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Chapter 17

Quadratic Hamiltonians

17.1 Bosonic Models

The general noninteracting bosonic Hamiltonian is written

$$\hat{H} = \tfrac{1}{2}\Psi_r^\dagger \, \mathcal{H}_{rs} \Psi_s \quad , \tag{17.1}$$

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

$$\Psi^\dagger = \big(\psi_1^\dagger \, , \, \cdots \, , \, \psi_N^\dagger \, , \, \psi_1 \, , \, \cdots \, , \, \psi_N\big) \quad . \tag{17.2}$$

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

$$\big[\Psi_r \, , \, \Psi_s^\dagger\big] = \Sigma_{rs} \quad , \quad \Sigma = \begin{pmatrix} \mathbb{I}_{N\times N} & 0 \\ 0 & -\mathbb{I}_{N\times N} \end{pmatrix} \quad , \tag{17.3}$$

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

$$\mathcal{H} = \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \tag{17.4}$$

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

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

$$\begin{pmatrix} \psi \\ \psi^\dagger \end{pmatrix} = \overbrace{\begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}}^{\mathcal{S}} \begin{pmatrix} \phi \\ \phi^\dagger \end{pmatrix} \quad , \tag{17.5}$$

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

$$\begin{aligned} \psi_i &= U_{ia}\,\phi_a + V^*_{ia}\,\phi^\dagger_a \\ \psi^\dagger_i &= V_{ia}\,\phi_a + U^*_{ia}\,\phi^\dagger_a \quad , \end{aligned} \tag{17.6}$$

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.*

$$\big[\Phi_r\,,\,\Phi^\dagger_s\big] = \Sigma_{rs} \quad . \tag{17.7}$$

This then requires

$$\mathcal{S}\,\Sigma\,\mathcal{S}^\dagger = \mathcal{S}^\dagger\,\Sigma\,\mathcal{S} = \Sigma \quad , \tag{17.8}$$

which entails

$$U^\dagger U - V^\dagger V = \mathbb{I} \qquad\qquad U^{\mathsf{t}} V - V^{\mathsf{t}} U = 0 \tag{17.9}$$

$$U U^\dagger - V^* V^{\mathsf{t}} = \mathbb{I} \qquad\qquad U^* V^{\mathsf{t}} - V U^\dagger = 0 \quad . \tag{17.10}$$

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

$$\mathcal{S}^{-1} = \Sigma\,\mathcal{S}^\dagger\,\Sigma = \begin{pmatrix} U^\dagger & -V^\dagger \\ -V^{\mathsf{t}} & U^{\mathsf{t}} \end{pmatrix} \quad . \tag{17.11}$$

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

$$\begin{aligned} \phi_a &= U^*_{ia}\,\psi_i - V^*_{ia}\,\psi^\dagger_i \\ \phi^\dagger_a &= -V_{ia}\,\psi_i + U_{ia}\,\psi^\dagger_i \quad , \end{aligned} \tag{17.12}$$

17.1.1 Bogoliubov equations

We are now in the position to demand

$$\mathcal{S}^\dagger \mathcal{H} \mathcal{S} = \mathcal{E} = \begin{pmatrix} E & 0 \\ 0 & E \end{pmatrix} \quad , \tag{17.13}$$

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

$$\mathcal{H}\,\mathcal{S} = \mathcal{S}^{\dagger\,-1}\mathcal{E} = \Sigma\,\mathcal{S}\,\Sigma\,\mathcal{E} \quad , \tag{17.14}$$

which is to say

$$\begin{pmatrix} A & B \\ B^* & A \end{pmatrix} \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} = \begin{pmatrix} U & -V^* \\ -V & U^* \end{pmatrix} \begin{pmatrix} E & 0 \\ 0 & E \end{pmatrix} \quad . \tag{17.15}$$

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

$$\begin{aligned} A_{ij}\, U_{ja} + B_{ij}\, V_{ja} &= +U_{ia}\, E_a \\ B^*_{ij}\, U_{ja} + A^*_{ij}\, V_{ja} &= -V_{ia}\, E_a \quad , \end{aligned} \tag{17.16}$$

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

$$\hat{H} = \sum_a E_a \left(\phi^\dagger_a \phi_a + \tfrac{1}{2}\right) \quad . \tag{17.17}$$

At temperature T, we have

$$\left\langle \phi^\dagger_a \, \phi_b \right\rangle = n(E_a)\, \delta_{ab} \quad , \tag{17.18}$$

where

$$n(E) = \frac{1}{\exp(E/k_{\rm B}T) - 1} \tag{17.19}$$

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

$$\langle \psi^\dagger_i \psi_j \rangle = \sum_a \Big\{ n_a\, U^*_{ia}\, U_{ja} + (1 + n_a)\, V_{ia}\, V^*_{ja} \Big\} \tag{17.20}$$

$$\langle \psi_i \psi_j \rangle = \sum_a \Big\{ n_a\, V^*_{ia}\, U_{ja} + (1 + n_a)\, U_{ia}\, V^*_{ja} \Big\} \quad , \tag{17.21}$$

where $n_a \equiv n(E_a)$.

17.1.2 Ground state

We have found

$$\varPhi = \mathcal{S}^{-1} \varPsi = \varSigma\, \mathcal{S}^\dagger \varSigma\, \varPsi \quad , \tag{17.22}$$

hence

$$\begin{aligned} \phi_a &= U^\dagger_{ai}\, \psi_i - V^\dagger_{ai}\, \psi^\dagger_i \\ &= \psi_i\, U^*_{ia} - \psi^\dagger_i\, V^*_{ia} \quad . \end{aligned} \tag{17.23}$$

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

$$|\, \mathrm{G}\, \rangle = C \, \exp\Big(\tfrac{1}{2} Q_{ij}\, \psi^\dagger_i \psi^\dagger_j \Big) \,|\, 0\, \rangle \quad , \tag{17.24}$$

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

$$\phi_a\, e^{\hat{Q}} \,|\, 0\, \rangle = e^{\hat{Q}} \Big(e^{-\hat{Q}}\, \phi_a\, e^{\hat{Q}} \Big) \,|\, 0\, \rangle \quad , \tag{17.25}$$

where

$$\hat{Q} \equiv \tfrac{1}{2} Q_{ij}\, \psi_i^\dagger \psi_j^\dagger \quad . \tag{17.26}$$

We now define

$$\psi_i(x) \equiv e^{-x\hat{Q}}\, \psi_i \, e^{x\hat{Q}} \tag{17.27}$$

and we find

$$\frac{d\psi_i(x)}{dx} = e^{-x\hat{Q}} \big[\psi_i \, , \, \hat{Q}\big] e^{x\hat{Q}} = Q_{ij}\, \psi_j^\dagger \quad , \tag{17.28}$$

and integrating[1] we obtain

$$\psi_i(x) \equiv e^{-x\hat{Q}}\, \psi_i \, e^{x\hat{Q}} = \psi_i(x) + x\, Q_{ij}\, \psi_j^\dagger \quad . \tag{17.29}$$

We may now write

$$e^{-\hat{Q}}\, \phi_a \, e^{\hat{Q}} = U_{ai}^\dagger \, \psi_i + \big(U_{ai}^\dagger \, Q_{ij} - V_{aj}^\dagger\big)\, \psi_j^\dagger \quad , \tag{17.30}$$

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

$$Q = \big(U^\dagger\big)^{-1} V^\dagger \quad , \tag{17.31}$$

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

17.1.3 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 $\mathcal{S}^\dagger = \Sigma \mathcal{S}^{-1} \Sigma$ and therefore

$$\mathcal{S}^\dagger \mathcal{H}\, \mathcal{S} = \Sigma\, \mathcal{S}^{-1}\, \Sigma\, \mathcal{H}\, \mathcal{S} \quad . \tag{17.32}$$

Now

$$\Sigma\, \mathcal{H} = \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \quad . \tag{17.33}$$

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

$$(\Sigma\, \mathcal{H})^{\mathrm{t}} = \begin{pmatrix} A^{\mathrm{t}} & -B^\dagger \\ B^{\mathrm{t}} & -A^\dagger \end{pmatrix} = \begin{pmatrix} A^* & -B^* \\ B & -A \end{pmatrix} = -\mathcal{J}^{-1} (\Sigma\, \mathcal{H})\, \mathcal{J} \quad , \tag{17.34}$$

where

$$\mathcal{J} = \begin{pmatrix} 0 & \mathbb{I} \\ -\mathbb{I} & 0 \end{pmatrix} \tag{17.35}$$

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

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

$$P(E) = \det(E - \Sigma\,\mathcal{H}) = \det(E + \mathcal{J}^{-1}\,\Sigma\,\mathcal{H}\,\mathcal{J}) = \det(E + \Sigma\,\mathcal{H}) = P(-E) \quad . \tag{17.36}$$

We conclude that the eigenvalues of $\Sigma\,\mathcal{H}$ come in $(+E,-E)$ pairs. To obtain the eigenenergies for the bosonic Hamiltonian $\hat{H}$, however, as per eqn. 17.32, we must multiply $\mathcal{S}^{-1}\Sigma\,\mathcal{H}\,\mathcal{S}$ 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).

17.2 Fermionic Models

The general noninteracting fermionic Hamiltonian is written

$$\hat{H} = \tfrac{1}{2}\Psi^\dagger_r\,\mathcal{H}_{rs}\Psi_s \quad , \tag{17.37}$$

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

$$\Psi^\dagger = \big(\psi^\dagger_1\,,\,\cdots\,,\,\psi^\dagger_N\,,\,\psi_1\,,\,\cdots\,,\,\psi_N\big) \quad . \tag{17.38}$$

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

$$\big\{\Psi_r\,,\,\Psi^\dagger_s\big\} = \delta_{rs} \quad . \tag{17.39}$$

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

$$\mathcal{H} = \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \quad , \tag{17.40}$$

where $A = A^\dagger$ is Hermitian and $B = -B^{\mathsf{t}}$ is antisymmetric. Since this is of the same form as eqn. 17.33, 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:

$$\begin{pmatrix} \psi \\ \psi^\dagger \end{pmatrix} = \overbrace{\begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}}^{\mathcal{S}} \begin{pmatrix} \phi \\ \phi^\dagger \end{pmatrix} \quad , \tag{17.41}$$

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

$$\begin{aligned} \psi_i &= U_{ia}\,\phi_a + V^*_{ia}\,\phi^\dagger_a \\ \psi^\dagger_i &= V_{ia}\,\phi_a + U^*_{ia}\,\phi^\dagger_a \quad . \end{aligned} \tag{17.42}$$

[2]This is true even though B in eqn. 17.33 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.

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

$$\{\Phi_r\,,\,\Phi_s^\dagger\}=\delta_{rs}\quad, \tag{17.43}$$

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

$$\mathcal{S}^\dagger\mathcal{S}=\mathcal{S}\mathcal{S}^\dagger=\mathcal{I}\quad, \tag{17.44}$$

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

$$U^\dagger U+V^\dagger V=\mathbb{I}\qquad\qquad U^{\mathsf{t}}V+V^{\mathsf{t}}U=0 \tag{17.45}$$

$$UU^\dagger+V^*V^{\mathsf{t}}=\mathbb{I}\qquad\qquad U^*V^{\mathsf{t}}+VU^\dagger=0\quad. \tag{17.46}$$

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

$$\begin{aligned}\phi_a&=U^*_{ia}\,\psi_i+V^*_{ia}\,\psi_i^\dagger\\ \phi_a^\dagger&=V_{ia}\,\psi_i+U_{ia}\,\psi_i^\dagger\quad,\end{aligned} \tag{17.47}$$

The transformed Hamiltonian matrix is

$$\mathcal{S}^\dagger\mathcal{H}\,\mathcal{S}=\mathcal{E}\equiv\begin{pmatrix}E&0\\0&-E\end{pmatrix}\quad. \tag{17.48}$$

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

$$\begin{aligned}A_{ij}\,U_{ja}+B_{ij}\,V_{ja}&=U_{ia}\,E_a\\ -B^*_{ij}\,U_{ja}-A^*_{ij}\,V_{ja}&=V_{ia}\,E_a\quad.\end{aligned} \tag{17.49}$$

The Hamiltonian then takes the form

$$\hat{H}=\sum_a E_a\left(\phi_a^\dagger\phi_a-\tfrac{1}{2}\right)\quad. \tag{17.50}$$

At temperature T, we have

$$\left\langle\phi_a^\dagger\phi_b\right\rangle=f(E_a)\,\delta_{ab}\quad, \tag{17.51}$$

where

$$f(E)=\frac{1}{\exp(E/k_{\rm B}T)+1} \tag{17.52}$$

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

$$\begin{aligned}\langle\psi_i^\dagger\psi_j\rangle&=\sum_a\Big\{f_a\,U^*_{ia}\,U_{ja}+(1-f_a)\,V_{ia}\,V^*_{ja}\Big\}\\ \langle\psi_i\psi_j\rangle&=\sum_a\Big\{f_a\,V^*_{ia}\,U_{ja}+(1-f_a)\,U_{ia}\,V^*_{ja}\Big\}\quad,\end{aligned} \tag{17.53}$$

where $f_a=f(E_a)$.

17.2.1 Ground state

We write

$$| \, \mathrm{G} \, \rangle = C \exp\Big(\tfrac{1}{2} Q_{ij} \, \psi_i^\dagger \psi_j^\dagger\Big) \, | \, 0 \, \rangle \quad , \tag{17.54}$$

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

$$\psi_i(x) = e^{-x\hat{Q}} \, \psi_i \, e^{x\hat{Q}} \quad . \tag{17.55}$$

We then have

$$\frac{d\psi_i(x)}{dx} = e^{-x\hat{Q}} \, \big[\psi_i, \hat{Q}\big] \, e^{x\hat{Q}} = Q_{ij} \, \psi_j^\dagger \quad \Rightarrow \quad \psi_i(x) = \psi_i + x \, Q_{ij} \, \psi_j^\dagger \quad . \tag{17.56}$$

Thus,

$$e^{-\hat{Q}} \, \phi_a \, e^{\hat{Q}} = U_{ai}^\dagger \, \psi_i + \big(V_{aj}^\dagger + U_{ai}^\dagger \, Q_{ij}\big) \, \psi_j^\dagger \quad , \tag{17.57}$$

from which we obtain

$$Q = -\big(U^\dagger\big)^{-1} V^\dagger \quad . \tag{17.58}$$

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

17.3 Majorana Fermion Models

Majorana fermions satisfy the anticommutation relations $\big\{\theta_i \, , \, \theta_j\big\} = 2\delta_{ij}$. 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 $\big\{c \, , \, c^\dagger\big\} = 1$, we may define Majorana fermions η and $\widetilde{\eta}$ as follows:

$$\eta = c + c^\dagger \qquad\qquad c = \tfrac{1}{2}(\eta - i\eta') \tag{17.59}$$

$$\widetilde{\eta} = i(c - c^\dagger) \qquad\qquad c^\dagger = \tfrac{1}{2}(\eta + i\widetilde{\eta}) \quad . \tag{17.60}$$

The most general noninteracting Majorana Hamiltonian is of the form

$$\hat{H} = \tfrac{i}{4} M_{ij} \, \theta_i \, \theta_j \quad , \tag{17.61}$$

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

$$\theta_i = \mathcal{R}_{ia} \, \xi_a \quad , \tag{17.62}$$

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

$$\mathcal{R}^{\rm t}\mathcal{M}\mathcal{R} = E\otimes i\sigma^y = \begin{pmatrix} 0 & -E_1 & 0 & 0 & \cdots \\ E_1 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & -E_2 & \cdots \\ 0 & 0 & E_2 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad . \tag{17.63}$$

Thus,

$$\hat{H} = -\tfrac{i}{2}\sum_{a=1}^{N} E_a\,\xi_{2a-1}\,\xi_{2a} = \sum_a E_a\big(c^\dagger_a c_a - \tfrac{1}{2}\big) \quad , \tag{17.64}$$

where

$$c_a \equiv \tfrac{1}{2}\big(\xi_{2a-1} - i\,\xi_{2a}\big) \quad , \quad c^\dagger_a \equiv \tfrac{1}{2}\big(\xi_{2a-1} + i\,\xi_{2a}\big) \quad . \tag{17.65}$$

17.3.1 Majorana chain

Consider the Hamiltonian

$$\hat{H} = -i\sum_{n=1}^{N} \sigma_n\,\alpha_n\,\alpha_{n+1} \tag{17.66}$$

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,

$$\theta_1 \equiv \alpha_1 \quad , \quad \theta_2 \equiv \sigma_1\alpha_2 \quad , \quad \theta_3 \equiv \sigma_1\sigma_2\,\alpha_3 \quad , \quad \ldots \quad , \quad \theta_N \equiv \sigma_1\sigma_2\cdots\sigma_{N-1}\,\alpha_N \quad . \tag{17.67}$$

The Hamiltonian may now be written as

$$\hat{H} = -i\sum_{n=1}^{N} \theta_n\,\theta_{n+1} \quad , \tag{17.68}$$

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

$$\hat{\theta}_k = \frac{1}{\sqrt{N}}\sum_{n=1}^{N} e^{-ikn}\,\theta_n \qquad , \qquad \theta_n = \frac{1}{\sqrt{N}}\sum_k e^{ikn}\,\hat{\theta}_k \quad . \tag{17.69}$$

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

$$\big\{\theta_m\,,\,\theta_n\big\} = 2\,\delta_{m-n\,,\,0\,{\rm mod}\,N} \qquad , \qquad \big\{\hat{\theta}_k\,,\,\hat{\theta}_p\big\} = 2\,\delta_{k+p\,,\,0\,{\rm mod}\,2\pi} \quad . \tag{17.70}$$

There are four cases to consider:

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

$$k \in \pm\frac{2\pi}{N} \times \Big\{1\,,\,\ldots\,,\,\tfrac{1}{2}N - 1\Big\} \quad , \quad k = 0 \quad , \quad k = \pi \quad . \tag{17.71}$$

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

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

$$k \in \pm\frac{2\pi}{N} \times \Big\{1\,,\,\ldots\,,\,\tfrac{1}{2}(N - 1)\Big\} \quad , \quad k = 0 \quad . \tag{17.72}$$

Only $k = 0$ is unpaired.

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

$$k \in \pm\frac{2\pi}{N} \times \Big\{\tfrac{1}{2}\,,\,\ldots\,,\,\tfrac{1}{2}(N - 1)\Big\} \quad . \tag{17.73}$$

All the crystal momenta are paired.

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

$$k \in \pm\frac{2\pi}{N} \times \Big\{\tfrac{1}{2}\,,\,\ldots\,,\,\tfrac{1}{2}N - 1\Big\} \quad , \quad k = \pi \quad . \tag{17.74}$$

Only $k = \pi$ is unpaired.

We may now write

$$\begin{aligned}\hat{H} &= -i\sum_k e^{-ik}\,\hat{\theta}_k\,\hat{\theta}_{-k} \\ &= -i\sum_{k\in(0,\pi)} \Big(e^{ik}\,\hat{\theta}_{-k}\,\hat{\theta}_k + e^{-ik}\,\hat{\theta}_k\,\hat{\theta}_{-k}\Big) - i\sum_{k\in\mathrm{U}} e^{-ik}\,\hat{\theta}_k^2 \\ &= \sum_{k\in(0,\pi)} 2\sin k\,\hat{\theta}_{-k}\,\hat{\theta}_k - 2i\sum_{k\in(0,\pi)} e^{-ik} - i\sum_{k\in\mathrm{U}} e^{-ik} \quad .\end{aligned} \tag{17.75}$$

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

$$\hat{H} = \sum_{k\in(0,\pi)} 4\sin k\,c_k^\dagger\,c_k + E_0 \quad , \tag{17.76}$$

where

$$E_0 = -2i\sum_{k\in(0,\pi)} e^{-ik} - i\sum_{k\in\mathrm{U}} e^{-ik} \quad . \tag{17.77}$$

We now proceed to evaluate E_0 for our four cases.

Case I : 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

$$E_0^{(\mathrm{I})} = -2i \sum_{\ell=1}^{\frac{N}{2}-1} e^{-2\pi i\ell/N} = -2\,\mathrm{ctn}\Big(\frac{\pi}{N}\Big) \quad . \tag{17.78}$$

Note that we have used the identity

$$\sum_{\ell=1}^{J-1} x^\ell = \frac{x - x^J}{1-x} \quad . \tag{17.79}$$

Case II : 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

$$E_0^{(\mathrm{II})} = -2i \sum_{\ell=1}^{\frac{N+1}{2}-1} e^{-2\pi i\ell/N} - i = -2i\left(\frac{e^{-2\pi i/N} + e^{-i\pi/N}}{1 - e^{-2\pi i/N}}\right) - i = -\,\mathrm{ctn}\left(\frac{\pi}{2N}\right) \quad . \tag{17.80}$$

Case III : 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

$$E_0^{(\mathrm{III})} = -2i\,e^{-i\pi/N} \sum_{\ell=0}^{\frac{N}{2}-1} e^{-2\pi\ell/N} = -2\csc\left(\frac{\pi}{N}\right) \quad . \tag{17.81}$$

Case IV : We have $\mathrm{U} = \{\pi\}$. 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,

$$E_0^{(\mathrm{IV})} = -2i\,e^{i\pi/N} \sum_{\ell=1}^{\frac{N+1}{2}-1} e^{-2\pi i\ell/N} + i = -2i\bigg(\frac{e^{-i\pi/N} + 1}{1 - e^{-2\pi i/N}}\bigg) + i = -\,\mathrm{ctn}\left(\frac{\pi}{2N}\right) \quad . \tag{17.82}$$

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

17.4 Jordan-Wigner Transformation

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

$$\begin{aligned} S^+_n &= \exp\bigg(i\pi \sum_{j=1}^{n-1} c^\dagger_j c_j\bigg)\, c^\dagger_n \\ S^-_n &= \exp\bigg(i\pi \sum_{j=1}^{n-1} c^\dagger_j c_j\bigg)\, c_n \\ S^z_n &= c^\dagger_n c_n - \tfrac{1}{2} \quad . \end{aligned} \tag{17.83}$$

The inverse is then

$$\begin{aligned} c^\dagger_n &= \exp\bigg(i\pi \sum_{j=1}^{n-1} \big(S^z_j + \tfrac{1}{2}\big)\bigg)\, S^+_n \\ c_n &= \exp\bigg(i\pi \sum_{j=1}^{n-1} \big(S^z_j + \tfrac{1}{2}\big)\bigg)\, S^-_n \quad . \end{aligned} \tag{17.84}$$

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

$$c\, e^{i\pi c^\dagger c} = -c \quad , \quad c^\dagger e^{i\pi c^\dagger c} = c^\dagger \quad . \tag{17.85}$$

Taking the Hermitian conjugate,

$$e^{i\pi c^\dagger c}\, c^\dagger = -c^\dagger \quad , \quad e^{i\pi c^\dagger c}\, c = c \quad . \tag{17.86}$$

The expression

$$\exp\bigg(i\pi \sum_{j=1}^{n-1} \big(S^z_j + \tfrac{1}{2}\big)\bigg) = \prod_{j=1}^{n-1} \exp\Big(i\pi\big(S^z_j + \tfrac{1}{2}\big)\Big) \tag{17.87}$$

is known as a *Jordan-Wigner string*.

The nearest-neighbor bilinear transverse spin interaction terms are

$$\begin{aligned} S^+_n\, S^-_{n+1} &= c^\dagger_n\, e^{i\pi c^\dagger_n c_n}\, c_{n+1} = c^\dagger_n\, c_{n+1} \\ S^-_n\, S^+_{n+1} &= c_n\, e^{i\pi c^\dagger_n c_n}\, c^\dagger_{n+1} = c^\dagger_{n+1}\, c_n \\ S^+_n\, S^+_{n+1} &= c^\dagger_n\, e^{i\pi c^\dagger_n c_n}\, c^\dagger_{n+1} = c^\dagger_n\, c^\dagger_{n+1} \\ S^-_n\, S^+_{n+1} &= c_n\, e^{i\pi c^\dagger_n c_n}\, c_{n+1} = c_{n+1}\, c_n \quad . \end{aligned} \tag{17.88}$$

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

$$\begin{aligned} S_N^+ \, S_1^- &= -e^{i\pi\hat{M}} \, c_N^\dagger c_1 \\ S_N^- \, S_1^+ &= -e^{i\pi\hat{M}} \, c_1^\dagger c_N \\ S_N^+ \, S_1^+ &= -e^{i\pi\hat{M}} \, c_N^\dagger c_1^\dagger \\ S_N^- \, S_1^+ &= -e^{i\pi\hat{M}} \, c_1 c_N \quad . \end{aligned} \tag{17.89}$$

where

$$\hat{M} = \sum_{j=1}^N c_j^\dagger c_j \quad . \tag{17.90}$$

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.

17.4.1 Anisotropic XY model

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

$$\begin{aligned} \hat{H}_{\text{chain}} &= \sum_{n=1}^{N-1} \Big\{ J_x \, S_n^x \, S_{n+1}^x + J_y \, S_n^y \, S_{n+1}^y \Big\} + h \sum_{n=1}^N S_n^z \\ &= \tfrac{1}{2} \sum_{n=1}^{N-1} \Big\{ J_+ \big(c_n^\dagger \, c_{n+1} + c_{n+1}^\dagger \, c_n \big) + J_- \big(c_n^\dagger \, c_{n+1}^\dagger + c_{n+1} \, c_n \big) \Big\} + h \sum_{n=1}^N \big(c_n^\dagger \, c_n - \tfrac{1}{2} \big) \quad , \end{aligned} \tag{17.91}$$

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

$$\begin{aligned} \Delta H &= J_x \, S_N^x \, S_1^x + J_y \, S_N^y \, S_1^y \\ &= -\tfrac{1}{2} \, e^{i\pi\hat{M}} \Big\{ J_+ \big(c_N^\dagger \, c_1 + c_1^\dagger \, c_N \big) + J_- \big(c_N^\dagger \, c_1^\dagger + c_1 \, c_N \big) \Big\} \quad . \end{aligned} \tag{17.92}$$

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 number sectors, respectively. We then define

$$c_1 \equiv \begin{cases} -c_{N+1} & \text{if } \eta = +1 \\ +c_{N+1} & \text{if } \eta = -1 \quad . \end{cases} \tag{17.93}$$

If we write

$$c_n = \frac{1}{\sqrt{N}} \sum_k e^{ikn} \, c_k \quad , \tag{17.94}$$

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

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

$$k_j = \begin{cases} 2\pi(j+\frac{1}{2})/N & \text{if } \eta = +1 \\ 2\pi j/N & \text{if } \eta = -1 \end{cases} \quad . \tag{17.95}$$

Thus, the Hamiltonian becomes

$$\begin{aligned} \hat{H}_{\text{ring}} &= \sum_k \Big\{ (J_+ \cos k + h)\, c_k^\dagger\, c_k + \tfrac{1}{2} J_-\, e^{ik}\, c_k^\dagger\, c_{-k}^\dagger + \tfrac{1}{2} J_-\, e^{-ik}\, c_{-k}\, c_k \Big\} + \tfrac{1}{2} N h \\ &= \sum_{k>0} \begin{pmatrix} c_k^\dagger & c_{-k} \end{pmatrix} \overbrace{\begin{pmatrix} \omega_k & \Delta_k \\ \Delta_k^* & -\omega_k \end{pmatrix}}^{H_k} \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix} \quad , \end{aligned} \tag{17.96}$$

where

$$\omega_k = J_+ \cos k + h \qquad . \qquad \Delta_k = i\, J_- \sin k \quad . \tag{17.97}$$

Diagonalizing via a unitary transformation, we obtain

$$\hat{H}_{\text{ring}} = \sum_k E_k \left(\gamma_k^\dagger \gamma_k - \tfrac{1}{2} \right) \quad , \tag{17.98}$$

where the dispersion relation is

$$E_k = \sqrt{\omega_k^2 + |\Delta_k|^2} = \sqrt{(J_+ \cos k + h)^2 + J_-^2 \sin^2 k} \quad . \tag{17.99}$$

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

$$S_k = \begin{pmatrix} u_k & -v_k^* \\ v_k & u_k \end{pmatrix} \tag{17.100}$$

where

$$u_k = \frac{E_k + \omega_k}{\sqrt{2E_k(E_k + \omega_k)}} \qquad , \qquad v_k = \frac{\Delta_k^*}{\sqrt{2E_k(E_k + \omega_k)}} \quad . \tag{17.101}$$

Thus,

$$\begin{aligned} \gamma_k &= u_k\, c_k - v_k^*\, c_{-k}^\dagger \\ \gamma_k^\dagger &= -v_k\, c_{-k} + u_k\, c_k^\dagger \quad . \end{aligned} \tag{17.102}$$

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

$$\begin{aligned} c_k &= u_k\, \gamma_k + v_k^*\, \gamma_{-k}^\dagger \\ c_k^\dagger &= v_k\, \gamma_{-k} + u_k\, \gamma_k^\dagger \quad . \end{aligned} \tag{17.103}$$

When we compute correlation functions, we use the fact that

$$e^{i\pi c^\dagger c} = (c^\dagger + c)(c^\dagger - c) = -(c^\dagger - c)(c^\dagger + c) \quad , \tag{17.104}$$

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

$$\begin{aligned}
\rho_x(\ell) &= \big\langle S_n^x \, S_{n+\ell}^x \big\rangle = \tfrac{1}{4} \big\langle B_n \, A_{n+1} \, B_{n+1} \cdots A_{n+\ell-1} \, B_{n+\ell-1} \, A_{n+\ell} \big\rangle \\
\rho_y(\ell) &= \big\langle S_n^y \, S_{n+\ell}^y \big\rangle = \tfrac{1}{4} \, (-1)^\ell \big\langle \, A_n \, B_{n+1} \, A_{n+1} \cdots B_{n+\ell-1} \, A_{n+\ell-1} \, B_{n+\ell} \big\rangle \\
\rho_z(\ell) &= \big\langle S_n^z \, S_{n+\ell}^z \big\rangle = \tfrac{1}{4} \big\langle A_n \, B_n \, A_{n+\ell} \, B_{n+\ell} \big\rangle \quad ,
\end{aligned} \tag{17.105}$$

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

$$\big\langle \mathcal{O}_1 \, \mathcal{O}_2 \, \cdots \, \mathcal{O}_{2m} \big\rangle = \sum_{\sigma \in \mathcal{C}_{2r}} (-1)^\sigma \big\langle \mathcal{O}_{\sigma(1)} \, \mathcal{O}_{\sigma(2)} \big\rangle \cdots \big\langle \mathcal{O}_{\sigma(2r-1)} \, \mathcal{O}_{\sigma(2r)} \big\rangle \quad , \tag{17.106}$$

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

$$\rho_z(\ell) = \tfrac{1}{4} \big\langle A_n B_n \big\rangle \big\langle A_{n+\ell} B_{n+\ell} \big\rangle - \tfrac{1}{4} \big\langle A_n A_{n+\ell} \big\rangle \big\langle B_n B_{n+\ell} \big\rangle + \tfrac{1}{4} \big\langle A_n B_{n+\ell} \big\rangle \big\langle B_n A_{n+\ell} \big\rangle \quad . \tag{17.107}$$

Now we need the following:

$$\big\langle A_n A_{n'} \big\rangle = \delta_{nn'} \qquad , \qquad \big\langle B_n B_{n'} \big\rangle = -\delta_{nn'} \qquad , \qquad \big\langle A_n B_{n'} \big\rangle \equiv G(n' - n) \tag{17.108}$$

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

$$\big\langle A_n A_{n'} \big\rangle = \big\langle A_{n'} A_n \big\rangle \quad \Rightarrow \quad \big\langle A_n A_{n'} \big\rangle = \tfrac{1}{2} \big\langle \{ A_n , A_{n'} \} \big\rangle = \delta_{nn'} \quad , \tag{17.109}$$

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

$$\begin{aligned}
G(n'-n) &= \big\langle (c_n^\dagger + c_n) \, (c_{n'}^\dagger - c_{n'}) \big\rangle \\
&= \frac{1}{N} \sum_{k,k'} \Big(\big\langle c_k^\dagger \, c_{k'}^\dagger \big\rangle - \big\langle c_{-k} c_{k'} \big\rangle + \big\langle c_{-k} c_{-k}^\dagger \big\rangle - \big\langle c_k^\dagger c_k \big\rangle \Big) \, e^{ik(n'-n)} \\
&= \frac{1}{N} \sum_k \Big(u_k^2 - |v_k|^2 + 2u_k v_k \Big) \, e^{-ikn} \, e^{ik'n'} = \frac{1}{N} \sum_k \bigg(\frac{\omega_k + \Delta_k}{E_k} \bigg) \, e^{ik(n'-n)}
\end{aligned} \tag{17.110}$$

for $n \neq n'$, and at $T = 0$. Note that $\big\langle B_{n'} A_n \big\rangle = -G(n - n')$ 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

$$\rho_z(\ell) = \tfrac{1}{4} \, G^2(0) - \tfrac{1}{4} \, G(\ell) \, G(-\ell) \tag{17.111}$$

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

$$\rho_x(\ell) = \det \begin{pmatrix} G(1) & G(2) & \cdots & G(\ell) \\ G(0) & G(1) & \cdots & G(\ell-1) \\ \vdots & \vdots & \ddots & \vdots \\ G(2-\ell) & G(3-\ell) & \cdots & G(1) \end{pmatrix} \tag{17.112}$$

and

$$\rho_y(\ell) = \det \begin{pmatrix} G(-1) & G(0) & \cdots & G(\ell-2) \\ G(-2) & G(-1) & \cdots & G(\ell-3) \\ \vdots & \vdots & \ddots & \vdots \\ G(-\ell) & G(1-\ell) & \cdots & G(-1) \end{pmatrix} \quad . \tag{17.113}$$

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

17.4.2 Majorana representation of the JW transformation

With Eqn. 17.65, 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:

$$\begin{aligned} X_n &= (i\,\alpha_1\,\beta_1)\,(i\,\alpha_2\,\beta_2)\cdots(i\,\alpha_{n-1}\,\beta_{n-1})\,\alpha_n \\ Y_n &= (i\,\alpha_1\,\beta_1)\,(i\,\alpha_2\,\beta_2)\cdots(i\,\alpha_{n-1}\,\beta_{n-1})\,\beta_n \\ Z_n &= -i\,\alpha_n\,\beta_n \quad . \end{aligned} \tag{17.114}$$

Here we write (X_n, Y_n, Z_n) for the Pauli matrices $(\sigma^x_n, \sigma^y_n, \sigma^z_n) = (2S^x_n, 2S^y_n, 2S^z_n)$. 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 $\alpha_n = c_n + c^\dagger_n$ and $\beta_n = i(c_n - c^\dagger_n)$, in terms of N Dirac fermions $\big\{(c_1, c^\dagger_1), \ldots, (c_N, c^\dagger_N)\big\}$. Note that

$$i\,\alpha_n\,\beta_n = -Z_n = \exp(i\pi c^\dagger_n c_n) = 1 - 2\,c^\dagger_n c_n \quad , \tag{17.115}$$

and we thereby recover Eqn. 17.84.