A model of interacting spins on a one-dimensional lattice.

In this problem you will investigate a model with Hamiltonian
\[ \hat{H}(\gamma, \lambda) = -\sum_j \left[ \frac{1}{2} (1 + \gamma) \hat{\sigma}_j^x \hat{\sigma}_{j+1}^x + \frac{1}{2} (1 - \gamma) \hat{\sigma}_j^y \hat{\sigma}_{j+1}^y + \lambda \hat{\sigma}_j^z \right]. \] (1)

The sum is over the sites \( j \) of a one-dimensional lattice. At each site there is a \( S = 1/2 \) spin \( \hat{S}_j = (\hbar/2) \hat{\sigma}_j \) where the \( \hat{\sigma}_\alpha^j \) operators (\( \alpha = x, y, z \)) can be represented by the standard Pauli matrices. The first two terms, which contain the parameter \( \gamma \), represent interactions between nearest-neighbor spins, while the last term, proportional to the parameter \( \lambda \), describes the coupling to an external magnetic field in the \( z \) direction. It is convenient to introduce the operators
\[ \hat{\sigma}_j^\pm = \frac{1}{2} (\hat{\sigma}_j^x \pm i \hat{\sigma}_j^y), \] (2)

in terms of which the Hamiltonian becomes (from now on I drop writing \( \gamma, \lambda \) as arguments of \( \hat{H} \))
\[ \hat{H} = -\sum_i \left[ (\hat{\sigma}_i^+ \hat{\sigma}_{i+1}^- + \hat{\sigma}_i^- \hat{\sigma}_{i+1}^+) + \gamma (\hat{\sigma}_i^+ \hat{\sigma}_{i+1}^- + \hat{\sigma}_i^- \hat{\sigma}_{i+1}^+) + \lambda \hat{\sigma}_i^z \right]. \] (3)

It is possible to solve this model exactly. The exact solution involves the following sequence of steps: (1) a Jordan-Wigner transformation, (2) a Fourier transformation, and (3) a Bogoliubov transformation. The Jordan-Wigner transformation maps the original spin model to one describing spinless fermions hopping on the same one-dimensional lattice. This fermionic model only contains quadratic (as opposed to quartic) terms and so can be diagonalized exactly. By doing a Fourier transformation to fermionic operators that create/annihilate fermions in definite \( k \) states, a partial diagonalization is accomplished, in the sense that fermionic operators with different \( |k| \)'s become decoupled. Operators associated with opposite wavevectors \( k \) and \( -k \) are however still coupled after the Fourier transformation; these can be decoupled by a subsequent Bogoliubov transformation.

We now introduce fermionic creation and annihilation operators \( \hat{c}_j^\dagger, \hat{c}_j \) where the index \( j = 1, 2, \ldots N \) refers to the lattice site. (These fermions are referred to as spinless because they have no spin index, just a site index.) These fermions obey standard fermionic anticommutation relations
\[ \{\hat{c}_j, \hat{c}_{j'}^\dagger\} = \delta_{j,j'}, \] (4)
\[ \{\hat{c}_j, \hat{c}_{j'}\} = \{\hat{c}_j^\dagger, \hat{c}_{j'}^\dagger\} = 0. \] (5)
The spin operators can be expressed in terms of these fermion operators by a Jordan-Wigner transformation:

\[
\hat{\sigma}^+_i = \left[ \prod_{j=1}^{i-1} (1 - 2\hat{n}_j) \right] \hat{c}_i, \tag{6}
\]

\[
\hat{\sigma}^-_i = \left[ \prod_{j=1}^{i-1} (1 - 2\hat{n}_j) \right] \hat{c}_i^\dagger, \tag{7}
\]

\[
\hat{\sigma}^z_i = 1 - 2\hat{n}_i, \tag{8}
\]

where \(\hat{n}_j = \hat{c}_j^\dagger \hat{c}_j\). The relation (8) shows that the two possible eigenvalues \(\pm 1\) of \(\hat{\sigma}^z_i\) corresponds to the absence or presence of a fermion at site \(i\). Note that spin operators belonging to different sites commute while fermion operators on different sites anticommute. The ”string operator” \(\prod_{j=1}^{i-1} (1 - 2\hat{n}_j)\) is crucial in bringing about the change from anticommutation to commutation.

(a) Use the fermionic operator algebra [see (4)-(5), (26)-(30)] and the Jordan-Wigner transformation to show that for \(i \neq j\),

\[
[\hat{\sigma}^+_i, \hat{\sigma}^-_j] = 0. \tag{9}
\]

(You may assume \(i < j\).)

(b) The product \(\hat{\sigma}^+_i \hat{\sigma}^+_i\) appears in (3). Show that in terms of the fermions it becomes

\[
\hat{\sigma}^+_i \hat{\sigma}^+_i = \hat{c}_i \hat{c}_i^\dagger. \tag{10}
\]

***

Expressing the other terms in (3) in fermionic form as well, one finds

\[
\hat{H} = -\sum_j \left[ (\hat{c}_j^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_{j+1}) + \gamma (\hat{c}_{j+1} \hat{c}_j + \hat{c}_j^\dagger \hat{c}_{j+1}^\dagger) - 2\lambda \hat{c}_j^\dagger \hat{c}_j + \lambda \right]. \tag{11}
\]

We will use periodic boundary conditions on the fermion operators,\(^1\) i.e. \(c_{N+1} = c_1\). Writing \(\hat{c}_j\) as a Fourier series,

\[
\hat{c}_j = \frac{1}{\sqrt{N}} \sum_k e^{ikj} \hat{c}_k, \tag{12}
\]

the periodic boundary conditions imply \(e^{i k N} = 1\), i.e.

\[
k = \frac{2\pi n}{N} \tag{13}
\]

\(^1\)This is actually not completely correct. The choice of periodic boundary conditions on the spin operators results in boundary conditions on the fermion operators which are periodic or anti-periodic, depending on the number of fermions in the system. However, for our purposes it is sufficiently accurate to simply use periodic boundary conditions on the fermions.
where \( n \) is an integer. Since there are \( N \) values for the site index \( j \), there must be \( N \) inequivalent values of the wavevectors \( k \). Take \( N \) to be odd and the \( N \) values of \( n \) to be
\[
-\frac{N-1}{2}, \ldots, -1, 0, 1, \ldots, \frac{N-1}{2}.
\] (14)

(c) Show that the Hamiltonian (11) becomes
\[
\hat{H} = \sum_k [2(\lambda - \cos k)\hat{c}_k^\dagger \hat{c}_k + i\gamma \sin k(\hat{c}_{-k} \hat{c}_k + \hat{c}_{-k}^\dagger \hat{c}_k^\dagger) - \lambda].
\] (15)

***

In (15) fermionic operators with different \( |k| \)'s have been decoupled, but there is still a coupling between \( k \) and \(-k\) operators. To get rid of this remaining coupling, we define operators
\[
\hat{d}_k = u_k \hat{c}_k - iv_k \hat{c}_{-k}^\dagger
\] (16)
and \( \hat{d}_k^\dagger \equiv (\hat{d}_k)^\dagger \), where
\[
u_k = \cos \theta_k^2, \quad v_k = \sin \theta_k^2,
\] (17)
where the real parameter (angle) \( \theta_k \) is so far unspecified, except that we take
\[
\theta_{-k} = -\theta_k \Rightarrow u_{-k} = u_k, \quad v_{-k} = -v_k.
\] (18)
This implies that the \( \hat{d}_k \)-operators satisfy standard fermionic anticommutation relations just like the \( \hat{c}_k \) operators, i.e.
\[
\{\hat{d}_k, \hat{d}_{k'}\} = 0, \quad \{\hat{d}_k, \hat{d}_{k'}^\dagger\} = \delta_{k,k'}.
\] (19)

(d) Show that the inverse transformation of (16) is
\[
\hat{c}_k = u_k \hat{d}_k + iv_k \hat{d}_{-k}^\dagger
\] (20)

***

We will choose the parameter \( \theta_k \) such that the coefficients of all “anomalous” terms in the Hamiltonian vanish when expressed in terms of the \( \hat{d}_k \) operators. (By definition, these anomalous terms contain products of two creation operators or two annihilation operators, i.e. terms of the form \( \hat{d}_k \hat{d}_{-k} \) and its hermitian conjugate).

(e) Show that this leads to the following condition on \( \theta_k \):
\[
\tan \theta_k = \frac{\gamma \sin k}{\lambda - \cos k}.
\] (21)

***

Two values of \( k \) are inequivalent if they do not differ by an integer multiple of \( 2\pi \).
Note that \( \cos^2 \theta_k = (1 + \tan^2 \theta_k)^{-1} = (\lambda - \cos k)^2/[\lambda - \cos k)^2 + \gamma^2 \sin^2 k] \) and that (21) leaves us with freedom to choose the sign of \( \cos \theta_k \). We will choose the sign such that

\[
\cos \theta_k = \frac{\lambda - \cos k}{\sqrt{\lambda - \cos k)^2 + \gamma^2 \sin^2 k}}.
\] (22)

(f) Using (21)-(22), show that the Hamiltonian is given on the diagonal form

\[
\hat{H} = \sum_k \varepsilon_k \hat{d}_k^\dagger \hat{d}_k + C
\] (23)

and give expressions for \( \varepsilon_k \geq 0 \) and \( C \).

(g) What is the ground state energy \( E_0(\gamma, \lambda) \) of the model?

***

The ground state of (23) can be written

\[
|G\rangle = \left( \prod_{k \geq 0} \hat{G}_k \right) |0\rangle,
\] (24)

where \(|0\rangle\) is the vacuum of the \( \hat{c}_k \)-operators (i.e. \( \hat{c}_k |0\rangle = 0 \) for all \( k \)).

(h) Show that the operator \( \hat{G}_k \) in (24) is, for \( k > 0 \), given by

\[
\hat{G}_k = \cos \frac{\theta_k}{2} + i \sin \frac{\theta_k}{2} \hat{c}_k^\dagger \hat{c}_k^\dagger.
\] (25)

(i) Let \( E_1(\gamma, \lambda) \) be the energy of the first excited state. Determine the region of parameter space \( (\gamma, \lambda) \) for which the excitation energy \( E_1(\gamma, \lambda) - E_0(\gamma, \lambda) = 0 \) (or approaches 0 in the thermodynamic limit \( N \to \infty \)).

**Some results that may be useful:**

\[
\hat{c}_j^2 = 0 = (\hat{c}_j^\dagger)^2,
\] (26)

\[
\hat{n}_j^2 = \hat{n}_j, \quad \text{(where } \hat{n}_j \equiv \hat{c}_j^\dagger \hat{c}_j \text{)}
\] (27)

\[
[\hat{n}_j, \hat{n}_j^\dagger] = 0,
\] (28)

\[
[\hat{n}_j, \hat{c}_{j'}] = -\delta_{j,j'} \hat{c}_j,
\] (29)

\[
[\hat{n}_j, \hat{c}_{j'}^\dagger] = \delta_{j,j'} \hat{c}_j^\dagger.
\] (30)

[Aside: While the first two lines here are only valid for fermions (being manifestations of fermionic anti-symmetry and the Pauli principle), the last three lines are valid also for bosons.]

If both \( k \) and \( k' \) are of the form (13) with \( n \) and \( n' \) taking values in the set (14), then

\[
\frac{1}{N} \sum_{j=1}^N e^{i(k \mp k')j} = \delta_{k,\pm k'}.
\] (31)