_r \, , \, \Psi_s^\dagger \big\} = \delta_{rs} \quad . \tag{39}$$

The matrix $\mathcal{H}$ is of the form

$$\mathcal{H} = \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \quad , \tag{40}$$

where $A = A^\dagger$ is Hermitian and $B = -B^{\mathsf{t}}$ is antisymmetric. Since this is of the same form as eqn. 33, we conclude that the eigenvalues of $\mathcal{H}$ come in $(+E, -E)$ pairs[2].

As with the bosonic case, the Hamiltonian is brought to diagonal form by a canonical transformation:

$$\begin{pmatrix} \psi \\ \psi^\dagger \end{pmatrix} = \overbrace{\begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}}^{\mathcal{S}} \begin{pmatrix} \phi \\ \phi^\dagger \end{pmatrix} \quad , \tag{41}$$

which is to say $\Psi = \mathcal{S}\, \Phi$, or in component form

$$\begin{aligned} \psi_i &= U_{ia}\, \phi_a + V_{ia}^*\, \phi_a^\dagger \\ \psi_i^\dagger &= V_{ia}\, \phi_a + U_{ia}^*\, \phi_a^\dagger \quad . \end{aligned} \tag{42}$$

In order that the transformation be canonical, we must preserve the anticommutation relations, *i.e.* $\big\{ \phi_a \, , \, \phi_b^\dagger \big\} = \delta_{ab}$, meaning

$$\big\{ \Phi_r \, , \, \Phi_s^\dagger \big\} = \delta_{rs} \quad , \tag{43}$$

which requires that $\mathcal{S}$ is unitary:

$$\mathcal{S}^\dagger \mathcal{S} = \mathcal{S}\mathcal{S}^\dagger = \mathcal{I} \quad , \tag{44}$$

where $\mathcal{I}$ is again the identity matrix of rank $2N$. Thus,

$$U^\dagger U + V^\dagger V = \mathbb{I} \qquad\qquad U^{\mathsf{t}} V + V^{\mathsf{t}} U = 0 \tag{45}$$

$$U U^\dagger + V^* V^{\mathsf{t}} = \mathbb{I} \qquad\qquad U^* V^{\mathsf{t}} + V U^\dagger = 0 \quad . \tag{46}$$

The inverse relation between the operators follows from $\Phi = \mathcal{S}^{-1}\Psi = \mathcal{S}^\dagger \Psi$:

$$\begin{aligned} \phi_a &= U_{ia}^*\, \psi_i + V_{ia}^*\, \psi_i^\dagger \\ \phi_a^\dagger &= V_{ia}\, \psi_i + U_{ia}\, \psi_i^\dagger \quad , \end{aligned} \tag{47}$$

The transformed Hamiltonian matrix is

$$\mathcal{S}^\dagger \mathcal{H}\, \mathcal{S} = \mathcal{E} \equiv \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix} \quad . \tag{48}$$

[2] This is true even though B in eqn. 33 is symmetric rather than antisymmetric. In proving the evenness of the characteristic polynomial $P(E) = P(-E)$, we did not appeal to the symmetry or antisymmetry of B.

Without loss of generality, we may take E to be a diagonal matrix with nonnegative entries. In component notation, the eigenvalue equations are

$$\begin{aligned} A_{ij}\,U_{ja} + B_{ij}\,V_{ja} &= U_{ia}\,E_a \\ -B^*_{ij}\,U_{ja} - A^*_{ij}\,V_{ja} &= V_{ia}\,E_a \quad . \end{aligned} \tag{49}$$

The Hamiltonian then takes the form

$$\hat{H} = \sum_a E_a\left(\phi^\dagger_a\phi_a - \tfrac{1}{2}\right) \quad . \tag{50}$$

At temperature T, we have

$$\left\langle \phi^\dagger_a\phi_b\right\rangle = f(E_a)\,\delta_{ab} \quad , \tag{51}$$

where

$$f(E) = \frac{1}{\exp(E/k_{\rm B}T)+1} \tag{52}$$

is the Fermi distribution. As for bosons, the anomalous correlators all vanish: $\langle\phi_a\phi_b\rangle = 0$. The finite temperature two-point correlation functions are then

$$\begin{aligned} \langle\psi^\dagger_i\psi_j\rangle &= \sum_a \Big\{ f_a\,U^*_{ia}\,U_{ja} + (1-f_a)\,V_{ia}\,V^*_{ja}\Big\} \\ \langle\psi_i\psi_j\rangle &= \sum_a \Big\{ f_a\,V^*_{ia}\,U_{ja} + (1-f_a)\,U_{ia}\,V^*_{ja}\Big\} \quad , \end{aligned} \tag{53}$$

where $f_a = f(E_a)$.

1.2.1 Ground state

We write

$$|\,\mathrm{G}\,\rangle = C\exp\left(\tfrac{1}{2}Q_{ij}\,\psi^\dagger_i\psi^\dagger_j\right)|\,0\,\rangle \quad , \tag{54}$$

with $Q = -Q^{\rm t}$, and we demand, as in the bosonic case, that $\phi_a\,|\,\mathrm{G}\,\rangle \equiv 0$. Again we define $\hat{Q} = \frac{1}{2}Q_{ij}\,\psi^\dagger_i\psi^\dagger_j$, and

$$\psi_i(x) = e^{-x\hat{Q}}\,\psi_i\,e^{x\hat{Q}} \quad . \tag{55}$$

We then have

$$\frac{d\psi_i(x)}{dx} = e^{-x\hat{Q}}\left[\psi_i,\hat{Q}\right]e^{x\hat{Q}} = Q_{ij}\,\psi^\dagger_j \quad \Rightarrow \quad \psi_i(x) = \psi_i + x\,Q_{ij}\,\psi^\dagger_j \quad . \tag{56}$$

Thus,

$$e^{-\hat{Q}}\,\phi_a\,e^{\hat{Q}} = U^\dagger_{ai}\,\psi_i + \left(V^\dagger_{aj} + U^\dagger_{ai}\,Q_{ij}\right)\psi^\dagger_j \quad , \tag{57}$$

from which we obtain

$$Q = -\left(U^\dagger\right)^{-1}V^\dagger \quad . \tag{58}$$

Since $U^\dagger V^* + V^\dagger U^* = 0$, we recover $Q = -Q^{\rm t}$.

1.3 Majorana Fermion Models

Majorana fermions satisfy the anticommutation relations $\{\theta_i\,,\,\theta_j\} = 2\delta_{ij}$. Thus, $(\theta_i)^2 = 1$ for every i. We also have $\theta_i^\dagger = \theta_i$ and for this reason they are sometimes called 'real' fermions. If c is the annihilator for a Dirac particle, with $\{c\,,\,c^\dagger\} = 1$, we may define Majorana fermions η and $\widetilde{\eta}$ as follows:

$$\eta = c + c^\dagger \qquad\qquad c = \tfrac{1}{2}(\eta - i\eta') \tag{59}$$

$$\widetilde{\eta} = i(c - c^\dagger) \qquad\qquad c^\dagger = \tfrac{1}{2}(\eta + i\widetilde{\eta}) \quad . \tag{60}$$

The most general noninteracting Majorana Hamiltonian is of the form

$$\hat{H} = \tfrac{i}{4} M_{ij}\,\theta_i\,\theta_j \quad , \tag{61}$$

where $M = -M^{\rm t} = M^*$ is a real antisymmetric matrix of even dimension $2N$. This is brought to canonical form by a real orthogonal transformation,

$$\theta_i = \mathcal{R}_{ia}\,\xi_a \quad , \tag{62}$$

where $\mathcal{R}^{\rm t}\mathcal{R} = \mathcal{I}$, and where $\{\xi_a\,,\,\xi_b\} = 2\delta_{ab}$. We have

$$\mathcal{R}^{\rm t}\mathcal{M}\mathcal{R} = E \otimes i\sigma^y = \begin{pmatrix} 0 & -E_1 & 0 & 0 & \cdots \\ E_1 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & -E_2 & \cdots \\ 0 & 0 & E_2 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad . \tag{63}$$

Thus,

$$\hat{H} = -\tfrac{i}{2}\sum_{a=1}^{N} E_a\,\xi_{2a-1}\,\xi_{2a} = \sum_a E_a\big(c_a^\dagger c_a - \tfrac{1}{2}\big) \quad , \tag{64}$$

where

$$c_a \equiv \tfrac{1}{2}\big(\xi_{2a-1} - i\,\xi_{2a}\big) \quad , \quad c_a^\dagger \equiv \tfrac{1}{2}\big(\xi_{2a-1} + i\,\xi_{2a}\big) \quad . \tag{65}$$

1.4 Majorana chain

Consider the Hamiltonian

$$\hat{H} = -i\sum_{n=1}^{N} \sigma_n\,\alpha_n\,\alpha_{n+1} \tag{66}$$

where $\sigma_n = \pm 1$ is a $\mathbb{Z}_2$ gauge field and $\{\alpha_m, \alpha_n\} = 2\,\delta_{mn}$ is the Majorana fermion anticommutator. Periodic boundary conditions are assumed, *i.e.* $\alpha_{N+1} = \alpha_1$. We now make a gauge transformation to a new set of Majorana fermions,

$$\theta_1 \equiv \alpha_1 \quad , \quad \theta_2 \equiv \sigma_1\alpha_2 \quad , \quad \theta_3 \equiv \sigma_1\sigma_2\,\alpha_3 \quad , \quad \ldots \quad , \quad \theta_N \equiv \sigma_1\sigma_2\cdots\sigma_{N-1}\,\alpha_N \quad . \tag{67}$$

The Hamiltonian may now be written as

$$\hat{H} = -i \sum_{n=1}^{N} \theta_n \, \theta_{n+1} \quad , \tag{68}$$

where $\theta_{N+1} = \sigma \, \theta_1$, with $\sigma = \prod_{j=1}^{N} \sigma_j$. So the boundary conditions on the θ Majoranas are either periodic ($\sigma = +1$) or antiperiodic ($\sigma = -1$). We now switch to crystal momentum space, defining

$$\hat{\theta}_k = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{-ikn} \, \theta_n \qquad , \qquad \theta_n = \frac{1}{\sqrt{N}} \sum_k e^{ikn} \, \hat{\theta}_k \quad . \tag{69}$$

The k-values are quantized according to $e^{ikN} = \sigma$. The anticommutators are

$$\big\{ \theta_m \, , \, \theta_n \big\} = 2 \, \delta_{m-n \, , \, 0 \bmod N} \qquad , \qquad \big\{ \hat{\theta}_k \, , \, \hat{\theta}_p \big\} = 2 \, \delta_{k+p \, , \, 0 \bmod 2\pi} \quad . \tag{70}$$

There are four cases to consider:

<u>Case I</u> : $\sigma = +1$, N even. We have $e^{ikN} = +1$, and the N allowed k values are

$$k \in \pm \frac{2\pi}{N} \times \Big\{ 1 \, , \, \ldots \, , \, \tfrac{1}{2} N - 1 \Big\} \quad , \quad k = 0 \quad , \quad k = \pi \quad . \tag{71}$$

Note that the allowed crystal momenta all occur in $\{+k, -k\}$ pairs, with the exception of $k = 0$ and $k = \pi$, which are unpaired.

<u>Case II</u> : $\sigma = +1$, N odd. We have $e^{ikN} = +1$, and the N allowed k values are

$$k \in \pm \frac{2\pi}{N} \times \Big\{ 1 \, , \, \ldots \, , \, \tfrac{1}{2} (N-1) \Big\} \quad , \quad k = 0 \quad . \tag{72}$$

Only $k = 0$ is unpaired.

<u>Case III</u> : $\sigma = 1$, N even. We have $e^{ikN} = -1$, and the N allowed k values are

$$k \in \pm \frac{2\pi}{N} \times \Big\{ \tfrac{1}{2} \, , \, \ldots \, , \, \tfrac{1}{2} (N-1) \Big\} \quad . \tag{73}$$

All the crystal momenta are paired.

<u>Case IV</u> : $\sigma = 1$, N odd. We have $e^{ikN} = -1$, and the N allowed k values are

$$k \in \pm \frac{2\pi}{N} \times \Big\{ \tfrac{1}{2} \, , \, \ldots \, , \, \tfrac{1}{2} N - 1 \Big\} \quad , \quad k = \pi \quad . \tag{74}$$

Only $k = \pi$ is unpaired.

We may now write

$$\begin{aligned}\hat{H} &= -i\sum_k e^{-ik}\,\hat{\theta}_k\,\hat{\theta}_{-k} \\ &= -i\sum_{k\in(0,\pi)} \Big(e^{ik}\,\hat{\theta}_{-k}\,\hat{\theta}_k + e^{-ik}\,\hat{\theta}_k\,\hat{\theta}_{-k}\Big) - i\sum_{k\in\mathrm{U}} e^{-ik}\,\hat{\theta}_k^2 \\ &= \sum_{k\in(0,\pi)} 2\sin k\,\hat{\theta}_{-k}\,\hat{\theta}_k - 2i\sum_{k\in(0,\pi)} e^{-ik} - i\sum_{k\in\mathrm{U}} e^{-ik} \quad .\end{aligned} \tag{75}$$

where U denotes the set of unpaired (or self-paired) crystal momenta, *i.e.* the set of k for which $e^{ik} = e^{-ik}$. Note that $\big\{\hat{\theta}_{-k}\,,\,\hat{\theta}_{k'}\big\} = 2\,\delta_{k,k'}$ and $\hat{\theta}_{-k} = \hat{\theta}_k^\dagger$, so we may define $\hat{\theta}_{-k} \equiv \sqrt{2}\,c_k^\dagger$ and $\hat{\theta}_k \equiv \sqrt{2}\,c_k$, where c_k is a complex fermion. Thus, we have

$$\hat{H} = \sum_{k\in(0,\pi)} 4\sin k\, c_k^\dagger\, c_k + E_0 \quad , \tag{76}$$

where

$$E_0 = -2i\sum_{k\in(0,\pi)} e^{-ik} - i\sum_{k\in\mathrm{U}} e^{-ik} \quad . \tag{77}$$

We now proceed to evaluate E_0 for our four cases.

<u>Case I</u> : Since $\mathrm{U} = \{0,\pi\}$, we have $\sum_{k\in\mathrm{U}} e^{-ik} = 0$. For $k\in(0,\pi)$ we may write $k = 2\pi\ell/N$ with $\ell\in\big\{1\,,\,\ldots\,,\,\frac{1}{2}N-1\big\}$. We then have

$$E_0^{(\mathrm{I})} = -2i\sum_{\ell=1}^{\frac{N}{2}-1} e^{-2\pi i\ell/N} = -2\,\mathrm{ctn}\Big(\frac{\pi}{N}\Big) \quad . \tag{78}$$

Note that we have used the identity

$$\sum_{\ell=1}^{J-1} x^\ell = \frac{x-x^J}{1-x} \quad . \tag{79}$$

<u>Case II</u> : We have $\mathrm{U} = \{0\}$. For the main set $k\in(0,\pi)$ we may write $k = 2\pi\ell/N$ with $\ell\in\big\{1\,,\,\ldots\,,\,\frac{1}{2}(N-1)\big\}$. We then have

$$E_0^{(\mathrm{II})} = -2i\sum_{\ell=1}^{\frac{N+1}{2}-1} e^{-2\pi i\ell/N} - i = -2i\left(\frac{e^{-2\pi i/N}+e^{-i\pi/N}}{1-e^{-2\pi i/N}}\right) - i = -\,\mathrm{ctn}\left(\frac{\pi}{2N}\right) \quad . \tag{80}$$

<u>Case III</u> : We have $\mathrm{U} = \{\emptyset\}$. For $k\in(0,\pi)$ we may write $k = 2\pi\ell/N + \pi/N$ with $\ell\in\big\{0\,,\,\ldots\,,\,\frac{1}{2}N-1\big\}$. Then

$$E_0^{(\mathrm{III})} = -2i\,e^{-i\pi/N}\sum_{\ell=0}^{\frac{N}{2}-1} e^{-2\pi\ell/N} = -2\csc\left(\frac{\pi}{N}\right) \quad . \tag{81}$$

<u>Case IV</u> : We have U $=\{\pi\}$. For $k\in(0,\pi)$ we may write $k=2\pi\ell/N-\pi/N$ with $\ell\in\big\{1\,,\,\ldots\,,\,\frac{1}{2}(N-1)\big\}$. Thus,

$$E_0^{(\mathrm{IV})}=-2i\,e^{i\pi/N}\sum_{\ell=1}^{\frac{N+1}{2}-1}e^{-2\pi i\ell/N}+i=-2i\bigg(\frac{e^{-i\pi/N}+1}{1-e^{-2\pi i/N}}\bigg)+i=-\operatorname{ctn}\Big(\frac{\pi}{2N}\Big)\quad. \tag{82}$$

Note that in the $N\to\infty$ limit, in all four cases we have $E_0=2N/\pi+\mathcal{O}(1)$.

2 Jordan-Wigner Transformation

The Jordan-Wigner transformation is an equivalence, in one-dimensional lattice systems, between the $S=\frac{1}{2}$ $\mathsf{SU}(2)$ algebra and the algebra of spinless fermions. Explicitly, we have

$$\begin{aligned} S^+_n&=\exp\Bigg(i\pi\sum_{j=1}^{n-1}c^\dagger_j c_j\Bigg)\,c^\dagger_n\\ S^-_n&=\exp\Bigg(i\pi\sum_{j=1}^{n-1}c^\dagger_j c_j\Bigg)\,c_n\\ S^z_n&=c^\dagger_n c_n-\tfrac{1}{2}\quad. \end{aligned} \tag{83}$$

The inverse is then

$$\begin{aligned} c^\dagger_n&=\exp\Bigg(i\pi\sum_{j=1}^{n-1}\big(S^z_j+\tfrac{1}{2}\big)\Bigg)\,S^+_n\\ c_n&=\exp\Bigg(i\pi\sum_{j=1}^{n-1}\big(S^z_j+\tfrac{1}{2}\big)\Bigg)\,S^-_n\quad. \end{aligned} \tag{84}$$

Note that $e^{i\pi c^\dagger c}$ has eigenvalues ±1, and that

$$c\,e^{i\pi c^\dagger c}=-c\quad,\quad c^\dagger e^{i\pi c^\dagger c}=c^\dagger\quad. \tag{85}$$

Taking the Hermitian conjugate,

$$e^{i\pi c^\dagger c}\,c^\dagger=-c^\dagger\quad,\quad e^{i\pi c^\dagger c}\,c=c\quad. \tag{86}$$

The expression

$$\exp\Bigg(i\pi\sum_{j=1}^{n-1}\big(S^z_j+\tfrac{1}{2}\big)\Bigg)=\prod_{j=1}^{n-1}\exp\Big(i\pi\big(S^z_j+\tfrac{1}{2}\big)\Big) \tag{87}$$

is known as a *Jordan-Wigner string*.

The nearest-neighbor bilinear transverse spin interaction terms are

$$
\begin{aligned}
S_n^+\,S_{n+1}^- &= c_n^\dagger\, e^{i\pi c_n^\dagger c_n}\, c_{n+1} = c_n^\dagger\, c_{n+1} \\
S_n^-\,S_{n+1}^+ &= c_n\, e^{i\pi c_n^\dagger c_n}\, c_{n+1}^\dagger = c_{n+1}^\dagger\, c_n \\
S_n^+\,S_{n+1}^+ &= c_n^\dagger\, e^{i\pi c_n^\dagger c_n}\, c_{n+1}^\dagger = c_n^\dagger\, c_{n+1}^\dagger \\
S_n^-\,S_{n+1}^+ &= c_n\, e^{i\pi c_n^\dagger c_n}\, c_{n+1} = c_{n+1}\, c_n \quad .
\end{aligned}
\tag{88}
$$

On an N-site ring, however, on the 'last' link, which connects site N back to site 1, yields

$$
\begin{aligned}
S_N^+\,S_1^- &= -e^{i\pi\hat{M}}\, c_N^\dagger c_1 \\
S_N^-\,S_1^+ &= -e^{i\pi\hat{M}}\, c_1^\dagger c_N \\
S_N^+\,S_1^+ &= -e^{i\pi\hat{M}}\, c_N^\dagger c_1^\dagger \\
S_N^-\,S_1^+ &= -e^{i\pi\hat{M}}\, c_1 c_N \quad .
\end{aligned}
\tag{89}
$$

where

$$
\hat{M} = \sum_{j=1}^{N} c_j^\dagger c_j \quad . \tag{90}
$$

Note that $e^{i\pi\hat{M}} = (-1)^{\hat{M}}$ must commute with every possible term we could write, since fermion number parity must be conserved.

2.1 Anisotropic XY model

Consider the anisotropic XY model in a perpendicular field on an N-site chain[3], with

$$
\begin{aligned}
\hat{H}_{\text{chain}} &= \sum_{n=1}^{N-1} \Big\{ J_x\, S_n^x\, S_{n+1}^x + J_y\, S_n^y\, S_{n+1}^y \Big\} + h \sum_{n=1}^{N} S_n^z \\
&= \tfrac{1}{2} \sum_{n=1}^{N-1} \Big\{ J_+\big(c_n^\dagger\, c_{n+1} + c_{n+1}^\dagger\, c_n\big) + J_-\big(c_n^\dagger\, c_{n+1}^\dagger + c_{n+1}\, c_n\big) \Big\} + h \sum_{n=1}^{N} \big(c_n^\dagger\, c_n - \tfrac{1}{2}\big) \quad ,
\end{aligned}
\tag{91}
$$

where $J_\pm = \frac{1}{2}(J_x \pm J_y)$. On an N-site ring, we add the term

$$
\begin{aligned}
\Delta H &= J_x\, S_N^x\, S_1^x + J_y\, S_N^y\, S_1^y \\
&= -\tfrac{1}{2}\, e^{i\pi\hat{M}} \Big\{ J_+\big(c_N^\dagger\, c_1 + c_1^\dagger\, c_N\big) + J_-\big(c_N^\dagger\, c_1^\dagger + c_1\, c_N\big) \Big\} \quad .
\end{aligned}
\tag{92}
$$

Since $e^{i\pi\hat{M}}$ commutes with $\hat{H}_{\text{chain}}$ and with all fermion bilinears (hence with ΔH as well), we can specify the eigenvalues as $\eta \equiv e^{i\pi\hat{M}} = \pm 1$, which are the even and odd fermion

[3]See E. Lieb, T. Schultz, and D. Mattis, *Ann. Phys.* **16**, 407 (1961).

number sectors, respectively. We then define

$$c_1 \equiv \begin{cases} -c_{N+1} & \text{if } \eta = +1 \\ +c_{N+1} & \text{if } \eta = -1 \end{cases} \quad . \tag{93}$$

If we write

$$c_n = \frac{1}{\sqrt{N}} \sum_k e^{ikn}\, c_k \quad , \tag{94}$$

where the index n refers to real space and k to momentum space, we have the wave vector quantization rule $e^{ikN} = -\eta$, *i.e.* for even and odd sectors

$$k_j = \begin{cases} 2\pi(j + \frac{1}{2})/N & \text{if } \eta = +1 \\ 2\pi j/N & \text{if } \eta = -1 \end{cases} \quad . \tag{95}$$

Thus, the Hamiltonian becomes

$$\begin{aligned} \hat{H}_{\text{ring}} &= \sum_k \Big\{ (J_+ \cos k + h)\, c_k^\dagger\, c_k + \tfrac{1}{2} J_-\, e^{ik}\, c_k^\dagger\, c_{-k}^\dagger + \tfrac{1}{2} J_-\, e^{-ik}\, c_{-k}\, c_k \Big\} + \tfrac{1}{2} N h \\ &= \sum_{k>0} \begin{pmatrix} c_k^\dagger & c_{-k} \end{pmatrix} \overbrace{\begin{pmatrix} \omega_k & \Delta_k \\ \Delta_k^* & -\omega_k \end{pmatrix}}^{H_k} \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix} \quad , \end{aligned} \tag{96}$$

where

$$\omega_k = J_+ \cos k + h \qquad . \qquad \Delta_k = i\, J_- \sin k \quad . \tag{97}$$

Diagonalizing via a unitary transformation, we obtain

$$\hat{H}_{\text{ring}} = \sum_k E_k \left(\gamma_k^\dagger \gamma_k - \tfrac{1}{2} \right) \quad , \tag{98}$$

where the dispersion relation is

$$E_k = \sqrt{\omega_k^2 + |\Delta_k|^2} = \sqrt{(J_+ \cos k + h)^2 + J_-^2 \sin^2 k} \quad . \tag{99}$$

Note that $S_k^\dagger\, H_k\, S_k = \mathsf{diag}(E_k, -E_k)$, where

$$S_k = \begin{pmatrix} u_k & -v_k^* \\ v_k & u_k \end{pmatrix} \tag{100}$$

where

$$u_k = \frac{E_k + \omega_k}{\sqrt{2E_k(E_k + \omega_k)}} \qquad , \qquad v_k = \frac{\Delta_k^*}{\sqrt{2E_k(E_k + \omega_k)}} \quad . \tag{101}$$

Thus,

$$\begin{aligned} \gamma_k &= u_k\, c_k - v_k^*\, c_{-k}^\dagger \\ \gamma_k^\dagger &= -v_k\, c_{-k} + u_k\, c_k^\dagger \quad . \end{aligned} \tag{102}$$

Note that $u_{-k} = u_k = u_k^*$ while $v_{-k} = -v_k = v_k^*$, and that

$$\begin{aligned} c_k &= u_k\,\gamma_k + v_k^*\,\gamma_{-k}^\dagger \\ c_k^\dagger &= v_k\,\gamma_{-k} + u_k\,\gamma_k^\dagger \quad . \end{aligned} \tag{103}$$

When we compute correlation functions, we use the fact that

$$e^{i\pi c^\dagger c} = (c^\dagger + c)(c^\dagger - c) = -(c^\dagger - c)(c^\dagger + c) \quad , \tag{104}$$

and, defining $A_j \equiv c_j^\dagger + c_j$ and $B_j \equiv c_j^\dagger - c_j$, Then the correlation functions are

$$\begin{aligned} \rho_x(\ell) &= \big\langle S_n^x\,S_{n+\ell}^x \big\rangle = \tfrac{1}{4}\,\big\langle B_n\,A_{n+1}\,B_{n+1}\cdots A_{n+\ell-1}\,B_{n+\ell-1}\,A_{n+\ell}\big\rangle \\ \rho_y(\ell) &= \big\langle S_n^y\,S_{n+\ell}^y \big\rangle = \tfrac{1}{4}\,(-1)^\ell \big\langle\, A_n\,B_{n+1}\,A_{n+1}\cdots B_{n+\ell-1}\,A_{n+\ell-1}\,B_{n+\ell}\big\rangle \\ \rho_z(\ell) &= \big\langle S_n^z\,S_{n+\ell}^z \big\rangle = \tfrac{1}{4}\,\big\langle A_n\,B_n\,A_{n+\ell}\,B_{n+\ell}\big\rangle \quad , \end{aligned} \tag{105}$$

where, without loss of generality, we presume $\ell > 0$. These expressions may be evaluated using Wick's theorem,

$$\big\langle \mathcal{O}_1\,\mathcal{O}_2\,\cdots\,\mathcal{O}_{2m}\big\rangle = \sum_{\sigma\in\mathcal{C}_{2r}} (-1)^\sigma\,\big\langle \mathcal{O}_{\sigma(1)}\,\mathcal{O}_{\sigma(2)}\big\rangle\cdots\big\langle \mathcal{O}_{\sigma(2r-1)}\,\mathcal{O}_{\sigma(2r)}\big\rangle \quad , \tag{106}$$

where σ is one of a special set of permutations $\mathcal{C}_{2r}$ of the set $\{1,\ldots,2r\}$ called *contractions*, which are arrangements of the $2r$ indices into r pairs. Exchanging any two pairs, or exchanging the indices within a pair results in the same contraction, so the number of such contractions is $|\mathcal{C}_{2r}| = (2r)!/(2^r\cdot r!)$. Here $(-1)^\sigma$ is the sign of the permutation σ. As an example, for $r = 2$ there are $4!/(4\cdot 2) = 3$ contractions. We then have

$$\rho_z(\ell) = \tfrac{1}{4}\,\big\langle A_n B_n\big\rangle\big\langle A_{n+\ell} B_{n+\ell}\big\rangle - \tfrac{1}{4}\,\big\langle A_n A_{n+\ell}\big\rangle\big\langle B_n B_{n+\ell}\big\rangle + \tfrac{1}{4}\,\big\langle A_n B_{n+\ell}\big\rangle\big\langle B_n A_{n+\ell}\big\rangle \quad . \tag{107}$$

Now we need the following:

$$\big\langle A_n A_{n'}\big\rangle = \delta_{nn'} \qquad , \qquad \big\langle B_n B_{n'}\big\rangle = -\delta_{nn'} \qquad , \qquad \big\langle A_n B_{n'}\big\rangle \equiv G(n'-n) \tag{108}$$

The first two of these relations follow by inversion symmetry, *i.e.*

$$\big\langle A_n A_{n'}\big\rangle = \big\langle A_{n'} A_n\big\rangle \quad \Rightarrow \quad \big\langle A_n A_{n'}\big\rangle = \tfrac{1}{2}\,\big\langle \{A_n, A_{n'}\}\big\rangle = \delta_{nn'} \quad , \tag{109}$$

with a corresponding argument showing $\big\langle B_n B_{n'}\big\rangle = -\delta_{nn'}$. We then have

$$\begin{aligned} G(n'-n) &= \big\langle (c_n^\dagger + c_n)\,(c_{n'}^\dagger - c_{n'})\big\rangle \\ &= \frac{1}{N}\sum_{k,k'} \Big(\big\langle c_k^\dagger\,c_{k'}^\dagger\big\rangle - \big\langle c_{-k} c_{k'}\big\rangle + \big\langle c_{-k} c_{-k}^\dagger\big\rangle - \big\langle c_k^\dagger c_k\big\rangle\Big)\, e^{ik(n'-n)} \\ &= \frac{1}{N}\sum_k \Big(u_k^2 - |v_k|^2 + 2u_k v_k\Big)\, e^{-ikn}\,e^{ik'n'} = \frac{1}{N}\sum_k \bigg(\frac{\omega_k + \Delta_k}{E_k}\bigg)\, e^{ik(n'-n)} \end{aligned} \tag{110}$$

for $n \neq n'$, and at $T = 0$. Note that $\langle B_{n'} A_n \rangle = -G(n-n')$ for $n \neq n'$ and that $G(0) = 1-2\nu$ where $\nu = \langle c_j^\dagger c_j \rangle$ is the fermion occupation per site, which is translationally invariant. Thus, we have

$$\rho_z(\ell) = \tfrac{1}{4}\, G^2(0) - \tfrac{1}{4}\, G(\ell)\, G(-\ell) \tag{111}$$

The transverse spin correlations may be expressed as determinants, *viz.*

$$\rho_x(\ell) = \mathsf{det} \begin{pmatrix} G(1) & G(2) & \cdots & G(\ell) \\ G(0) & G(1) & \cdots & G(\ell-1) \\ \vdots & \vdots & \ddots & \vdots \\ G(2-\ell) & G(3-\ell) & \cdots & G(1) \end{pmatrix} \tag{112}$$

and

$$\rho_y(\ell) = \mathsf{det} \begin{pmatrix} G(-1) & G(0) & \cdots & G(\ell-2) \\ G(-2) & G(-1) & \cdots & G(\ell-3) \\ \vdots & \vdots & \ddots & \vdots \\ G(-\ell) & G(1-\ell) & \cdots & G(-1) \end{pmatrix} \quad . \tag{113}$$

Matrices like these which are constant along the diagonals are called *Toeplitz matrices*. A matrix M is Toeplitz if $M_{i,j} = M_{i+1,j+1} = m(i-j)$.

2.2 Majorana representation of the JW transformation

With Eqn. 65, which describes how one can write a single Dirac fermion with operators c and $c^\dagger$ in terms of two Majorana fermions α and β, *i.e.* $\alpha = c + c^\dagger$ and $\beta = i(c - c^\dagger)$, we can write the JW transformation as follows:

$$\begin{aligned} X_n &= (i\,\alpha_1\,\beta_1)\,(i\,\alpha_2\,\beta_2)\cdots(i\,\alpha_{n-1}\,\beta_{n-1})\,\alpha_n \\ Y_n &= (i\,\alpha_1\,\beta_1)\,(i\,\alpha_2\,\beta_2)\cdots(i\,\alpha_{n-1}\,\beta_{n-1})\,\beta_n \\ Z_n &= -i\,\alpha_n\,\beta_n \quad . \end{aligned} \tag{114}$$

Here we write (X_n, Y_n, Z_n) for the Pauli matrices $(\sigma_n^x, \sigma_n^y, \sigma_n^z) = (2S_n^x, 2S_n^y, 2S_n^z)$. Note that $X_n\, Y_n = i\, Z_n$. Thus, we have written the N spin operators along the chain in terms of $2N$ Majorana fermions $\{\alpha_1, \beta_1, \ldots, \alpha_N, \beta_N\}$, and, through the relations $\alpha_n = c_n + c_n^\dagger$ and $\beta_n = i(c_n - c_n^\dagger)$, in terms of N Dirac fermions $\big\{(c_1, c_1^\dagger), \ldots, (c_N, c_N^\dagger)\big\}$. Note that

$$i\,\alpha_n\,\beta_n = -Z_n = \exp(i\pi c_n^\dagger c_n) = 1 - 2\,c_n^\dagger c_n \quad , \tag{115}$$

and we thereby recover Eqn. 84.