TFY4210 Quantum theory of many-particle systems, 2016: Tutorial 10

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

In this problem you will investigate a model with Hamiltonian

$$\hat{H}(\gamma,\lambda) = -\sum_j \left[\frac{1+\gamma}{2}\hat{\sigma}_j^x\hat{\sigma}_{j+1}^x + \frac{1-\gamma}{2}\hat{\sigma}_j^y\hat{\sigma}_{j+1}^y + \lambda\hat{\sigma}_j^z\right]. \tag{1}$$

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

$$\hat{\sigma}_j^\pm = \frac{1}{2}(\hat{\sigma}_j^x \pm i\hat{\sigma}_j^y), \tag{2}$$

in terms of which the Hamiltonian becomes (from now on I drop writing γ, λ as arguments of $\hat{H}$)

$$\hat{H} = -\sum_i \left[(\hat{\sigma}_i^+\hat{\sigma}_{i+1}^- + \hat{\sigma}_i^-\hat{\sigma}_{i+1}^+) + \gamma(\hat{\sigma}_i^+\hat{\sigma}_{i+1}^+ + \hat{\sigma}_i^-\hat{\sigma}_{i+1}^-) + \lambda\hat{\sigma}_i^z\right]. \tag{3}$$

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 anti-commutation relations

$$\{\hat{c}_j, \hat{c}_{j'}^\dagger\} = \delta_{j,j'}, \tag{4}$$

$$\{\hat{c}_j, \hat{c}_{j'}\} = \{\hat{c}_j^\dagger, \hat{c}_{j'}^\dagger\} = 0. \tag{5}$$

The spin operators can be expressed in terms of these fermion operators by a Jordan-Wigner transformation:

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

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

$$\hat{\sigma}_i^z = 1-2\hat{n}_i, \tag{8}$$

where $\hat{n}_j = \hat{c}_j^\dagger \hat{c}_j$. The relation (8) shows that the two possible eigenvalues ± 1 of $\hat{\sigma}_i^z$ 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 $\hat{\sigma}_i^+\hat{\sigma}_{i+1}^+$ appears in (3). Show that in terms of the fermions it becomes

$$\hat{\sigma}_i^+\hat{\sigma}_{i+1}^+ = \hat{c}_{i+1}\hat{c}_i. \tag{10}$$

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

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

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 $e^{ikN} = 1$, 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[2] values of the wavevectors k. Take N to be odd and the N values of n to be

$$n = -\frac{N-1}{2}, \ldots, -1, 0, 1, \ldots, \frac{N-1}{2}. \tag{14}$$

(c) Show that the Hamiltonian (11) becomes

$$\hat{H} = \sum_k [2(\lambda - \cos k)\hat{c}_k^\dagger \hat{c}_k + i\gamma \sin k(\hat{c}_{-k}\hat{c}_k + \hat{c}_{-k}^\dagger \hat{c}_k^\dagger) - \lambda]. \tag{15}$$

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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

$$\hat{d}_k = u_k \hat{c}_k - i v_k \hat{c}_{-k}^\dagger \tag{16}$$

and $\hat{d}_k^\dagger \equiv (\hat{d}_k)^\dagger$, where

$$u_k = \cos\frac{\theta_k}{2}, \quad v_k = \sin\frac{\theta_k}{2}, \tag{17}$$

where the real parameter (angle) θ_k is so far unspecified, except that we take

$$\theta_{-k} = -\theta_k \quad \Rightarrow \quad u_{-k} = u_k, \quad v_{-k} = -v_k. \tag{18}$$

This implies that the $\hat{d}_k$-operators satisfy standard fermionic anticommutation relations just like the $\hat{c}_k$ operators, i.e.

$$\{\hat{d}_k, \hat{d}_{k'}\} = 0, \quad \{\hat{d}_k, \hat{d}_{k'}^\dagger\} = \delta_{k,k'}. \tag{19}$$

(d) Show that the inverse transformation of (16) is

$$\hat{c}_k = u_k \hat{d}_k + i v_k \hat{d}_{-k}^\dagger. \tag{20}$$

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We will choose the parameter θ_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 θ_k:

$$\tan\theta_k = \frac{\gamma \sin k}{\lambda - \cos k}. \tag{21}$$

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[2] Two values of k are inequivalent if they do not differ by an integer multiple of 2π.

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

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

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

$$\hat{H} = \sum_k \varepsilon_k \hat{d}_k^\dagger \hat{d}_k + C \tag{23}$$

and give expressions for $\varepsilon_k \geq 0$ and C.

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

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The ground state of (23) can be written

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

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

$$\hat{G}_k = \cos\frac{\theta_k}{2} + i\sin\frac{\theta_k}{2}\hat{c}_k^\dagger\hat{c}_{-k}^\dagger. \tag{25}$$

(i) Let $E_1(\gamma,\lambda)$ be the energy of the first excited state. Determine the region of parameter space (γ,λ) 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:

$$\begin{aligned}
\hat{c}_j^2 &= 0 = (\hat{c}_j^\dagger)^2, && (26)\\
\hat{n}_j^2 &= \hat{n}_j, \quad (\text{where } \hat{n}_j \equiv \hat{c}_j^\dagger\hat{c}_j) && (27)\\
[\hat{n}_j,\hat{n}_{j'}] &= 0, && (28)\\
[\hat{n}_j,\hat{c}_{j'}] &= -\delta_{j,j'}\hat{c}_j, && (29)\\
[\hat{n}_j,\hat{c}_{j'}^\dagger] &= \delta_{j,j'}\hat{c}_j^\dagger. && (30)
\end{aligned}$$

[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

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