Phys 506 lecture 31: Ion traps and quantum simulation

1 Trapped ion Hamiltonian

Ions are trapped in a linear Paul trap via harmonic confinement plus Coulomb repulsion:

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \sum_{i>j}^{N} \frac{e^2}{|\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j|} + \sum_{i=1}^{N} \left(\frac{1}{2} m\omega_x^2 \hat{r}_{ix}^2 + \frac{1}{2} m\omega_y^2 \hat{r}_{iy}^2 + \frac{1}{2} m\omega_z^2 \hat{r}_{iz}^2 \right)$$

Use classical mechanics to solve for equilibrium positions and for harmonic deviations about equilibrium to find

$$\hat{H} = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i,j=1}^{N} \left(\frac{1}{2} r_{ix} K_{ij}^x r_{jx} + \frac{1}{2} r_{iy} K_{ij}^y r_{jy} + \frac{1}{2} r_{iz} K_{ij}^z r_{jz} \right)$$

where K_{ij} is the spring constant matrix. Introduce normal modes b_i^α which are eigenvectors of the K matrices.

$$\sum_j K_{ij}^x b_j = k_\alpha^x b_i$$

and similarly for y and z. Define frequencies via

$$\omega_\alpha^x = \sqrt{\frac{k_\alpha^x}{m}}$$

and similarly for y and z. Then, the quantized phonon Hamiltonian is

$$H_{\text{phonon}} = \sum_{i=x,y,z} \sum_{\alpha=1}^{N} \hbar\omega_\alpha^j \left(\hat{a}_{\alpha,j}^\dagger \hat{a}_{\alpha,j} + \frac{1}{2} \right),$$

where $a_{\alpha,j}$ is the phonon destruction operator in the αth normal mode in the j-direction.

2 Example: Three site chain

The transverse normal modes are

1. (Center of Mass) $\mathbf{b}^{com} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 & 1 \end{pmatrix}$
2. (Tilt) $\mathbf{b}^{tilt} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & -1 \end{pmatrix}$
3. (Zig Zag) $\mathbf{b}^{zigzag} = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 & -2 & 1 \end{pmatrix}$

In general, we have N phonon modes for each direction. Each ion has a complicated level structure. For the Yb+ ion, we shine two lasers detuned from from the excited state but with a high enough power to drive transitions from the up state to the down state.

This looks like a $(\sigma_+ + \sigma_-)$ interaction since the spins flip periodically with period Ω_j given by the Rabi frequency. But $\sigma_+ + \sigma_- \propto \sigma_x$. So we have found a σ_x operation on our ions.

The ions also couple to the spatial profile of the laser beam. Because we have two beams at different frequencies and different k-vectors, we find the laser ion interaction is

$$\hat{H}_{\text{laser-ion}} = -\sum_{j=1}^{N} \hbar\Omega_j (\delta\mathbf{k}\cdot\delta\hat{\mathbf{R}}_j)\sigma_j^x \sin\mu t$$

where Ω_j is the Rabi frequency, $\delta\mathbf{k}$ is the difference in the wavevectors of the lasers, $\delta\hat{\mathbf{R}}_j$ is the position of the jth ion relative to equilibrium, and σ_j^x is the Pauli spin matrix at the jth location. We write

$$\delta\hat{\mathbf{R}}_j = \sum_{\alpha=1}^{N} b_j^{\alpha x}\sqrt{\frac{\hbar}{2m\omega_\alpha}}(\hat{a}_\alpha^{\dagger,x} + \hat{a}_\alpha^x) + y \text{ and } z \text{ terms.}$$

For experiments $\delta\mathbf{k}$ is in the x-direction only, so we get

$$\hat{H} = \sum_{\alpha=1}^{N} \hbar\omega_\alpha\left(\hat{a}_\alpha^\dagger\hat{a}_\alpha + \frac{1}{2}\right) - \sum_{j=1}^{N}\hbar\Omega_j\delta k\sum_{\alpha=1}^{N}\sqrt{\frac{\hbar}{2m\omega_\alpha}}(\hat{a}_\alpha^\dagger + \hat{a}_\alpha)b_j^\alpha\sigma_j^x\sin\mu t.$$

Notice that this is of the form $\hat{H} = \hat{H}_0 + \hat{V}(t)$. Go to the interaction representation and note

$$e^{\frac{i}{\hbar}\hat{H}_0 t}a_\alpha^\dagger e^{-\frac{i}{\hbar}\hat{H}_0 t} = e^{i\omega_\alpha t}\hat{a}_\alpha^\dagger$$
$$e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{a}_\alpha e^{-\frac{i}{\hbar}\hat{H}_0 t} = e^{-i\omega_\alpha t}\hat{a}_\alpha.$$

We need to add a transverse magnetic field as well

$$\hat{H}_B(t) = \sum_{j=1}^{N} B(t)\sigma_j^y,$$

which will be our control parameter for quantum simulation.

3 Adiabatic quantum simulation

Start system polarized along the y-direction with $B(t{=}0)$ large. Turn the laser-ion interaction on and ramp the B field slowly to zero.

The system evolves from a state polarized along the y-axis to the ground state of the system in no artificial magnetic field.

The evolution operator in the interaction representation can be written as

$$\hat{U}(t) = e^{-i\hat{H}_{\text{phonon}}t}T\exp\left(-\frac{i}{\hbar}\int_0^t\left(\hat{V}_I(t') + \hat{H}_B(t')\right)\,dt'\right),$$

where

$$\hat{V}_I(t) = -\sum_{j=1}^{N}\sum_{\alpha=1}^{N}\hbar\Omega_j\delta_k\sqrt{\frac{\hbar}{2m\omega_\alpha}}b_j^\alpha(\hat{a}_\alpha^\dagger e^{i\omega_\alpha t} + \hat{a}_\alpha e^{-i\omega_\alpha t})\sigma_j^x\sin\mu t.$$

Note that

$$[\hat{V}_I(t), \hat{V}_I(t')] = -\sum_{j=1}^{N}\sum_{\alpha=1}^{N} \frac{\hbar^2\Omega_j^2\delta k^2\hbar}{2m\omega_\alpha} b_j^\alpha b_i^\alpha \sigma_j^\alpha \sigma_i^\alpha \left(-e^{i\omega_\alpha(t-t')} + e^{-i\omega_\alpha(t-t')}\right)\sin\mu t \sin\mu t'$$

$$= -\sum_{i,j=1}^{N}\sum_{\alpha=1}^{N} \frac{\hbar^3\Omega_j^2\delta k^2}{2m\omega_\alpha} b_i^\alpha b_j^\alpha(-2i\sin\omega_\alpha(t-t'))\sigma_j^\alpha\sigma_i^\alpha \sin\mu t\sin\mu t'.$$

But, this commutator commutes with everything else except for the $\hat{H}_B(t)$ term.

If we assume $\int_0^t B(t')\, dt' \ll 1$ then any terms coming from commutators of $\hat{H}_B(t)$ are small because the term in front is small. So we proceed as before—define

$$\hat{W}_I(t) = \int_0^t \hat{V}_I(t')\, dt'$$

and we find

$$\hat{U}(t) = e^{-\frac{i}{\hbar}\hat{H}_{\text{phonon}}t} e^{-\frac{i}{\hbar}\hat{W}_I(t)}\hat{U}_{\text{spin}}(t)$$

where

$$\hat{U}_{\text{spin}}(t) = T\exp\left(-\frac{i}{\hbar}\int_0^t dt' \left\{\sum_{ij} J_{ij}(t)\sigma_i^x\sigma_j^x + \sum_i B(t)\sigma_j^y\right\}\right)$$

with $J_{ij}(t)$ found by performing some integrals

$$J_{ij}(t) - \frac{\hbar}{2}\sum_{\alpha=1}^{N}\Omega_i\Omega_j b_i^\alpha b_j^\alpha \frac{\delta k^2\hbar}{2m\omega_\alpha}\frac{1}{\omega_\alpha^2-\mu^2}(\omega_\alpha - \omega_\alpha\cos 2\mu t - 2\mu\sin\omega_\alpha t\sin\mu t).$$

The constant piece looks like an Ising model

$$\hat{H}_{\text{Ising}} = \sum_{ij} J_{ij}\sigma_i^x\sigma_j^x.$$

On a triangle, we can have ferromagnetic states or frustrated states.

The full spin problem looks like an Ising model in a transverse field. For the moment, let us neglect the time dependent exchange.

$$\hat{H}_{\text{transverse}} = \sum_{ij} J_{ij}\sigma_i^x\sigma_j^x + B(t)\sum_i \sigma_i^y$$

This Hamiltonian has two symmetries on the chain:

1. Spin Inversion symmetry: If we take $\sigma_x \to -\sigma_x$ and $\sigma_z \to -\sigma_z$ then $\hat{H}$ is invariant as are the spin commutation relations. Therefore, we can classify states as even or odd under change of sign of spin.

2. Spatial Reflection symmetry: The ion traps are symmetric, reflected about the center so we can classify states as even or odd under spatial reflection.

Returning to our three site chain example, $J_{12} = J_{23} \implies$ spatial symmetry. We classify the states in the x spin basis.

Even in both spin and space:

$$\frac{1}{\sqrt{2}}(|\uparrow\uparrow\uparrow\rangle + |\downarrow\downarrow\downarrow\rangle)$$
$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\uparrow\rangle + |\downarrow\uparrow\downarrow\rangle)$$
$$\frac{1}{2}(|\uparrow\uparrow\downarrow\rangle + |\downarrow\uparrow\uparrow\rangle + |\downarrow\downarrow\uparrow\rangle + |\uparrow\downarrow\downarrow\rangle)$$

Odd in spin and even in space:

$$\frac{1}{\sqrt{2}}(|\uparrow\uparrow\uparrow\rangle - |\downarrow\downarrow\downarrow\rangle)$$
$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\uparrow\rangle - |\downarrow\uparrow\downarrow\rangle)$$
$$\frac{1}{2}(|\uparrow\uparrow\downarrow\rangle + |\downarrow\uparrow\uparrow\rangle - |\downarrow\downarrow\uparrow\rangle - |\uparrow\downarrow\uparrow\rangle)$$

Even in spin and odd in space:

$$\frac{1}{2}(|\uparrow\uparrow\downarrow\rangle - |\downarrow\uparrow\uparrow\rangle + |\downarrow\downarrow\uparrow\rangle - |\uparrow\downarrow\downarrow\rangle)$$

and finally, odd in both spin and space:

$$\frac{1}{2}(|\uparrow\uparrow\downarrow\rangle - |\downarrow\uparrow\uparrow\rangle - |\downarrow\downarrow\uparrow\rangle + |\uparrow\downarrow\downarrow\rangle)$$

From this we can compute $\hat{H}$ in each symmetry sector (block diagonalization). It turns out the ground state is in the odd spin even space sector. You will explore this on the homework.

4 Other approximation schemes for time evolution

1.) Adiabatic spin evolution
a.) Ignore time-dependent exchange terms.
b.) Assume $B(t)$ changes slow enough that the system remains in the instantaneous ground state.
c.) For each t, find $B(t)$, diagonalize $\hat{H}$ taking the ground state at each t as the eigenstate.

2.) Sudden approximation
Same as above except start state along y-direction and turn J and B on together. Project the polarized state onto eigenstates to get initial probabilities. Then, evolve each state adiabatically, fixing the initial probabilities.

3.) Full time dependent spin evolution
Evaluate the spin evolution operator by discretizing time and the so-called Trotter formula

$$\hat{U}(t + \Delta t) = e^{-\frac{i}{\hbar}\hat{H}(t+\Delta t/2)\Delta t}\hat{U}(t)$$

Start from $\hat{U}(0) = 1$ to get

$$\hat{U}(t + \Delta t) = e^{-\frac{i}{\hbar}\hat{H}(t+\Delta t/2)\Delta t} e^{-\frac{i}{\hbar}\hat{H}(t-\Delta t/2)\Delta t} \cdots e^{-\frac{i}{\hbar}\hat{H}(\Delta t/2)\Delta t}$$

and evolve states forward in time.

4.) Full evolution including phonons
Evolve the wavefunction including phonons from its initial state.

Surprisingly, over a wide range of parameters 4 and 2 agree very well and agree with experiments.