Week 2

Outline:

* Fermions and the Heisenberg model
  - XYZ chain: fermion representation
  - Goldstone modes: magnons
  - Magnons and their excitation energy
  - Example: ferromagnets and magnon dispersion, (quadratic dispersion in Heisenberg model and linear dispersion in XY)...

* Topological superconductivity in 1D and majorana fermions
  - Noninteracting chain, Kitaev chain and localized edge Majorana fermions
  - Degenerate ground state ~~and~~

* Properties of Majorana fermions

* Interacting systems
  - Interaction Hamiltonian.

* **Perturbation theory**
  - QM of a single particle
  - [illegible] diagrams

Let us start with fermionized XXZ spin chain:

$$\boxed{H = -\frac{J}{2}\sum_j \left(f_{j+1}^+ f_j + f_j^+ f_{j+1}\right) + J_z \sum_j n_j - J_z \sum_j n_j n_{j+1}}$$

and transform it to momentum space:

$$f_j = \frac{1}{\sqrt{N}}\sum_k c_k e^{i\vec{k}\vec{R}_j},$$ where c_k^+ creates a "spin"/fermi[on] excitation in momentum space with momentum k.

The single particle terms will acquire the following form:

$$J_z \sum_j \hat{n}_j = J_z \sum_k c_k^+ c_k$$

$$-\frac{J}{2}\sum_j \left[f_{j+1}^+ f_j + H.c.\right] = -\frac{J}{2N}\sum_{k,k'}\left[e^{-ika} + e^{ika}\right] c_k^+ c_{k'} \underbrace{\sum_j e^{-i(k-k')R_j}}_{N\cdot\delta_{kk'}}$$

$$= -J\sum_k \cos(ka) c_k^+ c_k$$

$$= -J\sum_k \cos(ka)\,\hat{n}_k$$

The XXZ Heisenberg Hamiltonian can thus be written as

$$H = \sum_k \left[J_z - J\cos(ka)\right] c_k^+ c_k - J_z \sum_j n_j n_{j+1}$$

or $$H = \sum_k \omega_k c_k^+ c_k - J_z \sum_j n_j n_{j+1},$$ where

$\boxed{\omega_k = J_z - J\cos(ka)}$ - defines a magnon excitation energy.

Consider the interaction term:

$$-J_z \sum_j \hat{n}_j \hat{n}_{j+1} = \sum_{i,j} V(i-j)\,\hat{n}_i \hat{n}_j \,,$$

where
$$V(i-j) = \begin{cases} -\dfrac{J_z}{2}, & \text{for } i-j = \pm 1 \\ 0, & \text{otherwise}. \end{cases}$$

Fourier transform of V reads: $V(q) = -J_z \cos(qa)$, so that the full Hamiltonian becomes:

$$\boxed{H = \sum_k \omega_k C_k^+ C_k - \frac{J_z}{N} \sum_{k,k',q} \cos(qa)\, C_{k-q}^+ C_{k'+q}^+ C_{k'} C_k}$$

while we remind that the original Hamiltonian was:

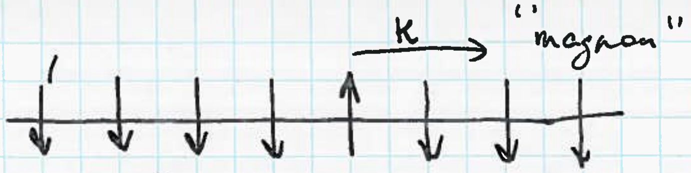
$$H = -J \sum_j \left[S_j^x S_{j+1}^x + S_j^y S_{j+1}^y \right] - J_z \sum_j S_j^z S_{j+1}^z =$$
$$= -\frac{J}{2} \sum \left[S_{j+1}^+ S_j^- + H.c. \right] - J_z \sum_j S_j^z S_{j+1}^z .$$

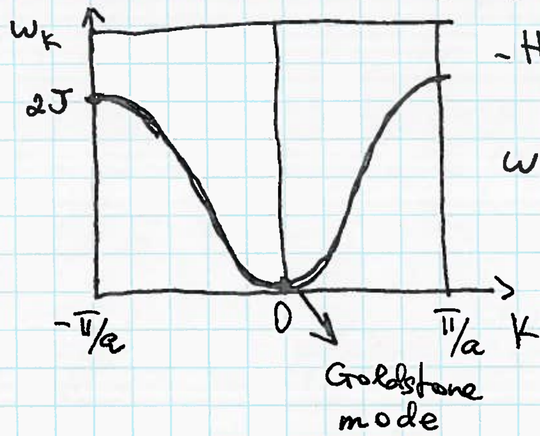
In fact, this is an <u>exactly solvable</u> model, and one could extract many properties of the magnet from the exact (Bethe ansatz) solution. Here we will just neglect the interaction (reasonable for Heisenberg ferromagnet $J_z = J$, and x-y model, $J_z = 0$).

1) Heisenberg ferromagnet, $J_z = J\,(>0)$.

In this case, the spectrum is $\omega_k = 2J \sin^2\left(\frac{ka}{2}\right)$.

- always positive => <u>no magnons in the ground state.</u>





– Heisenberg ferromagnet

$$\omega_k = 2J \sin^2\left(\frac{ka}{2}\right)$$

The ground state thus is: $|0\rangle = |\downarrow\downarrow\cdots\downarrow\rangle$, corresponding to a state with spontaneous magnetization $M = \underbrace{-\frac{1}{2} - \frac{1}{2} \cdots - \frac{1}{2}}_{N} = -\frac{N}{2}$.

Interestingly enough, since $\omega_{k=0} = 0 \Rightarrow$ it costs nothing to add a <u>magnon of arbitrarily long wavelength</u>! This is an example of a Goldstone mode. The reason it shows up is that spontaneous magnetization could point in any direction.

Suppose we want to rotate the magnetization by an infinitesimal angle $\delta\theta \ll \pi$ about x-axis $\Rightarrow$ $\Rightarrow$ the new state is

$$|\Psi_{rotated}\rangle = e^{i\delta\theta S_x} |\downarrow\downarrow\cdots\downarrow\rangle =$$

$$= |\downarrow\downarrow\cdots\downarrow\rangle + i\frac{\delta\theta}{2}\sum_j \left(S_j^+ + S_j^-\right)|\downarrow\downarrow\cdots\downarrow\rangle + O(\delta\theta^2)$$

$$= |\downarrow\downarrow\cdots\downarrow\rangle + i\frac{\delta\theta}{2}\sum_j S_j^+ |\downarrow\downarrow\cdots\downarrow\rangle + O(\delta\theta)^2$$

The change in the wavefunction $\frac{\delta\theta}{2}$ is

$$i\frac{\delta\theta}{2}\cdot S^{+}_{total}\,|\downarrow\downarrow\dots\downarrow\rangle \equiv \left(i\frac{\delta\theta}{2}\right)\cdot\sum_j f_j^{+}\underbrace{e^{i\hat{\phi}_j}}_{\text{gives } 1}|0\rangle$$

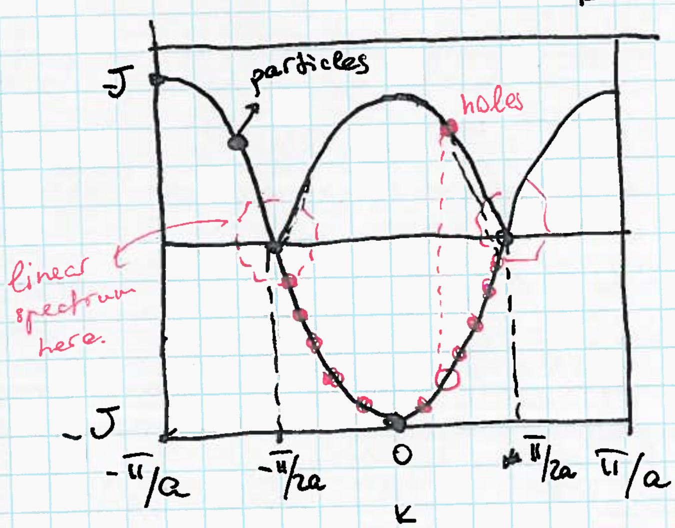
$$= \left(i\frac{\delta\theta}{2}\right)\cdot\sum_j f_j^{+}|0\rangle = \left(i\frac{\delta\theta}{2}\right)\cdot\sqrt{N}\cdot c^{+}_{k=0}|0\rangle$$

$\Rightarrow$ the action of adding a single magnon at $q=0$ rotates the magnetization infinitesimally upwards.

Rotating the magnetization should cost no energy
$\Rightarrow$ the $k=0$ magnon is a zero-energy excitation.

2) XY ferromagnet ($J_z=0$): When $|J_z| < J$, the spectrum develops a negative part, and magnon states with negative energy will become occupied. At $J_z=0$ one has

$$\omega_k = -J\cos(ka).$$



$\Rightarrow$ all negative-energy fermion states ~~are~~ with $|k| < \frac{2\pi}{a}$ are occupied.

The ground state is:

$$|\psi\rangle_{G.S.} = \prod_{|k|<\frac{2\pi}{a}} c_k^{+}|0\rangle.$$

The band of magnons is half-filled $\Rightarrow$

$$\Rightarrow \langle S_z\rangle = \langle n_f - \tfrac{1}{2}\rangle = 0. \Rightarrow \text{no G.S. magnetization.}$$

The loss of G.S. magnetization upon going from Heisenberg (XXX) to XY ferromagnet is due to the growth of spin fluctuations.

<u>Excitations:</u> can be made by adding a magnon at wavevectors $|k| > \frac{2\pi}{a}$ or by annihilating a magnon at wavevectors $|k| < \frac{2\pi}{a}$ to form a hole. The energy ~~of~~ to form a hole is $-\omega_k$.

To represent the hole excitations, we make particle-hole transformation for the occupied states, introducing

$$\tilde{C}_k = \begin{cases} C_k, & \text{if } |k| > \pi/2a \\ C^+_{-k}, & \text{if } |k| < \pi/2a \end{cases}$$

$\omega_{-k} = +\omega_k =$
$= -J \cos(ka)$

$-\omega_k = J \cos(ka)$

We have $C_k^+ C_k = 1 - C_k C_k^+$ and the Hamiltonian of the XY model can be written as

$$H_{XY} = \sum_k J \left| \cos ka \right| \left(\tilde{C}_k^+ \tilde{C}_k - 1/2 \right)$$

Notice that, unlike Heisenberg ferromagnet, the magnon excitation spectrum is now linear.

The G.S. energy is

$$E_{G.S.} = -\frac{1}{2} \sum_k J \left| \cos ka \right| = -a \int_{-\pi/2a}^{\pi/2a} \frac{dk}{2\pi} J \cos(ka) = -\frac{J}{\pi}.$$

No magnetization but zero-energy magnon modes at $q = \pm \pi/a \Leftrightarrow$ $\Leftrightarrow$ no long range order, but power-law spin-spin correlations!

Topological superconductivity in 1D and Majorana fermions

Can we have ~~excitation~~ quasiparticle (low-energy) excitations which are different from regular fermions and bosons? Majorana fermions are one example of such excitations. MFs are their own anti-particles, i.e. it is its "own hole".

Consider a 1D tight-binding chain with p-wave superconducting pairing:

$$H_{chain} = -\sum_{i=1}^{N-1}\left(t\, c_i^+ c_{i+1} + \Delta c_i c_{i+1} + H.c.\right) - \mu \sum_{i=1}^{N} n_i$$

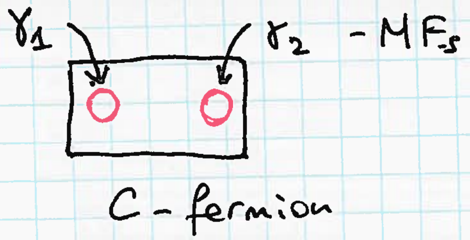
where μ is the chemical potential. The superconducting gap Δ and hopping t are assumed to be the same for all sites. We can assume superconducting phase to be zero: $\Delta = |\Delta|$. [Compare this Hamiltonian with the solution ~~of~~ prob 1 and 4 of HW1].

We can now rewrite H_{chain} in terms of Majorana operators

$$\boxed{\begin{aligned} c_i &= \frac{1}{2}\left(\gamma_{i,1} + i\gamma_{i,2}\right) \\ c_i^+ &= \frac{1}{2}\left(\gamma_{i,1} - i\gamma_{i,2}\right) \end{aligned}} \Rightarrow \begin{aligned} \gamma_{i,1} &= c_i^+ + c_i \\ \gamma_{i,2} &= i\left(c_i^+ - c_i\right) \end{aligned}$$

$\Downarrow$

are clearly Hermitian: $\gamma^+ = \gamma$.



One can easily rewrite the Hamiltonian in terms of MF-s.

In case when $\mu = 0$ and $t = \Delta$, the Hamiltonian is particularly simple:

$$H_{chain}(\mu=0, t=\Delta) = -\sum_{i=1}^{N-1} t\left(c_i^+ c_{i+1} + c_{i+1}^+ c_i + c_i c_{i+1} + c_{i+1}^+ c_i^+ \right) =$$

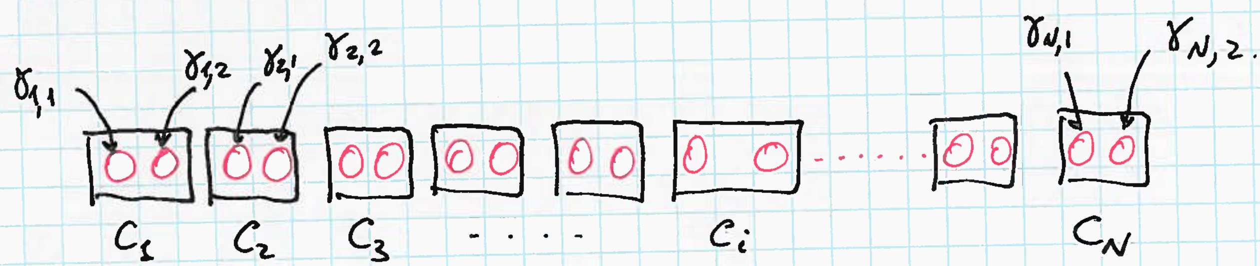
$$= -it \sum_{i=1}^{N-1} \gamma_{i,2}\, \gamma_{i+1,1}$$

since

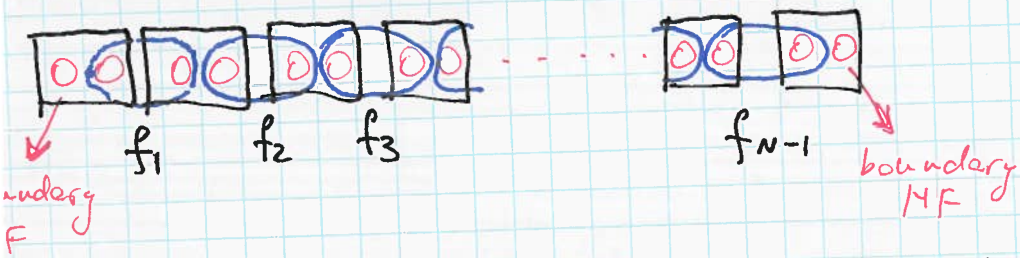
$$\gamma_{i,1}\,\gamma_{i+1,2} = (c_i^+ + c_i)\cdot i\,(c_{i+1}^+ - c_{i+1}) = i\left(c_i^+ c_{i+1}^+ - c_i c_{i+1} - \right.$$

$$\left. - c_i^+ c_{i+1} + c_i c_{i+1}^+ \right) = -i\left(c_i^+ c_{i+1} + c_i^+ c_i + c_i c_{i+1} + c_{i+1}^+ c_i^+ \right).$$

This is an alternative way of writing the diagonalized Hamiltonian.



Let us now go back to the fermion (not MF) representation by noting that, where a fermion on site i was split into two Majorana's living on site i, we can construct new fermion operators f_i, by combining Majorana operators on neighboring sites!



=> In the limit $\mu = 0$, $t = \Delta$, the Hamiltonian is diagonal in fermion operators which are obtained by combining instead Majorana operators on neighboring sites: $\gamma_{i+1,1}$ and $\gamma_{i,2}$.

=> there are 2 MF-s left, $\gamma_{1,2}$ and $\gamma_{N,1}$, which can be combined to form one zero-energy <u>nonlocal</u> fermion operator f_M.

Define:

$$\hat{f}_i = \frac{1}{2}\left(\gamma_{i+1,1} + i\gamma_{i,2}\right)$$

$$\hat{f}_i^+ = \frac{1}{2}\left(\gamma_{i+1,1} - i\gamma_{i,2}\right)$$

=>

$$\gamma_{i+1,1} = \left(\hat{f}_i^+ + \hat{f}_i\right)$$

$$\gamma_{i,2} = i\left(\hat{f}_i^+ - \hat{f}_i\right)$$

In terms of operators f, f^+ we find

$$-i\,\gamma_{i,2}\,\gamma_{i+1,1} = \left(f_i^+ - f_i\right)\left(f_i^+ + f_i\right) = 2 f_i^+ f_i = 2\tilde{n}_i$$

$$\Rightarrow \quad H_{chain} = 2t \sum_{i=1}^{N-1} \hat{f}_i^+ f_i \quad \text{- is diagonal.}$$

$\hat{f}_i$ are the annihilation operators corresponding to the eigenstates; the energy cost for creating a f-fermion is $2t$.

Notice that the Majorana operators $\gamma_{N,2}$ and $\gamma_{1,1}$, which are localized at the two ends of the wire, are completely missing from the Hamiltonian H_{chain}! These two operators can equivalently be described by a single fermionic state with operator

$$f_M = \frac{1}{2}\left(\gamma_{N,2} + i\gamma_{1,1}\right).$$

This state is a highly non local state a $\gamma_{N,2}$ and $\gamma_{1,1}$ are localized on opposite ends of the chain.

f_M - is absent from the Hamiltonian => occupying the corresponding state costs zero energy!

Superconducting state = condensate of Cooper pairs => ~~ev~~ has even number of fermions. This state thus has odd # of quasiparticles at zero-energy cost.

The ground state => is degenerate two-fold, corresponding to having in total an even and odd # of electrons in the superconductor.

→ this even-odd'ness is called parity, corresponding to the eigenvalue of the # operator of the ~~zero~~-energy fermion: ~~f_M~~ $n_M = f_M^\dagger f_M$

$$n_M = \begin{cases} 0 & \text{for even parity} \\ 1 & \text{for odd parity} \end{cases}$$

In fact, one can show that the Majorana end states remain as long as the chemical potential lies within the gap: $\underline{|\mu| < 2t}$.
In this general case, the MF-s are not completely localized at the two edge states of the wire, but decay exponentially away from the edges.

The Hamiltonian for the continuum version in 1D reads:

$$H_{1D} = \int dx \left[\psi^{+}(x) \left(\frac{p_x^2}{2m} - \mu \right) \psi(x) + \psi(x) |\Delta| e^{i\phi} p_x \psi(x) + + H.c. \right],$$

Properties of MF-s:

Let us consider a system of $2N$ spacially well-separated MFs: $\gamma_1, \gamma_2, \ldots, \gamma_{2N}$. The # of MFs is even $= 2N$ as ~~[illegible]~~ 1 MF contains half the degree of freedom of a fermion:

$$f_i = \frac{1}{2}\left(\gamma_{2i-1} + i\gamma_{2i} \right)$$

$$\Rightarrow \quad \left. \begin{aligned} \gamma_{2i-1} &= f^{+} + f \\ \gamma_{2i} &= i(f^{+} - f) \end{aligned} \right| \Rightarrow \quad \gamma_j = \gamma_j^{+}.$$

Using ~~as~~ fermionic anti-commutation relations of f-s, one can obtain:

$$\{\gamma_i \gamma_j\} = 2\delta_{ij} \quad - \quad \text{~~[illegible]~~}$$

$\Rightarrow$ we see $\gamma_i^2 = 1$.

$\Rightarrow$ Acting 2x by a Majorana operator, one gets ~~b~~ back to the initial state.

$\Rightarrow$ No Pauli principle for MFs. [unlike for fermions $c_i^2 = (c_i^+)^2 = 0$].

There is no notion of occupancy of MFs, since if $n_i^{MF} = \gamma_i^+ \gamma_i = \gamma_i^2 = 1$.

$\Rightarrow$ for Majorana's $n_i^{MF} \equiv 1$.

Similarly: $\gamma_i \gamma_i^+ \equiv 1$ so that Majorana mode is always filled and always empty $\Rightarrow$ counting them does not make sence.

There are a number of states $|n_1 \ldots n_N\rangle$, which are eigenstates of fermion # operators $n_i = f_i^+ f_i$ with eigenvalue $n_i = 0, 1$.

If 2 MFs come close to each other, they one can combine them into a fermion. To describe an overlap, t, between γ_{2i-1} and γ_{2i}, the only term one can introduce into H is

$$\frac{i}{2} t \gamma_{2i-1} \gamma_{2i} = t\left(n_i - \frac{1}{2}\right)$$

which corresponds to a finite energy cost for occupying the corresponding fermionic state $(t > 0)$
If the MFs do not overlap, the ground state is 2^N degenerate, correspondin to each n_i being 0 or 1.

Interaction Hamiltonian

So far we discussed 1D non-interacting systems in 2nd quantization formulation. In fact, 2nd quantization is easily extended to interactions. Classically, we know that the interaction potential energy of a continuous system of particles is:

$$V_{class.} = \frac{1}{2}\int d^D r\, d^D r'\, V(r-r')\,\rho(r)\rho(r')$$

$\Rightarrow$ one may expect that $\frac{1}{2}\int d^D r\, d^D r' V(r-r')\,\hat{\rho}(r)\hat{\rho}(r')$ will be the second quantized expression for $\hat{H}_{int} = \hat{V}$.
This is wrong, as this expression includes energy contribution corresponding to a single particle interacting with itself.

The requirement is that the action of the potential on the vacuum, or a one-particle state, gives zero:

$$\hat{V}|0\rangle = \hat{V}|\vec{r}\rangle = 0.$$

To guarantee this, we need to be careful that we normal order the field operators, by permuting them so that all destruction operators are on the RHS.
All additional terms that are generated by permuting the operators are dropped, but the signs associated with the permutation are preserved:

$$:\rho(x)\rho(y): \; = \; :\psi^+(x)\psi(x)\psi^+(y)\psi(y): \; =$$

for fermions

$$= \mp :\psi^+(x)\psi^+(y)\psi(x)\psi(y): = -\psi^+(x)\psi^+(y)\psi(x)\psi(y)$$

for bosons

$$= \psi^+(y)\psi^+(x)\psi(x)\psi(y),$$

where one can remove : : once all annihilation operators are on the RHS.

$$\Rightarrow \quad \hat{V} = \frac{1}{2}\int d^D r\, d^D r'\, V(r-r') :\hat{\rho}(r)\hat{\rho}(r'):$$

$$= \sum_{\alpha,\beta} \int d^D r\, d^D r'\, V(r-r')\, \psi_\alpha^+(r')\psi_\beta^+(r)\psi_\beta(r)\psi_\alpha(r')$$

where we have writtem a more general expersion for fields with spin/pseudospin degrees of freedom α, β.

Let us now show that the action of $\hat{V}$ on the many-body state $|r_1 \dots r_N\rangle$ is given by:

$$\hat{V}|r_1 \dots r_N\rangle = \sum_{i<j} V(r_i - r_j)\, |r_1, r_2, \dots, r_N\rangle .$$

<u>Proof</u>: To prove this, let us show that

$$[\hat{V}, \psi^+(r)] = \int d^D r'\, \hat{V}(r-r')\, \hat{\psi}^+(r)\hat{\rho}(r')$$

We have $[\hat{V}, \psi^+(x)] = \frac{1}{2}\int dy\, dy'\, V(y-y')\psi^+(y)\psi^+(y') \times$

$$\times \underbrace{[\psi(y')\psi(y), \psi^+(x)]_{\mp}}_{\delta(y-x)\psi(y') \pm \delta(y'-x)\psi(y)} =$$

here lower sign is for fermions upper – for bosons

$$= \psi^+(x) \frac{1}{2} \int dy' \, V(x-y') \rho(y') \pm$$

$$\pm \frac{1}{2} \int dy \, V(y-x) \underbrace{\psi^+(y)\psi^+(x)}_{\pm \psi^+(x)\psi^+(y)} \psi(y) =$$

$$= \int dy \, V(x-y) \psi^+(x) \rho(y).$$

Let us now ~~calculate~~: $\hat{V}|x_1 \dots x_N\rangle = \hat{V}\psi^+(x_N) \dots \psi^+(x_1)|0\rangle$ by commuting $\hat{V}$ successively to the right until it annihilates with the vacuum. Each time we hop $\hat{V}$ to the right over a field operator, we generate a remainder term. Commuting $\hat{V}$ past the j-th creation operator:

$$\psi^+(x_N) \dots \hat{V}\psi^+(x_j) \dots \psi^+(x_1)|0\rangle = \psi^+(x_N) \dots \psi^+(x_j)\hat{V} \dots \psi^+(x_1)|0\rangle$$

$$+ R_j,$$

where $R_j = \int d y \, \psi^+(x_N) \dots V(y-x_j)\psi^+(x_j)\rho(y) \dots \psi^+(x_1)|0\rangle$

Using $\rho(y)\psi^+(x_i) = \psi^+(x_i)\rho(y) + \psi^+(x_i)\rho(y-x_i)$,

we can commute the density operator to the right until it annihilates the vacuum. The terms generated by this procedure can be written

$$R_j = \sum_{i=1}^{j-1} V(x_i - x_j)\psi^+(x_N) \dots \psi^+(x_j) \dots \psi^+(x_i) \dots \psi^+(x_1)|0\rangle$$

$$= \sum_{i=1}^{j-1} V(x_i - x_j)|x_1 \dots x_N\rangle.$$

Thus, our final result is the sum of R_j:

$$\hat{V}\,\psi^{+}(x_N)\ldots\psi^{+}(x_1)\,|0\rangle = \sum_{j=2}^{N} R_j =$$

$$= \sum_{i<j} V(x_i - x_j)\,|x_1 \ldots x_N\rangle .$$

This makes sence: the state $|x_1 \ldots x_N\rangle$ is an eigenstate of the interection operator, with eigenvalue given by the classical interaction potential energy.

Momentum space representation of the interection Hamiltonian

This is very useful in <u>translationally invariant</u> systems, where momentum is conserved in parti collisions.

Let us consider fermions with spin $= s$

$$\Rightarrow \quad \Psi_\sigma(x) = \int \frac{d\vec{k}}{(2\pi)^D}\, C_{\vec{k}\sigma}\, e^{i\vec{k}\cdot\vec{x}}$$

$$\Psi^{+}_\sigma(x) = \int \frac{d\vec{k}}{(2\pi)^D}\, C^{+}_{\vec{k}\sigma}\, e^{-i\vec{k}\cdot\vec{x}} ,$$

where $\{ C_{\vec{k}\sigma},\, C^{+}_{\vec{k}',\sigma} \} = (2\pi)^D\, \delta^D(\vec{k}-\vec{k}')\, \delta_{\sigma\sigma'}$, (take $D=3$) are canonical fermion operators in momentum space.

Interaction term gives:

$$V(x-x') = \int \frac{d\vec{q}}{(2\pi)^3}\, V(\vec{q})\, e^{i\vec{q}(\vec{x}-\vec{x}')} .$$

Substituting these expressions into $\hat{V}$ we obtain

$$\hat{V} = \frac{1}{2}\int d^3x\, d^3x'\, V(x-x')\, \psi^{+}_\alpha(x')\, \psi^{+}_\beta(x)\, \psi_\beta(x)\, \psi_\alpha(x') =$$

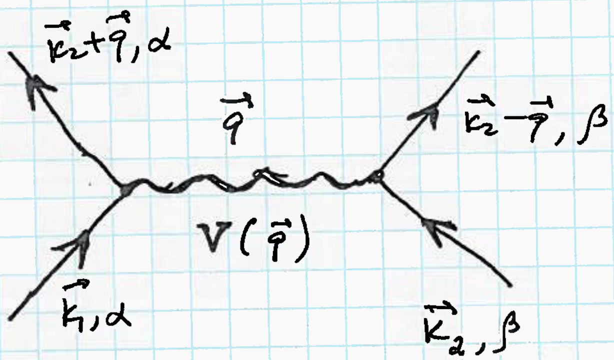
$$\hat{V} = \frac{1}{2}\sum_{\sigma\sigma'}\int \frac{d\vec{k}_1}{(2\pi)^3}\frac{d\vec{k}_2}{(2\pi)^3}\frac{d\vec{k}_3}{(2\pi)^3}\frac{d\vec{k}_4}{(2\pi)^3}\frac{d\vec{q}}{(2\pi)^3} V(\vec{q})\, C^{+}_{\vec{k}_4,\sigma} C_{\vec{k}_3,\sigma'} C_{\vec{k}_2\sigma'} C_{\vec{k}_1\sigma} \times$$

$$\times \underbrace{\int d^3x\, d^3x'\, e^{i(\vec{k}_1-\vec{k}_4+\vec{q})\vec{x}}\, e^{i(\vec{k}_2-\vec{k}_3-\vec{q})\vec{x}'}}_{=(2\pi)^6\delta^{(3)}[\vec{k}_4-\vec{k}_1-\vec{q}]\,\delta^{(3)}[\vec{k}_3-\vec{k}_2+\vec{q}]}.$$

Special integral here imposes momentum conservation at each scattering event. Thus we find

$$\hat{V} = \frac{1}{2}\sum_{\alpha,\beta}\int \frac{d\vec{k}_1}{(2\pi)^3}\frac{d\vec{k}_2}{(2\pi)^3}\frac{d\vec{q}}{(2\pi)^3} V(\vec{q})\, C^{+}_{\vec{k}_1+\vec{q},\alpha} C^{+}_{\vec{k}_2-\vec{q},\beta} C_{\vec{k}_2\beta} C_{\vec{k}_1\alpha}$$

$\Rightarrow$ when particles scatter at positions x, x', momentum is conserved.



Part. 1: $\vec{k}_1 \to \vec{k}_1+\vec{q}$

Particle 2: $\vec{k}_2 \to \vec{k}_2-\vec{q}$.

The matrix element associated with this scattering is the Fourier transform of the potential $V(\vec{q})$.

<u>Example:</u> δ-function interaction: $V(x) = U a^3 \delta^{(3)}(x)$

$\Rightarrow$ $V(q) = \int d^3x\, U a^3 \delta(x)\, e^{-i\vec{q}\vec{x}} = U(a^3)$ $\Rightarrow$ the interaction Hamiltonian in momentum space is:

$$\hat{V} = \sum_{\alpha,\beta}\frac{Ua^3}{2}\int \frac{d\vec{k}_1}{(2\pi)^3}\frac{d\vec{k}_2}{(2\pi)^3}\frac{d\vec{q}}{(2\pi)^3} C^{+}_{\vec{k}_1-\vec{q},\alpha} C^{+}_{\vec{k}_2+\vec{q},\beta} C_{\vec{k}_2\beta} C_{\vec{k}_1\alpha}$$

~~Cou~~ Screened Coulomb (Yukawa) potential:

$$V(r) = \frac{A e^{-\lambda r}}{r}$$

$$\Rightarrow \quad \hat{V} = \frac{1}{2} \sum_{\alpha,\beta} \frac{d\vec{k}_1}{(2\pi)^3} \frac{d\vec{k}_2}{(2\pi)^3} \frac{d\vec{q}}{(2\pi)^3} V(\vec{q}) C^+_{\vec{k}_1+\vec{q}\alpha} C^+_{\vec{k}_2-\vec{q}\beta} C_{\vec{k}_2\beta} C_{\vec{k}_1\alpha},$$

where $V(\vec{q}) = \int d^3\vec{r} \, \frac{A e^{-\lambda r}}{r} e^{-i\vec{q}\vec{r}} =$

$$= \int_0^\infty 4\pi r^2 dr \, V(r) \underbrace{\frac{1}{2} \int_{-1}^{1} d\cos\theta \, e^{-iqr\cos\theta}}_{= \frac{\sin qr}{qr}} =$$

$$= \frac{4\pi A}{q} \int_0^\infty dr e^{-\lambda r} \sin(qr) = \frac{4\pi A}{q^2+\lambda^2}, \quad \text{where}$$

we used $d^3\vec{r} = r^2 d\phi \, d\cos\theta \to 2\pi r^2 d\cos\theta$ in polar coordinates.

In case of Coulomb interaction: $V(r) = \frac{e^2}{4\pi\varepsilon_0 r} \Rightarrow$

$$\Rightarrow V(\vec{q}) = \frac{e^2}{q^2 \varepsilon_0} \quad \text{– in 3D.}$$

Quantum mechanics of a single particle

Consider a nonrelativistic particle. Our aim here is to show the connection between quantum-mechanical perturbation theory and Green's functions and diagrammatic technique.

Dynamics of a nonrelativistic particle is given by

$$i\hbar \frac{\partial \psi(r,t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi(r,t) + V(r)\psi(r,t).$$

In QM people usually are interested in finding the energy spectrum of the system and transition amplitudes caused by the scattering or time-dependent external field.

The first problem demands solving stationary Schroedinger eq.

$$\varepsilon\psi(r) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right)\psi(r).$$

Discrete spectrum here corresponds to bound states, while the continuous one corresponds to free states.

The wavefunction $\psi_k(r) = e^{i\vec{k}\vec{r}} + \chi_k(r)$

corresponds to the scattering of the free wave $e^{i\vec{k}}$ by a potential $V(\vec{r})$, where $\chi_k(r)$ has an asymptotic form of a spherical wave:

$$\chi_k(r) = f(\vec{k}, k\cdot\vec{n}) \cdot \frac{e^{ik|r|}}{|r|}, \quad r \to \infty$$

where $\vec{n} = \frac{\vec{r}}{r}$. Function $f\left(\vec{k}, k\cdot\frac{\vec{r}}{r}\right)$ is the so called scattering amplitude.

Let us solve the Schroedinger equation perturbatively; i.e. by writing it in powers of $V(r)$

$$\psi(r) = \psi^0(r) + \psi^{(1)}(r) + \psi^{(2)}(r) + \ldots$$

Easy to see, that one will have:

$$\left(\mathcal{E} + \frac{\hbar^2}{2m}\nabla^2\right)\psi^{(0)}(\vec{r}) = 0$$

$$\left(\mathcal{E} + \frac{\hbar^2}{2m}\nabla^2\right)\psi^{(1)}(\vec{r}) = V(\vec{r})\,\psi^{(0)}(\vec{r})$$

$$\left(\mathcal{E} + \frac{\hbar^2}{2m}\nabla^2\right)\psi^{(2)}(\vec{r}) = V(\vec{r})\,\psi^{(1)}(\vec{r})$$

$$\ldots$$

The solution of the free Schroedinger eq is can be chosen as

$\psi^{(0)}(r) = \exp(i\,\vec{k}\cdot\vec{r})$. If potential $V(r)$ is weak, it would be sufficient to account for first few equations here.

Formally, these series ~~[illegible]~~ give correct results even if $V(r)$ is strong, if one analytically continues these series ~~[illegible]~~ over ε from high-energies when $|\varepsilon| \gg V(r)$, where the series are convergent.

In order to establish a connection with diagrammatic technique, consider the Green's function corresponding to ~~t~~ Schroedinger eq:

$$\left[i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 - V(r)\right] G(\vec{r}, t; \vec{r}\,', t') = \delta(t-t')\,\delta(\vec{r}-\vec{r}\,').$$

If $V(r)=0$, the motion is free

$$G_0(t-t', \vec{r}-\vec{r}\,') = \iint \frac{d\varepsilon}{2\pi} \frac{d^3p}{(2\pi)^3}\, G_0(\varepsilon, \vec{p})\, e^{i\vec{p}(\vec{r}-\vec{r}\,') - i\varepsilon(t-t')},$$

$$G_0(\varepsilon, \vec{p}) = \frac{1}{\varepsilon - p^2/2m + i\delta}$$

The sign of the imaginary part $+i\delta$ is ~~ta~~ chosen in such a way, that $G_0(\varepsilon, \vec{p})$ is regular in upper half-plane of complex ε. This condition insures causality:

$G_0(t-t') = 0$ at $t<t'$. In general, the Greens function can be written as

$$= \left[i\frac{\partial}{\partial t} - \frac{\hat{p}^2}{2m} - V(r) \right]^{-1} = \left(G_0^{-1} - \hat{V} \right)^{-1} = \left(1 - \hat{V}\hat{G}_0 \right)^{-1} \hat{G}_0 .$$

f small $V(r)$, this expression can be expanded:

$$\hat{G} = \hat{G}_0 + \hat{G}_0 \hat{V} \hat{G}_0 + \hat{G}_0 \hat{V} \hat{G}_0 \hat{V} \hat{G}_0 + \dots$$

Interacting particles:

Construction of diagrams:

e Green's function gives an information about the ground state of the system and about the excitations.

The Green's function is

$$G(x_2, x_1) = -i \langle T \psi(x_2) \psi^+(x_1) \rangle =$$

For noninteracting fermions:

$$G_0(\varepsilon, \vec{p}) = \frac{1}{\varepsilon - \xi(\vec{p}) + i\delta(\vec{p})} = n_p G_A + (1 - n_p) G_R .$$

Here $\xi(p) = \frac{p^2}{2m} - E_F$ - fermion dispersion relation. The sign of the imaginary part depends on the occupation of the state with $\vec{p}$ - momentum:

$$\delta(\vec{p}) = 0 \cdot \text{sign}\left[\xi(\vec{p})\right] = \begin{cases} +0, & \text{if the state is empty} \\ -0, & \text{if it is occupied.} \end{cases}$$

Perturbation theory for the Green's function admits a graphical representation.

For a 2-particle interaction

$$U(x-x') = U(r-r', t-t')$$

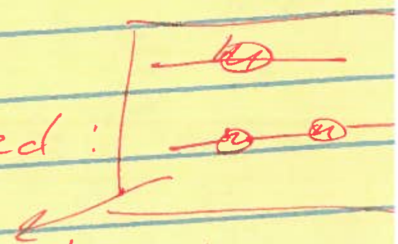
we have:

1) All diagrams consist of 2-elements: . → describes particle spreading, → corresponds to interactions between particles

2) One has vertices:  as constituent elements of diagrams

3) n-th order (in interaction) diagrams contain 2n vertices. If one is computing a Green's function ⇒ the diagram must have 2 external ends:

G = 

4) All diagrams must be connected: 

e.g., cannot have this.

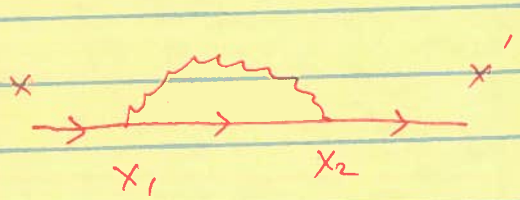
5) We associate a Green's function with each line $\underset{x \qquad x'}{\longrightarrow} = G_0(x-x')$, where x is the initial point and x' is the final one. Each wavy line is associated with the $\underset{x \quad x'}{\sim\sim} = U(x-x')$.

6). The expression of the diagram must be integrated over all vertex coordinates.

7) Each diagram comes with a factor $i^n(-1)^F$, where n is # of wavy lines (order of diagram), F is # of closed fermion loops:

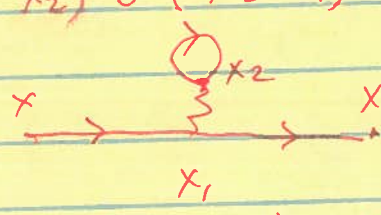
Examples:

a) $\delta G_a =$



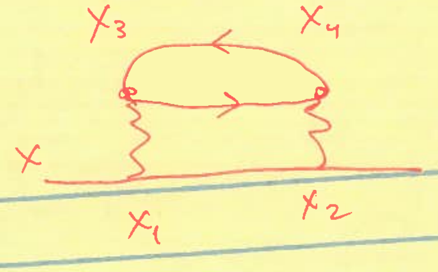
$= i\int d^4x_1\, d^4x_2\, G(x_1-x)\, G(x_2-x)$ $\times\, G(x'-x_2)\, U(x_2-x_1)$

b) $\delta G_b =$



$= -i\int d^4x_1\, d^4x_2\, G(x_1-x)\, G(0)\, \times$ $\times\, G(x'-x_1)\, U(x_2-x_1)$.

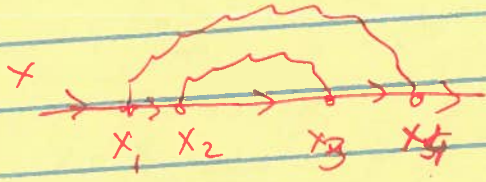
c) $\delta G_c =$



$=$

$$= \int d^4x_1\, d^4x_2\, d^4x_3\, d^4x_4\, G(x_3-x_4)\, G(x_4-x_3)\, G(x_2-x_1) \times$$
$$\times G(x'-x_2)\, G(x_1-x)\, U(x_3-x_1)\, U(x_4-x_2)$$

d) $\delta G_d =$

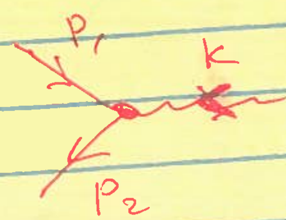


$=$

$$= -\int d^4x_1\, d^4x_2\, d^4x_3\, d^4x_4\, G(x_3-x_2)\, G(x_4-x_3)\, G(x_2-x_1) \times$$
$$\times G(x'-x_4)\, G(x_1-x)\, U(x_4-x_1)\, U(x_3-x_2).$$

Sometimes, momentum representation of diagrams is more convenient to deal with.

Then one uses Fourier transformed form of G and U, and each vertex ~~has mom~~ leads to momentum conservation: $\sim (2\pi)^4\, \delta(p_1 + k - p_2)$, where p_{i}, k are 4-momenta $(\vec{p}, \omega)$.



$\sim (2\pi)^4\, \delta(p_1 + k - p_2).$

In CM physics, there are several interacting situations with interactions.

* Coulomb interaction: $U(\omega, k) = \dfrac{4\pi e^2}{\varepsilon(\omega)|\vec{k}|^2}$, $k \gg \omega/c$,

where $\varepsilon(\omega)$ is dielectric permittivity

$$U(\vec{r}-\vec{r}\,', t-t') = \frac{e^2}{|\vec{r}-\vec{r}\,'|} \cdot \int \frac{e^{-i\omega(t-t')}}{\varepsilon(\omega)} \frac{d\omega}{2\pi}.$$

* Electron-phonon interaction

$U(\omega, \vec{k}) = g^2 D(\omega, \vec{k})$, g is interaction constant

$D(\omega, k) = \dfrac{\omega_0^2(\vec{k})}{\omega^2 - \omega_0^2(\vec{k}) + i0}$ - phonon's Green's function.

For acoustical phonons $\omega_0(\vec{k}) = c|\vec{k}|$, c is speed of light.