12

V. QUANTUM SIMULATIONS

We have seen that solving quantum-many-body problems ~~frequently~~ almost always requires smart approximations ($\langle\hat{\Psi}\rangle \approx \phi$, $\langle\hat{\Psi}\hat{\Psi}\rangle \approx \Delta$) or ~~pa~~ validity of perturbation theory.

In principle we could use a brute force approach

$$|\Psi(t)\rangle = \sum_{\vec{N}_1 \ldots \vec{N}_M} c_{\vec{N}_1 \ldots \vec{N}_M}(t) \underbrace{|\vec{N}_1 \ldots \vec{N}_M\rangle}_{(2.14)} \qquad (5.1)$$

and solve Many-Body SE in Fock-state representation

$$\boxed{i\hbar\, \dot{c}_{\vec{N}_1 \ldots \vec{N}_M}(t) = \sum_{\vec{N}'_1 \ldots \vec{N}'_M} \langle \vec{N}_1 \ldots \vec{N}_M | \hat{H} | \vec{N}'_1 \ldots \vec{N}'_M \rangle\, c_{\vec{N}'_1 \ldots \vec{N}'_M}} \qquad (5.2)$$

- excercise: Derive this from $i\hbar|\dot{\Psi}(t)\rangle = \hat{H}\Psi(t)$

However, if we allow at most N particles in M modes (single particle basis states), the size of Fock-space is

Fockspace dimension for max N bosons in M modes

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

- e.g. 9 particles, 10 modes $\quad d = 10^{10}$!

This very quickly cannot fit into a computer. $\Rightarrow$

Quantum-simulation concept (Richard Feynman)

Find an experimentally accessible system, with same Hamiltonian (mathematically), but on which I 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 IV, when discussing atomic-spin, we reffered to two selected Hyperfine-states, e.g.

$$|\uparrow\rangle = |F=\tfrac{1}{2}, m_F=+\tfrac{1}{2}\rangle \qquad |\downarrow\rangle = |F=\tfrac{1}{2}, m_F=-\tfrac{1}{2}\rangle$$

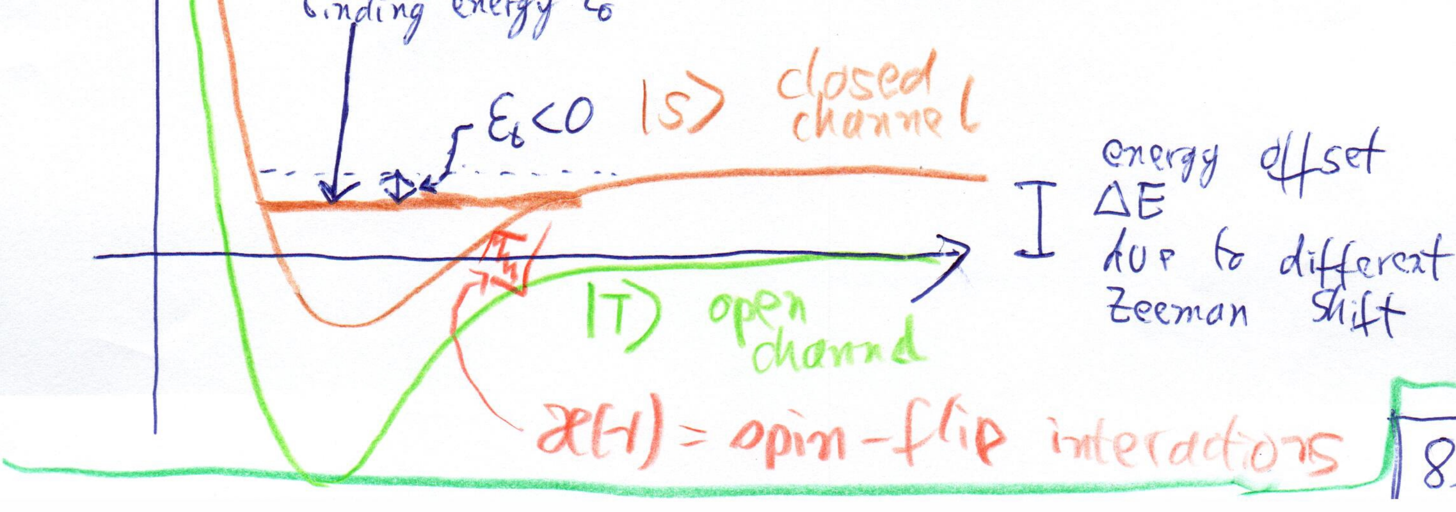
The states entering scattering properties are (pair) electron-spin singlett $|S\rangle = |S=0, m_S=0\rangle$ and triplett $|T\rangle = |S=1, m_S=+1,0,-1\rangle$

- Due to the uncpecified 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 PHY 402, p.25) of the Hyperfine structure

We can have the following picture: To find scattering length $a_s(|\uparrow\downarrow\rangle)$:

Multi-channel scattering

channel "=" certain choice of initial/final state quantum numbers



- Consider two incoming scattering partners in $|\uparrow\downarrow\rangle$ with energy $E \gtrsim 0$ (ultra-cold regime)

- Calculate 2nd order perturbation theory (in $\mathcal{H}(r)$, spin-flip Hamiltonian) energy correction for scattering state.

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

[see QM lecture]

- Schematically here

$$|n^{(0)}\rangle \sim |\uparrow\downarrow\rangle \otimes |E \simeq 0\rangle \qquad E_n^{(0)} \simeq 0$$

$$|k^{(0)}\rangle \sim |\uparrow\uparrow\rangle \otimes |\text{bound state}\rangle \qquad E_k^{(0)} \simeq \Delta E$$

$$|\langle k^{(0)}|\hat{V}|n^{(0)}\rangle|^2 \sim |\mathcal{H}|^2, \quad \frac{1}{E_n^{(0)} - E_k^{(0)}} \sim -\frac{1}{\Delta E}$$

- If $\Delta E \to 0$ (Resonance) $E_n^{(2)} \mapsto \infty$
  $\Delta E < 0$; $E_n^{(2)} > 0$ → (More) repulsive interactions
  $\Delta E > 0$; $E_n^{(2)} < 0$ (More) attractive interactions

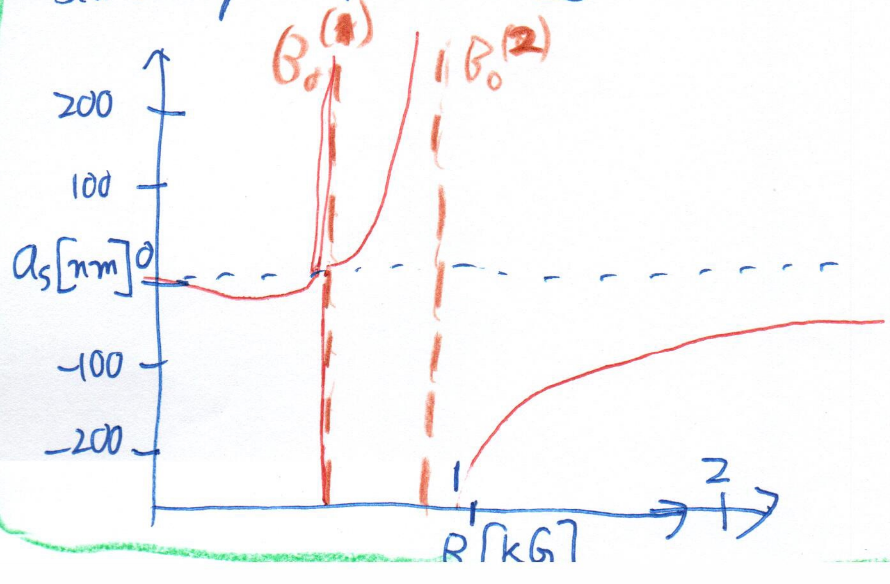
- Since ΔE depends on magnetic field B:

Scattering length near Feshbach resonance:

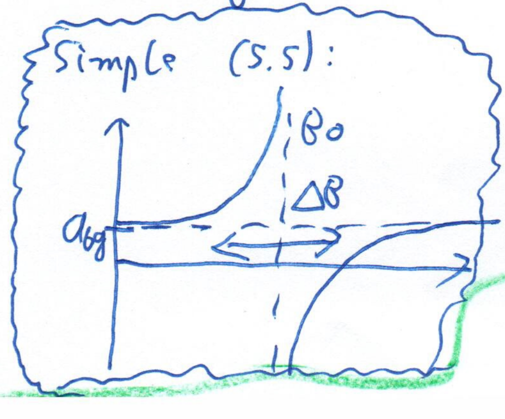
$$a_s(B) = a_{bg}\left(1 - \frac{\Delta B}{B - B_0}\right) \qquad (5.5)$$

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

Example: Scattering length with 2 Feshbach resonces [^6Li, $B_0^{(1)} = 543\,G$, $B_0^{(2)} = 834\,G$]



$\Delta_B^{(2)} \gg \Delta_B^{(1)}$



- Feshbach resonances effectivly make the interaction strength an experimentally controllable parameter

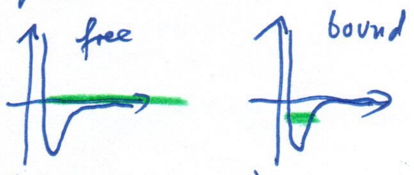
- We can reach $a_s = 0$, $a_s > 0$, $a_s < 0$ and (almost) $a_s = \infty$

5.2. BEC-BCS Crossover

- Using Feshbach resonances, we can now realize DGP with interactions ranging from ~~[illegible]~~ repulsive to attractive (see week 10 vs week 11).

- Let us re-consider the repulsive $a_s > 0$ side: Do we get a Fermi-liquid as groundstate as in section 4.8.1.?

- Answer: that ~~we~~ 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.



- Now bound-states are sth. like a Cooper pair. It turns out, with rigorous renormalisation we can actually apply ~~[illegible]~~ BCS theory <u>all the way</u> from $U_0 = \infty$ to $U_0 = -\infty$. In partical gap-equation (4.53) then can also be solved for $U_0 < 0$.

5.2.1. From Cooper-pairs to Molecules

Review: (New) p. 80c

Let us again look at the pair creation operator

$$\hat{C}^+ = \sum_k \varphi_k \hat{a}^+_{k\uparrow} \hat{a}^+_{(-k)\downarrow} \qquad (4.51e \text{ or } 4.43)$$

Commutator:

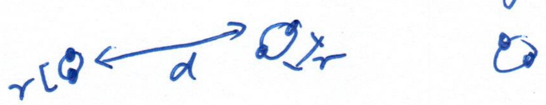
$$[\hat{C}, \hat{C}^+] = \sum_{k,k'} \varphi^*_k \varphi_{k'} [\hat{a}_{(-k)\downarrow} \hat{a}_{k\uparrow}, \hat{a}^+_{k'\uparrow} \hat{a}^+_{(-k')\downarrow}] \underset{\text{excercise}}{=}$$

$$= \sum_k |\varphi_k|^2 \left(1 - \hat{n}_{k\uparrow} - \hat{n}_{k\downarrow}\right) \qquad (5.6)$$

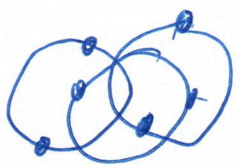
We can show (from p. 80d) that $\sum_k |\varphi_k|^2 = 1$ due to normalisation of our starting pair state $\varphi_0(\vec{x} - \vec{y})$.

Thus when acting on states with <u>few</u> Fermions "per momentum mode", we have $[\hat{c}, \hat{c}^\dagger] = 1$, and our <u>pair behaves like a Boson</u>. (You can also show $[\hat{c}, \hat{c}] = [\hat{c}^\dagger, \hat{c}^\dagger] = 0$)

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



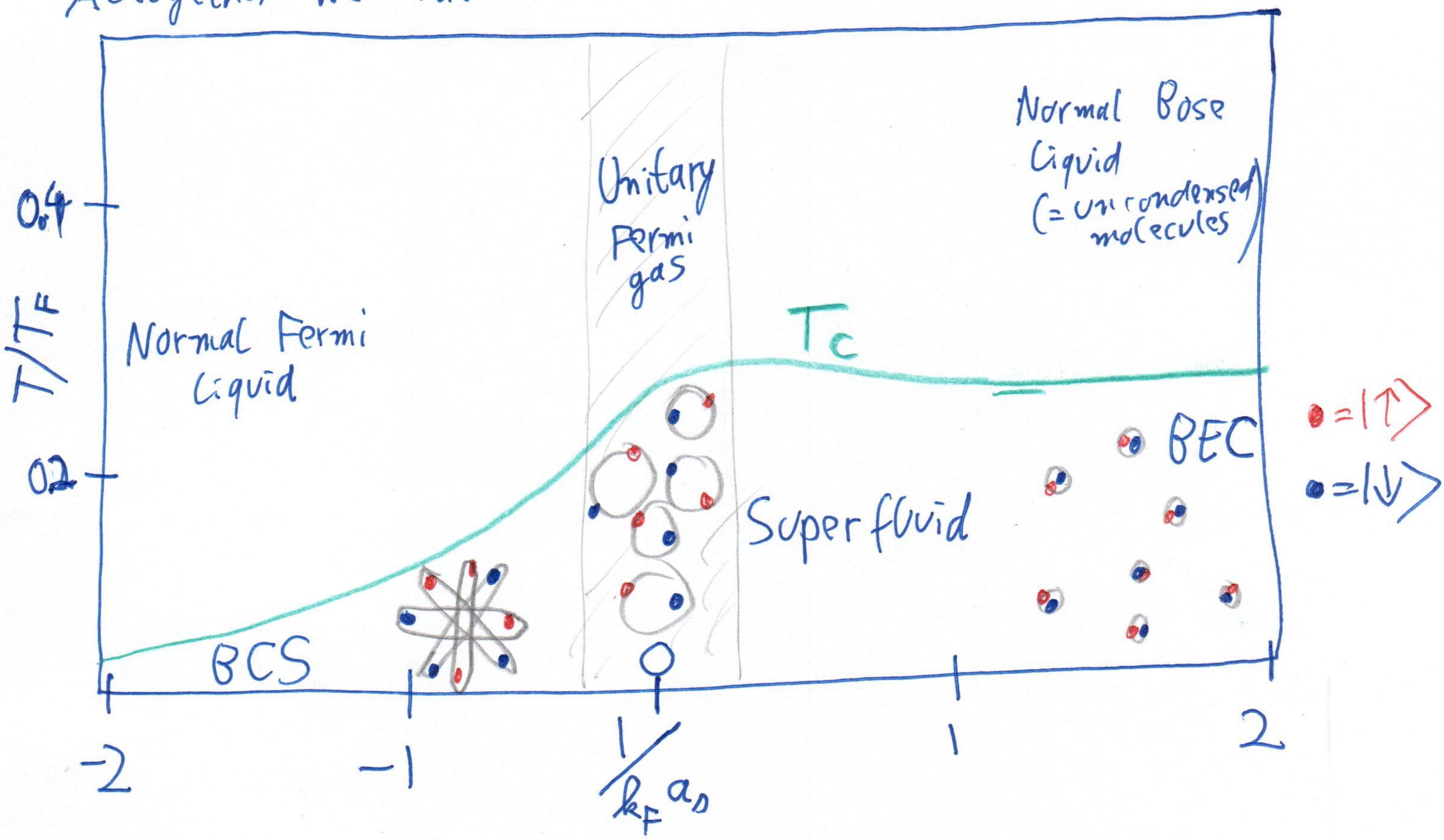
In the other limit, where $r \gg d$, we will have high occupations of all momentum modes ($\hat{n} \sim 1$), and we talk of <u>Cooper-pairs</u> (that are not quite bosons, but have some "bosonic character").

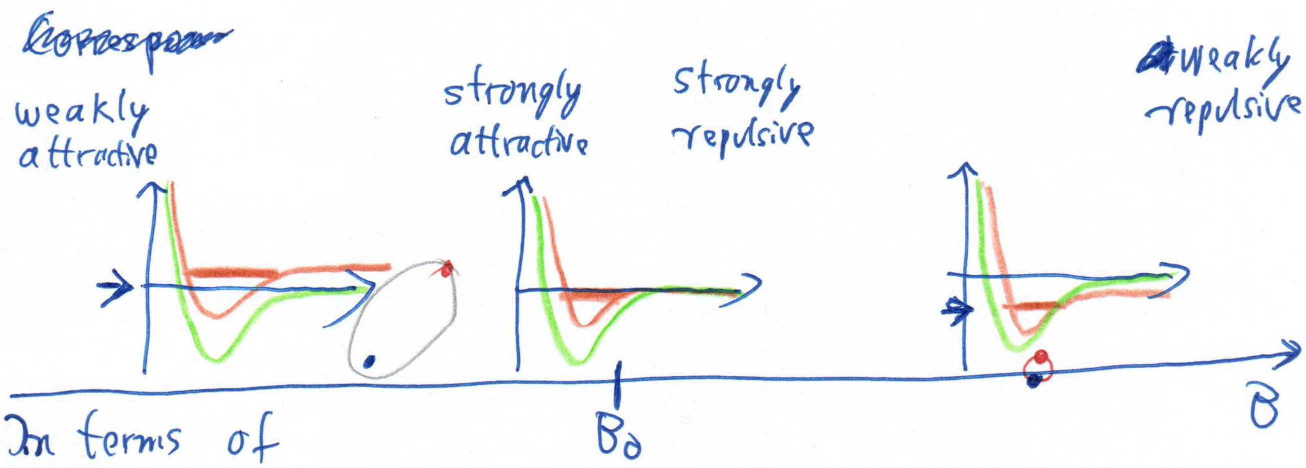


Through this change of the interpretation/details of the many-body paired state, we are able to smoothly interpolate between a BEC of bosonic molecules (made of two fermionic atoms) at $a_s > 0$ and a BCS-superfluid due to Cooper pairing at $a_s < 0$.

5.2.2. Crossover phase diagram:

Altogether we have:





In terms of Feshbach resonance

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

BCS

$$\mu = E_F > 0$$

$$\Delta \approx E_F e^{-\frac{\pi}{2k_F|a_s|}}$$

BEC <0

$$\mu = -\frac{1}{2}\underbrace{\left(\frac{\hbar^2}{m a_s^2}\right)}_{\epsilon_b} + \underbrace{U_m}_{\frac{4\pi\hbar^2 a_s}{m_{at}}} n_m$$

5.3. Quantum-simulation aspects of BEC-BCS cross-over

High-T_c superconductivity

While not being directly related, these share several features with the cross-over region:

- pair size ~ 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 these also apply to other DGF systems than ultracold gases, such as neutron stars (see 4.3.2.).

This is particularly useful, since calculations in this strongly interacting regime are very challenging.