Second quantization - additional examples

In these notes we continue to explore the physics of Hamiltonians written in the language of 2^{nd} quantization. To begin, let us explore a bit more the double well problem for Bosons. In particular, I want to look at it from a dynamical point of view.

The Hamiltonian is

$$H = \sum_{i=L,R} \left\{ \epsilon a_i^\dagger a_i + \frac{U}{2} a_i^\dagger a_i (a_i^\dagger a_i - 1) \right\} + J (a_L^\dagger a_R + a_R^\dagger a_L) \tag{1}$$

And what I want to do is solve Schrödinger's equation

$$i \partial_t |\psi\rangle = H |\psi\rangle \tag{2}$$

We can expand $|\psi\rangle$ in the Fock basis

$$|\psi_t\rangle = \sum_{n_L, n_R = 0}^{\infty} \psi_t(n_L, n_R) \, |n_L, n_R\rangle \tag{3}$$

But a state like this is a superposition of states with different numbers of particles. Which seems a bit strange. Instead, it is more natural to have a situation where the number of particles is well defined. This is where particle conservation comes in. If we start with N particles at t=0, we will continue to have N particles for all further times.

So, for instance, let us assume that we have only $N=2$ particles. Then there are only 3 Fock states: $|2,0\rangle$, $|1,1\rangle$, $|0,2\rangle$. Thus, any $|\psi_t\rangle$ may be parametrized as

$$|\psi_t\rangle = \psi_+(t)|2,0\rangle + \psi_0(t)|1,1\rangle + \psi_-(t)|0,2\rangle \qquad (4)$$

where, for simplicity, I'm writting $\psi_+ = \psi(2,0)$ and so on.

Now let's see how H in Eq (1) acts on these 3 Fock states.

Note that

$$\begin{aligned}
(a_L^\dagger a_R + a_R^\dagger a_L)|2,0\rangle &= \sqrt{2}\,|1,1\rangle \\
(a_L^\dagger a_R + a_R^\dagger a_L)|1,1\rangle &= \sqrt{2}\,|2,0\rangle + \sqrt{2}\,|0,2\rangle \qquad (5)\\
(a_L^\dagger a_R + a_R^\dagger a_L)|0,2\rangle &= \sqrt{2}\,|1,1\rangle
\end{aligned}$$

Thus

$$H|2,0\rangle = (2\epsilon + U)|2,0\rangle + \sqrt{2}\,J\,|1,1\rangle \qquad (6a)$$

$$H|1,1\rangle = 2\epsilon\,|1,1\rangle + \sqrt{2}\,J\,|2,0\rangle + \sqrt{2}\,J\,|0,2\rangle \qquad (6b)$$

$$H|0,2\rangle = (2\epsilon + U)|0,2\rangle + \sqrt{2}\,J\,|1,1\rangle \qquad (6c)$$

From this we then reconstruct the Hamiltonian matrix in the $N=2$ subspace. For instance, from (6a) we find that

$$\langle 2,0|H|2,0\rangle = 2\epsilon + U$$

$$\langle 1,1|H|2,0\rangle = \sqrt{2}\,J$$

$$\langle 0,2|H|2,0\rangle = 0$$

this represents the first column of the matrix.

We then get

$$H_2 = \begin{pmatrix} 2\epsilon + U & \sqrt{2}\,J & 0 \\ \sqrt{2}\,J & 2\epsilon & \sqrt{2}\,J \\ 0 & \sqrt{2}\,J & 2\epsilon + U \end{pmatrix} \qquad (7)$$

within this $N=2$ subspace, the state (4) will thus evolve according to

$$i\frac{d}{dt}\begin{pmatrix} \psi_+ \\ \psi_0 \\ \psi_- \end{pmatrix} = H_2 \begin{pmatrix} \psi_+ \\ \psi_0 \\ \psi_- \end{pmatrix} \qquad (8)$$

the important conclusion that I want you to take from this is that if we start in the subspace $\{|2,0\rangle, |1,1\rangle, |0,2\rangle\}$ we continue in this sub-space throughout.

From now on I will set $\epsilon = 0$ in Eq (7), since energy is defined only up to a constant. I will also, for simplicity, define

$$\alpha = 4J \qquad (9)$$

Then (7) becomes

$$H_2 = \begin{pmatrix} U & \alpha/2\sqrt{2} & 0 \\ \alpha/2\sqrt{2} & 0 & \alpha/2\sqrt{2} \\ 0 & \alpha/2\sqrt{2} & U \end{pmatrix} \qquad (10)$$

the eigenvalues of H_2 are then

$$\lambda_+ = \frac{1}{2}\left(U + \sqrt{U^2 + \alpha^2}\right) \tag{11a}$$

$$\lambda_0 = U \tag{11b}$$

$$\lambda_- = \frac{1}{2}\left(U - \sqrt{U^2 + \alpha^2}\right) \tag{11c}$$

the ground-state is always λ_-.

As for the matrix of eigenvectors, with some fooling on Mathematica one may show that we can write

$$S = \begin{pmatrix} -\frac{\cos\theta}{\sqrt{2}} & 1/\sqrt{2} & \frac{\sin\theta}{\sqrt{2}} \\ \sin\theta & 0 & \cos\theta \\ -\frac{\cos\theta}{\sqrt{2}} & -1/\sqrt{2} & \frac{\sin\theta}{\sqrt{2}} \end{pmatrix} \tag{12}$$

where

$$\tan(2\theta) = -\frac{\alpha}{U} \tag{13}$$

We then get

$$H_2 = S \Lambda S^\dagger \tag{14}$$

$$\Lambda = \mathrm{diag}\,(\lambda_+, \lambda_0, \lambda_-)$$

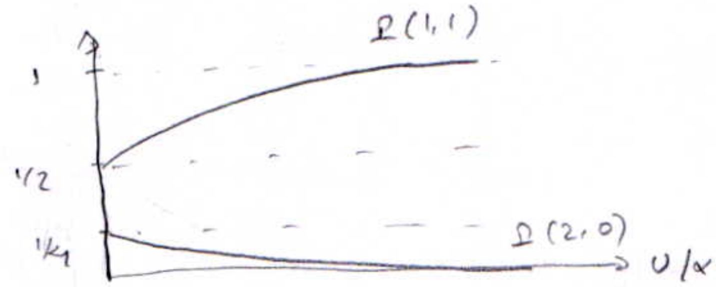
It is interesting to analyze these eigenvectors. In particular the ground state λ_-. the corresponding eigenvector is

$$\vec{v}_- = \begin{pmatrix} \sin\theta/\sqrt{2} \\ \cos\theta \\ \sin\theta/\sqrt{2} \end{pmatrix} \tag{15}$$

we can then analyze the probabilities of finding the system in $|2,0\rangle$, $|1,1\rangle$, $|0,2\rangle$, given it is in the GS:

$$P(2,0) = P(0,2) = \frac{\sin^2\theta}{2} \qquad P(1,1) = \cos^2\theta \tag{16}$$

If we plot these guys as a function of U/α, we get



Remember that U has the tendency of localizing the wavefunction. If $U=0$ we see that $P(2,0) = 1/4$ and $P(1,1) = 1/2$. the state is highly delocalized. conversely, as U becomes large, $P(1,1)$ becomes dominant. Large U penalizes tunneling, forcing the particles to stay each in its own site.

Finally, we can study the dynamics of Eq (8). We simply need to write

$$e^{-iH_2 t} = S\, e^{-i\Lambda t}\, S^{+} \tag{17}$$

For instance, suppose that at $t=0$ the system was prepared on $|1,1\rangle$. That is

$$|\psi_0\rangle = |1,1\rangle .$$

then at time t we will have

$$\psi_+(t) = \psi_-(t) = \frac{\sin 2\theta}{2\sqrt{2}}\left(e^{-i\lambda_- t} - e^{-i\lambda_+ t}\right) \tag{18}$$

$$\psi_0(t) = e^{-i\lambda_- t}\cos^2\theta + e^{-i\lambda_+ t}\sin^2\theta \tag{19}$$

Let

$$\Omega = \frac{1}{2}\sqrt{U^2+\alpha^2}$$

Then

$$\psi_\pm(t) = \frac{\sin 2\theta}{2\sqrt{2}}\, e^{-iUt}\left(e^{i\Omega t} - e^{-i\Omega t}\right)$$

$$= \frac{e^{-iUt}}{\sqrt{2}}\, \frac{(-\alpha)}{\sqrt{U^2+\alpha^2}}\, i \sin\Omega t$$

Thus, the probabilities becomes

$$\boxed{|\psi_\pm|^2 = \frac{1}{2}\,\frac{\alpha^2}{U^2+\alpha^2}\,\sin^2 \Omega t} \qquad (20)$$

Sanity check: if $\alpha = 0$ we get $\psi_\pm = 0$ because then there can be no tunneling.

We can also do another cool thing, which is to look at the reduced density matrix of the left site. Yes, everything we learned about density matrices, entanglement, and so on, continues to hold in this case.

So, we start with a general state like (4) and compute.

$$\begin{aligned}
\rho = |\psi\rangle\langle\psi| = {} & |\psi_+|^2\,|2,0\rangle\langle 2,0| + \psi_+\psi_0^*\,|2,0\rangle\langle 1,1| + \psi_+\psi_-^*\,|2,0\rangle\langle 0,2| \\
& + \psi_0\psi_+^*\,|1,1\rangle\langle 2,0| + |\psi_0|^2\,|1,1\rangle\langle 1,1| + \psi_0\psi_-^*\,|1,1\rangle\langle 0,2| \\
& + \psi_-\psi_+^*\,|0,2\rangle\langle 2,0| + \psi_-\psi_0^*\,|0,2\rangle\langle 2,0| + |\psi_-|^2\,|0,2\rangle\langle 0,2|
\end{aligned}$$

Now we take the partial trace, for instance over R. We then get terms like

$$\begin{aligned}
\mathrm{tr}_R\, |2,0\rangle\langle 2,0| &= |2\rangle\langle 2|\, \mathrm{tr}\,(|0\rangle\langle 0|) \\
&= |2\rangle\langle 2|
\end{aligned}$$

and

$$\begin{aligned}
\mathrm{tr}_R\, |2,0\rangle\langle 1,1| &= |2\rangle\langle 1|\, \mathrm{tr}\,(|0\rangle\langle 1|) \\
&= 0
\end{aligned}$$

Thus

$$\rho_L = |\psi_+|^2 |2\rangle\langle 2| + |\psi_0|^2 |1\rangle\langle 1| + |\psi_-|^2 |0\rangle\langle 0| \qquad (21)$$

the state of L is now in general mixed, so L and R are entangled. We can quantify the entanglement using the purity

$$\mathcal{P} = \mathrm{tr}\,\rho_L^2 = |\psi_+|^4 + |\psi_0|^4 + |\psi_-|^4 \qquad (22)$$

Using (20) and writing $q = |\psi_+|^2 = |\psi_-|^2$, we get

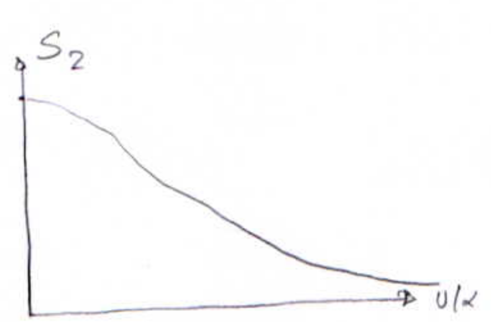
$$\mathcal{P} = q^2 + q^2 + (1-2q)^2$$

$$= 1 - 4q + 6q^2$$

$$q = \frac{1}{2}\frac{\alpha^2}{U^2+\alpha^2}\sin^2\Omega t.$$

If we plot this, for instance, for $\sin^2\Omega t = 1/2$, we get something like

It is common to plot the Rényi-2 entropy, $S_2 = -\ln \mathcal{P}$. It would then look like



The tight-binding model

Ok. Warm-up phase is over. Now let's talk about the real deal. This next section is extremely important. We are going to talk about how to deal with quadratic Hamiltonians. That is, Hamiltonians containing only products of two operators. For instance, in the case of bosons we could have something like

$$H = \sum_{ij} w_{ij} a_i^\dagger a_j \tag{23}$$

where w_{ij} are a set of coefficients. This is not the most general quadratic Hamiltonian. We could also have something like $a_i^\dagger a_j^\dagger + a_i a_j$. But we will not look into these right now.

To have a concrete example in mind, we can talk about a lattice containing only kinetic terms. Assuming for now we are in 1D, we get

The Hamiltonian would then read

$$H = \sum_{i=1}^{L} \epsilon\, a_i^\dagger a_i - J \sum_{i=1}^{L-1} (a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i) \tag{24}$$

This is called the tight-binding model

By inspection, we can read off what should the matrix W in (23) should be for the Hamiltonian (24); e.g for $L=5$,

$$W = \begin{pmatrix} \epsilon & -J & 0 & 0 & 0 \\ -J & \epsilon & -J & 0 & 0 \\ 0 & -J & \epsilon & -J & 0 \\ 0 & 0 & -J & \epsilon & -J \\ 0 & 0 & 0 & -J & \epsilon \end{pmatrix} \tag{25}$$

this should now start to remind you of our discussion about phonons. The idea is quite similar, except that there we had (q,p) and here we have $(a,a^\dagger)$.

Before we get our hands dirty, let me just mention that this same problem also holds for Fermions. that is, we could consider a quadratic fermionic Hamiltonian of the form

$$H = \sum_{ij\sigma,\sigma'} W_{ij}^{\sigma\sigma'} c_{i\sigma}^{\dagger} c_{j\sigma'} \tag{26}$$

Now the coefficients W also have a spin index (the internal structure). the tight-binding model (24) would then read

$$H = \sum_{\sigma,i=1}^{L} \epsilon_\sigma c_{i\sigma}^{\dagger} c_{i\sigma} - J \sum_{\sigma,i=1}^{L-1} (c_{i\sigma}^{\dagger} c_{i+1,\sigma} + c_{i+1,\sigma}^{\dagger} c_{i\sigma}) \tag{27}$$

Here I am assuming the hopping J is spin independent, which is a reasonable assumption. You then see that we have essentially two independent tight-binding models, one for each σ.