Week 12

PHY 635 Many-body Quantum Mechanics of Degenerate Gases
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5 Quantum Simulations

We have seen that solving quantum many-body problems almost always requires smart approximations ($\langle\hat{\psi}\rangle \approx \phi$, $\langle\hat{\psi}\hat{\psi}\rangle \approx \Delta$) or validity of perturbation theory. In principle, we could use a brute force approach

$$|\,\psi(t)\,\rangle = \sum_{N_1\ldots N_n} c_{N_1\ldots N_n}(t)\underbrace{|\,N_1\ldots N_n\,\rangle}_{Eq.\ (2.2)} \tag{5.1}$$

and solve the

Many-body SE in the Fock-state representation

$$i\hbar\dot{c}_{N_1\ldots N_n}(t) = \sum_{N'_1\ldots N'_n} \langle\,N_1\ldots N_n\,|\hat{H}|\,N'_1\ldots N'_n\,\rangle c_{N'_1\ldots N'_n} \tag{5.2}$$

• Exercise: derive this from $i\hbar|\,\dot{\psi}(t)\,\rangle = \hat{H}|\,\psi\,\rangle$.

However, even if we allow at most N particles in M modes (single particle basis states), we have

Dimension of Fock space d: Fock-space dimension for max N bosons in M modes

$$d = (N+1)^M \tag{5.3}$$

• e.g 9 particles, 10 modes $\Rightarrow d = 10^{10}$!
This very quickly cannot fit into a computer. $\Rightarrow$

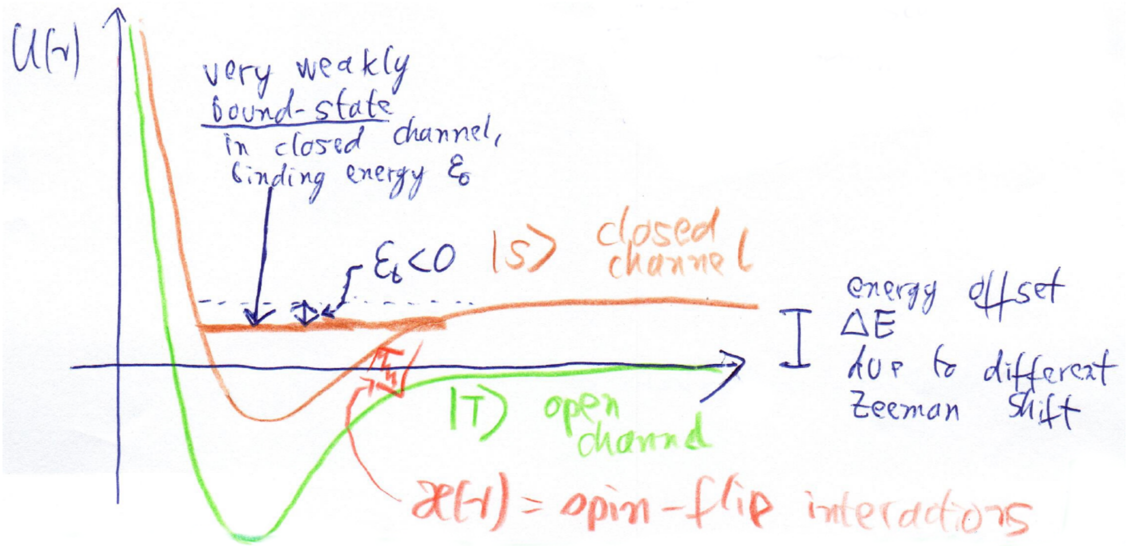
Quantum simulation concept: (Richard Feynman)
Find an experimentally accessible system, with the same Hamiltonian (mathematically) but on which we can do easier measurements and where parameters in the Hamiltonian are experimentally controllable.

- Disambiguation: the term "quantum simulation" can also refer to numerical simulation of any quantum problem.
- We now will sketch two examples using cold degenerate gases.
- Before that, let us revisit atomic interactions.

5.1 Fano-Feshbach Resonances

- So far, we have ignored electron spin dependence of atomic interactions (we had only looked at symmetry (boson/fermion)).
- In reality, interactions depend slightly on **electron**-spin.
- Careful: In chapter 4, when discussing atomic spin, we referred to two selected Hyperfine-states e.g
$$|\uparrow\rangle = \left|F = \frac{1}{2}, m_F = +\frac{1}{2}\right\rangle \quad \text{and,} \quad |\downarrow\rangle = \left|F = \frac{1}{2}, m_F = -\frac{1}{2}\right\rangle$$
The states entering scattering properties are (pair) electron spin singlet $|S\rangle = |s = 0, m_s = 0\rangle$ and triplet $|T\rangle = |s = 1, m_s = +1, 0, -1\rangle$.
- Due to unspecified nuclear spin, both $|\uparrow\uparrow\rangle, |\downarrow\uparrow\rangle$ may contain both $|S\rangle, |T\rangle$.
- Energy of $|S\rangle, |T\rangle$ depends differently on magnetic field through Zeeman-shift (see PHY402, pg. 25) of the Hyperfine structure.

Multi-channel scattering: (channel "=" certain choice of initial/final state quantum numbers) We can have the following picture: To find scattering length a_s ($|\uparrow\downarrow\rangle$):



- Consider two incoming scattering partners in $|\uparrow\downarrow\rangle$ with energy $E \gtrsim 0$ (ultra-cold regime)
- Calculate 2nd order perturbation theory (in $\kappa(r)$, spin-flip Hamiltonian) energy correction to scattering state

$$E_n^{(2)} = \sum_{k \neq n} \frac{\left|\langle k^{(0)}|\hat{V}|n^{(0)}\rangle\right|^2}{E_n^{(0)} - E_k^{(0)}} \tag{5.4}$$

(see QM lecture).

- Schematically here

$$
\begin{aligned}
&|\, n^{(0)}\,\rangle \sim |\uparrow\downarrow\rangle \otimes |\, E \approx 0\,\rangle, && E_n^{(0)} \approx 0 \\
&|\, k^{(0)}\,\rangle \sim |\uparrow\uparrow\rangle \otimes |\, \text{bound state}\,\rangle, && E_k^{(0)} \approx \Delta E \\
&\left|\langle\, k^{(0)}\,|\hat{V}|\, n^{(0)}\,\rangle\right|^2 \sim |\kappa|^2, && \frac{1}{E_n^{(0)} - E_k^{(0)}} \sim -\frac{1}{\Delta E}
\end{aligned}
$$

Three cases: If
$\Delta E \to 0$ (Resonance), $E_n^{(2)} \to \infty$
$\Delta E < 0$, $E_n^{(2)} > 0 \Rightarrow$ (more) repulsive interactions
$\Delta E > 0$, $E_n^{(2)} < 0 \Rightarrow$ (more) attractive interaction

- Since ΔE depends on magnetic field B:

> **Scattering length near Feshbach resonance**
>
> $$a_s(B) = a_{\text{bg}}\Big(1 - \frac{\Delta B}{B - B_0}\Big) \tag{5.5}$$

a_{bg} = background scattering length,
B_0 = position of resonance,
ΔB = width of resonance.

> **Example:** Scattering length with 2 Feshbach resonances [^{6}Li: $B_0^{(1)} = 543$ G, $B_0^{(2)} = 834$ G]
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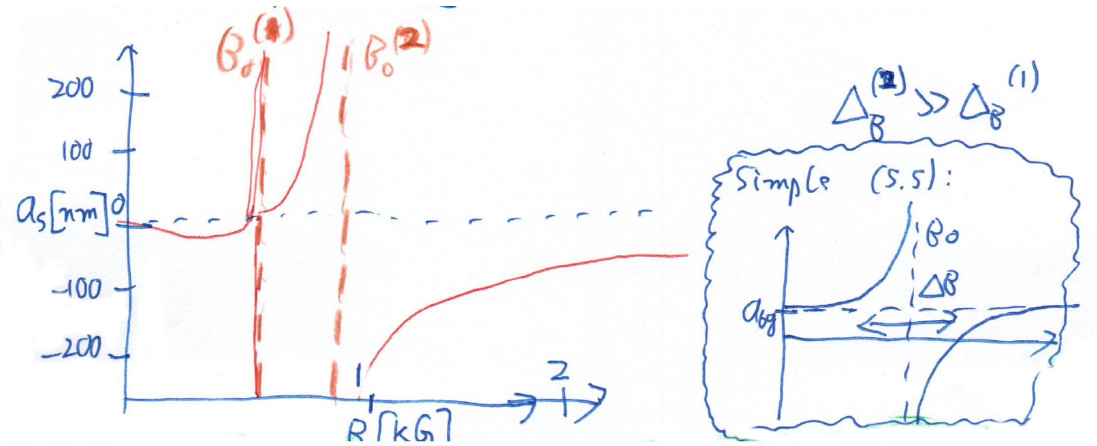
> 
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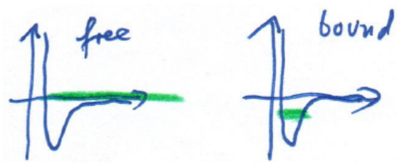
- Feshbach resonances effectively make the interaction strength an experimentally controllable parameter.
- We can reach $a_s = 0$, $a_s > 0$, $a_s < 0$ and (almost) $a_s = \infty$.

5.2 BEC-BCS Crossover

- Using Feshbach resonances, we can now realize DFG with interactions ranging from repulsive to attractive (see week 10 vs week 11).
- Let us reconsider the repulsive $a_s > 0$ side: Do we get a Fermi-liquid as ground state as in section 4.40?
- Answer: when considering the scenario with a Feshbach resonance, that would be only a meta-stable (excited) state/phase, since the scattering state with $E \approx 0$ for which we found $a_s > 0$ in section 5.1 has higher energy than a bound state in the closed channel.



- Bound-states and Cooper pairs are related (the latter *are* a type of weak bound state). It turns out, with rigorous renormalization we can actually apply BCS theory all the way from $U_0 = -\infty$ to $U_0 = \infty$. The gap-equation (4.75) then can be solved for $U_0 < 0$.

5.2.1 From Cooper-pairs to Molecules

Let us again look at the pair creation operator

$$\hat{C}^\dagger = \sum_{\mathbf{k}} \varphi_{\mathbf{k}} \hat{a}^\dagger_{\mathbf{k}\uparrow} \hat{a}^\dagger_{(-\mathbf{k})\downarrow} \tag{5.6}$$

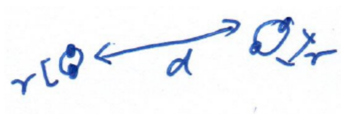
Commutator:

$$\left[\hat{C}, \hat{C}^\dagger\right] = \sum_{\mathbf{k},\mathbf{k}'} \varphi^*_{\mathbf{k}} \varphi_{\mathbf{k}'} \left[\hat{a}_{(-\mathbf{k})\downarrow} \hat{a}_{\mathbf{k}\uparrow}, \hat{a}^\dagger_{\mathbf{k}'\uparrow} \hat{a}^\dagger_{(-\mathbf{k}')\downarrow}\right] \overset{\text{(exercise)}}{=} \sum_{\mathbf{k}} |\varphi_{\mathbf{k}}|^2 (1 - \hat{n}_{\mathbf{k}\uparrow} - \hat{n}_{\mathbf{k}\downarrow}) \tag{5.7}$$

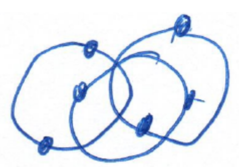
We can show (see steps on page 95) that $\sum_{\mathbf{k}} |\varphi_{\mathbf{k}}|^2 = 1$ due to normalization of our starting pair state $\varphi_0(\mathbf{x} - \mathbf{y})$.

Thus when acting on states with few fermions "per momentum mode", we have $\left[\hat{C}, \hat{C}^\dagger\right] = 1$, and our pair behaves like a boson. (You can show $\left[\hat{C}, \hat{C}\right] = \left[\hat{C}^\dagger, \hat{C}^\dagger\right] = 0$ also).

For this we require a broad Fourier transform $\tilde{\varphi}_0(k) \rightarrow$ tightly bound pairs in position space. This corresponds to molecules with spacing $d \gg$ orbital radius r,



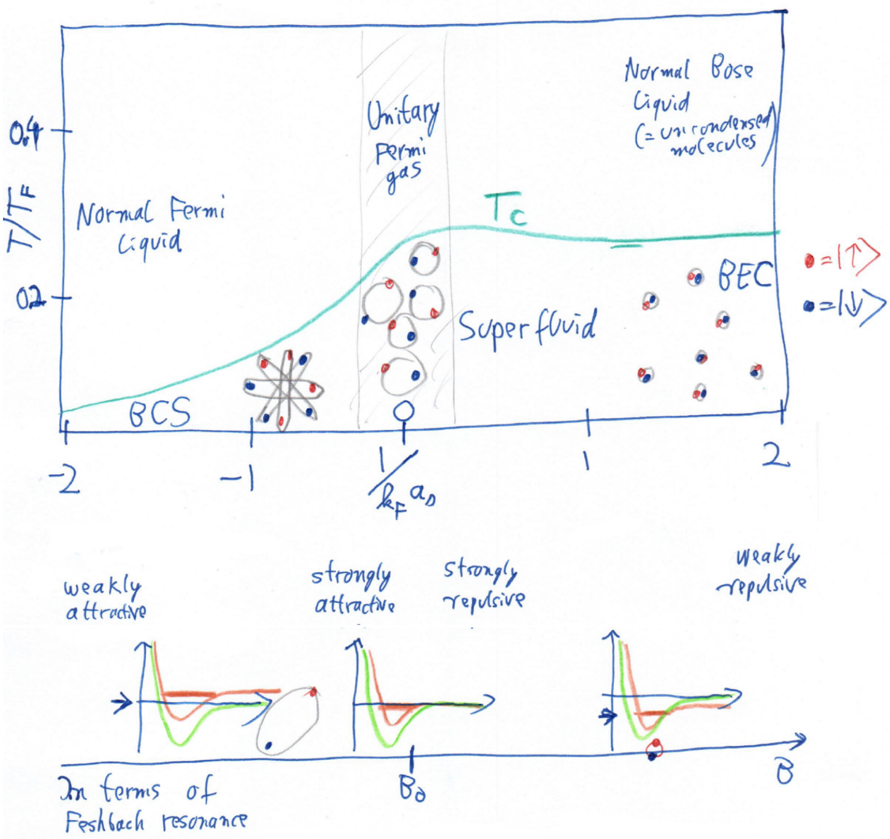
In other limit, where $r \gg d$, we will have high occupations of all momentum modes ($\hat{n} \sim 1$), and we talk of Cooper-pairs (that are not quite bosons, but have some "bosonic-character").



Through this change of the interpretation/details of the many-body paired state, we are able to smoothly interpolate between a BEC of bosonic molecules (made of two fermionic atoms) at $a_s > 0$ and a BCS-superfluid due to Cooper-pairing at $a_s < 0$.

5.2.2 Crossover phase diagram

Altogether we have the following phase diagram:



- Very close to resonance, interactions are very large, such that $r_{\text{range}} \ll k_F^{-1} \ll a_s$. This is called unitary case (for non-obvious reasons), here the only scale is k_F (physics universal).

on the left: BCS | on the right: BEC

$$\mu = E_F > 0 \qquad \mu = -\frac{1}{2}\underbrace{\left(\frac{\hbar^2}{m a_s}\right)}_{\varepsilon_b} + U_m \rho_m < 0$$

$$\Delta \approx E_F e^{-\frac{\pi}{2k_F|a_s|}} \qquad U_m = \frac{\pi \hbar^2 a_s}{m_{\text{at}}}$$

5.3 Quantum-simulation aspects of BEC-BCS crossover

High T_C superconductivity
While not being directly related, these share several features with the crossover region:

- Pair size $\sim$ average distance (see p. 89)
- Normal state (above T_C) not ordinary Fermi-liquid

Neutron stars/ Quark matter
Particularly in the unitary limit, there is only one scale in the interacting fermion problem (details don't matter). It should thus also apply to other DFG systems than ultra-cold gases, such as neutron stars (see section 4.4.2). This is particularly useful, since calculations in this strongly interacting regime are very challenging.