Summer Project on Condensed Matter Physics - IISc, Bangalore 2023

Lecture 9: Some Analytical Calculations

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In this lecture, some analystical calculations were done to show the correspondence/mapping in 1-D between spin-1/2 systems and fermions ↔ bosons.

1 Spin Chain

At site n,

$$\vec{s}_n = \left(\frac{\hbar}{2}\sigma_n^x, \frac{\hbar}{2}\sigma_n^y, \frac{\hbar}{2}\sigma_n^z\right) \tag{1}$$

At any site, the anticommutator and commutator relations are:

$$\{\sigma_n^x, \sigma_n^y\} = 0$$
$$[\sigma_n^x, \sigma_n^y] = i2\hbar\sigma_n^z$$
$$[S_n^x, S_n^y] = i\hbar S_n^z$$

At different sites,

$$[S_n^x, S_m^y] = \delta_{nm} i\hbar S_n^z$$

At different sites, the operators commute, and is boson-like. At a particular site, the operators are fermion-like.
Recall:
Bosonic operators: $b_n, b_n^\dagger$

$$[b_n, b_m^\dagger] = \delta_{nm}$$
$$[b_n, b_m] = 0$$
$$[b_n^\dagger, b_m^\dagger] = 0$$

Fermionic operators: $c_n, c_n^\dagger$

$$\{c_n, c_m^\dagger\} = \delta_{nm}$$
$$\{c_n, c_m\} = 0$$
$$\{c_n^\dagger, c_m^\dagger\} = 0$$

Let's look at the Hamiltonian:

$$H = J\sum_{n}(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + S_n^z S_{n+1}^z) \tag{2}$$

$(J > 0) \rightarrow$ isotropic anti-ferromagnetic chain

Think of $H = J\sum_n \vec{s}_n \cdot \vec{s}_{n+1}$
Minimum energy configuration is : $\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow$; called Neel configuration, with no net magnetization.
Consider $H = -J\sum_n \vec{s}_n \cdot \vec{s}_{n+1}$
Minimum energy configuration is : $\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow$; called isotropic ferromagnetic chain, with net magnetization.
There are different magnetic materials depending upon the orientations of the spins and teh relative strength of magnetic moments of the spins:

- Ferromagnetic
- Antiferromagnetic
- Ferrimagnetic
- Paramagnetic

Consider again:

$$\begin{aligned} H &= -J\sum_{n} \vec{s}_n \cdot \vec{s}_{n+1} \\ &= -J\sum_{n=1}^{L}[S_n^z S_{n+1}^z + \frac{1}{2}(S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+)] \end{aligned}$$

Try the ansatz: $|\psi\rangle = |\uparrow\uparrow\uparrow\uparrow\rangle$
Then, $H|\psi\rangle = -J\frac{L\hbar^2}{4}|\psi\rangle$
This is the ground state of the system, It is not unique. $\rightarrow L+1$ degenerate ground states.

But now consider,

$$H == J\sum_{n=1}^{L}[S_n^z S_{n+1}^z + \frac{1}{2}(S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+)]$$

Try the Neel state: $|\psi\rangle = |\uparrow\downarrow\uparrow\downarrow\rangle$
Then, $H|\psi\rangle = -J\frac{L\hbar^2}{4}|\psi\rangle +$ other states
Just finding the ground state is a hard problem. $\rightarrow$ Solved by Hans Bethe (1931 - Bethe ansatz)

We will try to solve the case for which there is no z-z coupling.

2 X-Y Model

$$H = J\sum_{n=1}^{L}(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y) \tag{3}$$

Note that here the sign of J is not important as we can flip the sign by a unitary transformation. Keep in mind that the following state: →←→←→←→←→← is not an eigenstate. TO find the ground state, we will need to something called the Jordan-Wigner transformation.

2.1 Jordan-Wigner Transformation

From spin-1/2 system, we need to go to spinless fermions. The fermionic operators will be as described before.
Mapping:

$$\begin{array}{ccccc} S_n^z & & & & c_n^\dagger c_n \\ \frac{\hbar}{2} & |\uparrow\rangle_n & \leftrightarrow & |1\rangle_n & 1 \\ -\frac{\hbar}{2} & |\downarrow\rangle_n & \leftrightarrow & |0\rangle_n & 0 \end{array}$$

The mapping between the operators is:

$$S_n^z = \hbar(c_n^\dagger c_n + 1/2) \tag{4}$$

$$\begin{aligned} S_n^+ &= S_n^x + iS_n^y \\ &= \frac{\hbar}{2}(\sigma^x + i\sigma^y) \\ &= \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \end{aligned}$$

Now the question is do the S_n^+ and S_n^- map directly to the $c_n^\dagger$ and c_n operators.

$$\begin{aligned} S_n^+ &\stackrel{?}{=} \hbar c_n^\dagger \\ S_n^- &\stackrel{?}{=} \hbar c_n \end{aligned}$$

The operators S_n^+ and S_n^- satisfy commutation relations at different n. The operators $c_n^\dagger$ and c_n satisfy anticommutation relations.
We know:

$$\sigma_n^z = \begin{pmatrix} 1 & 0 \\ - & -1 \end{pmatrix}$$

And,

$$\begin{aligned} \sigma_n^z\sigma_n^x &= -\sigma_n^x\sigma_n^z \\ \sigma_n^z\sigma_n^y &= -\sigma_n^y\sigma_n^z \end{aligned}$$

Taking $\hbar = 1$, we can take the fermionic operators to be a string of σ operators.

$$c_n^\dagger = S_n^+ \prod_{j=-\infty}^{n-1} \sigma_j^z \tag{5}$$

$$c_n = S_n^- \prod_{j=-\infty}^{n-1} \sigma_j^z \tag{6}$$

Doing so, we can have c_m and c_n satisfy teh correct antimmutation relations.
→But why is $\{c_m, c_n\} = 0$?
For $m = n$, $c_n^2 = 0$
$\implies c_n^2 = (S_n^-)^2 = 0$, since $S_n^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$
Next, $c_n c_m = -c_m c_n$ if $n \neq m$

The σ_j^z's for $j = -\infty$ to $m-1$ cancel since $(\sigma_j^z)^2 = 1$

$$\implies c_n = \sigma_m^z \sigma_{m+1}^z ......\sigma_{n-1}^z S_n^-$$
$$c_m = S_m^-$$

$\because \sigma_m^z$ anticommutes with $S_m^- \implies c_n$ and c_m anticommute if $m \neq n$
$\implies c_n^\dagger$ anticommutes with $c_m^\dagger$ by just taking Hermitian conjugate.

Next up: $\{c_n, c_m^\dagger\} = \delta_{mn}$
For $m = n$: $\{c_n, c_n^\dagger\} = 1$
So, $c_n c_n^\dagger + c_n^\dagger c_n = S_n^- S_n^+ + S_n^+ S_b^- = 1$ since,

$$S_n^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, S_n^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

The $m \neq n$ case follows as before.

Now we can inverse the relation and write:

$$S_n^+ = c_n^\dagger \prod_{j=-\infty}^{n-1} \sigma_j^z \tag{7}$$

$$S_n^- = c_n \prod_{j=-\infty}^{n-1} \sigma_j^z \tag{8}$$

and,

$$\sigma_j^z = 2(c_n^\dagger c_n - 1/2) \tag{9}$$

Then,

$$H = J\sum_{n=1}^{L}(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y) \tag{10}$$

$$= \frac{J}{2}\sum_n (S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+) \tag{11}$$

Using the same logic as before, we get:

$$S_n^+ \simeq c_n^\dagger \tag{12}$$

$$S_{n+1}^- \simeq \sigma_{n+1}^z c_{n+1} \tag{13}$$

Then, we can write:

$$H = \frac{J}{2}\sum_n [c_n^\dagger \sigma_n^z c_{n+1} + h.c.] \tag{14}$$

Consider the foloowing:

$$S_n^+\sigma_n^z \left|\uparrow\right\rangle_n = 0$$
$$S_n^+\sigma_n^z \left|\downarrow\right\rangle_n = -\left|\downarrow\right\rangle_n$$

And claiming that: $S_n^+\sigma_n^z = -S_n^+$,

$$c_n^\dagger \sigma_n^z = -c_n^\dagger \tag{15}$$

$$\therefore H = -\frac{J}{2}\sum_n (c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n) \tag{16}$$

This completes the Jordan-Wigner transformation. The X-Y model has been converted into a tight-binding Hamiltonian of spinless fermions.

Note: This trick will only work for 10D because in 2-D, it will be difficult to come up with the string of σ's when defining S_n^+ in terms of $c_n^\dagger$.

Now to solve for the energies, we will go to Fourier space:

$$c_k = \frac{1}{\sqrt{L}}\sum_n c_n e^{ikn} \tag{17}$$

$$c_n = \frac{1}{\sqrt{L}}\sum_k c_k e^{-ikn} \tag{18}$$

$$c_k^\dagger = \frac{1}{\sqrt{L}}\sum_n c_n^\dagger e^{ikn} \tag{19}$$

$$c_n^\dagger = \frac{1}{\sqrt{L}}\sum_k c_k^\dagger e^{-ikn} \tag{20}$$

Then, the Hamiltonian becomes,

$$H = \sum_k E_k c_k^\dagger c_k \tag{21}$$

where,

$$E_k = -Jcos(k) \tag{22}$$

Particles can be added to the bands by adding a chemical potential in the Hamiltonian.

$$H = \frac{J}{2}\sum_n (c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n) - \mu \sum_n c_n^\dagger c_n \tag{23}$$

$$\implies H = J\sum_n (S_n^x S_{n+1}^x + S_n^y S_{n+1}^y) - \mu \sum_n \left(S_n^z + \frac{1}{2}\right) \tag{24}$$

Here, the chemical potential μ acts like a magnetic field in the z direction.

3 Correlation Functions

3.1 Two-point Correlation Functions

Let us calculate the following quantity:

$$\langle GS| S_n^z S_m^z |GS\rangle = \langle GS| (c_n^\dagger c_n + 1/2)(c_m^\dagger c_m + 1/2) |GS\rangle \tag{25}$$

With no cross terms:

$$\langle GS| c^\dagger c_n |GS\rangle = \frac{1}{L}\sum_{k_1,k_2} \langle GS| c_{k_1}^\dagger c_{k_2} |GS\rangle e^{i(k_1-k_2)n} \tag{26}$$

$$\left(\text{To get non-zero terms: } -\frac{\pi}{2} < k_1 = k_2 < \frac{\pi}{2}\right) = \frac{1}{L}\sum_k^{L/2} = \frac{1}{2} \tag{27}$$

$$\implies \langle GS| c_m^\dagger c_m |GS\rangle = \frac{1}{2} \tag{28}$$

Then cross terms:

$$\langle GS| c_n^\dagger c_n c_m^\dagger c_m |GS\rangle = \frac{1}{L^2}\sum_{k_1,k_2,k_3,k_4} \langle GS| c_{k_1}^\dagger c_{k_2} c_{k_3}^\dagger c_{k_4} |GS\rangle e^{i(-k_1 n + k_2 n - k_3 m + k_4 m)} \tag{29}$$

$c_{k_4} |GS\rangle$ →annihilates k_4 if $-\frac{\pi}{4} < k_4 < \frac{\pi}{4}$
$c_{k_3}^\dagger c_{k_4} |GS\rangle$ →annihilates k_4 if $-\frac{\pi}{4} < k_4 < \frac{\pi}{4}$ and either creates that particle back ($k_3 = k_4$) or creates a new particle ($k_3 \neq k_4$) if $\frac{\pi}{2} < k_3 < \frac{3\pi}{2}$

Wick Contraction:

- $$k_3 = k_4$$
  $$k_1 = k_2$$
  $$\rightarrow \left(\frac{L}{2}\right)^2 = \frac{1}{4}$$
- $$k_3 \neq k_4$$
  $$k_1 \neq k_2$$
  $$k_1 = k_4$$
  $$k_2 = k_3$$

$$\langle GS| c_{k_1}^\dagger c_{k_2} c_{k_3}^\dagger c_{k_4} |GS\rangle = \langle GS| c_{k_2} c_{k_3}^\dagger c_{k_1}^\dagger c_{k_4} |GS\rangle \tag{30}$$

Phases: $e^{i(-k_1 n + k_1 m + k_2 n - k_2 m)}$

$$\sum_{-\pi/2<k_1<\pi/2} = \int_{-\pi/2}^{\pi/2} \frac{dk_1}{\frac{2\pi}{L}}$$

$$\begin{aligned}
\therefore \langle GS| S_n^z S_m^z |GS\rangle &= \frac{1}{L^2}\int_{-\pi/2}^{\pi/2} \frac{dk_1}{\frac{2\pi}{L}} \int_{\pi/2}^{3\pi/2} \frac{dk_2}{\frac{2\pi}{L}} e^{-i(k_1-k_2)(n-m)} && (31)\\
&= \int_{-\pi/2}^{\pi/2} \frac{dk_1}{2\pi} e^{-ik_1(n-m)} \int_{\pi/2}^{3\pi/2} \frac{dk_2}{2\pi} e^{-ik_2(n-m)} && (32)\\
&= \frac{1}{4\pi^2}\left(\frac{1}{-i(n-m)}[e^{ik_1(n-m)}]_{-\pi/2}^{\pi/2}\right)\left(\frac{1}{i(n-m)}[e^{ik_2(n-m)}]_{-\pi/2}^{\pi/2}\right) && (33)\\
&= \frac{1}{4\pi^2(n-m)^2}\left(-\left(e^{-i\frac{\pi}{2}(n-m)} - e^{i\frac{\pi}{2}(n-m)}\right)\right)\left(e^{i\frac{3\pi}{2}(n-m)} - e^{i\frac{\pi}{2}(n-m)}\right) && (34)\\
&= \frac{1}{4\pi^2(n-m)^2}(-2i)\sin\left(\frac{\pi}{2}(n-m)\right) e^{i\pi(n-m)}(2i)\sin\left(\frac{\pi}{2}(n-m)\right) && (35)\\
&= \frac{1}{\pi^2(n-m)^2}\sin^2\left(\frac{\pi}{2}(n-m)\right) e^{i\pi(n-m)} && (36)\\
&= 0, \text{ if } m-n = \text{even} && (37)\\
&= -\frac{1}{\pi^2(n-m)^2}, \text{ if } m-n = \text{odd} && (38)
\end{aligned}$$

In conclusion,

- gapless system :

$$\left\langle \vec{S_n} \cdot \vec{S_m} \right\rangle \sim \frac{1}{|m-n|^{power}}$$

- gapped system:

$$\left\langle \vec{S_n} \cdot \vec{S_m} \right\rangle \sim e^{-|m-n|/\xi}$$

3.2 A "cute" result

$$\sum_m \langle GS| S_n^z S_m^z |GS\rangle = \langle GS| S_n^z \sum_m S_m^z |GS\rangle \tag{39}$$

Here, $\sum_m S_m^z = \sum_m (c_m^\dagger c_m - 1/2) = \sum_m c_m^\dagger c_m - L/2$ Then,

$$\sum_m \langle GS| S_n^z S_m^z |GS\rangle = \frac{1}{4} - \frac{2}{\pi^2}\left(\frac{1}{1^2} + \frac{1}{3^2} + \frac{1}{5^2} + ...\right) \tag{40}$$

$$= 0 \tag{41}$$