Quantum Many-Body Physics

Lectures: Michael Knap

Monday 8:30 - 10:00 H3
Wednesday 16:00 - 17:30 H2

TAs: Stefan Birnkammer, Julian Bösl, Gloria Isbrandt, Caterina Zerba

Open tutorial: Mondays 10:00 - 11:30 HS 3344 / zoom
Tutorials: Wednesdays 10:00 - 12:00 HS 3344 / zoom

Literature: Altland and Simons "Condensed Matter Field theory"
Subir Sachdev "Quantum phases of matter" (2023)
Girvin and Yang "Modern Condensed Matter Physics" (2019)
Chaikin and Lubensky "Principles of Condensed Matter Physics"
Coleman "Introduction to QMB physics"
Wen, "Quantum Field Theory of Many-Body Systems"

Why should I attend this Lecture course?

- P.W. Anderson: "More is different"
- Modern introduction many-body physics
- Comprehensive review of basic tools and theoretical methods
- applications to various condensed matter problems and comparison to experiments

1. Introduction

- Motivation
- Recap of classical phases and mean field theory
- Quantum phases of matter
- Second quantization

When many particles interact, new physics can emerge!

A single H_2O molecule is neither a liquid, solid, or gas but 10^{23} of them are!

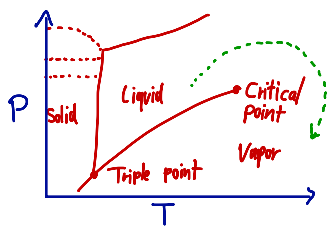
Underlying "fundamental" model "well" known:

$$\hat{T}_n = -\sum_i \frac{\hbar^2}{2M_i}\nabla^2_{\mathbf{R}_i} \quad \hat{T}_e = -\sum_i \frac{\hbar^2}{2m_e}\nabla^2_{\mathbf{r}_i} \quad \hat{U}_{ee} = \frac{1}{2}\sum_i\sum_{j\neq i}\frac{e^2}{4\pi\epsilon_0\,|\mathbf{r}_i-\mathbf{r}_j|} = \sum_i\sum_{j>i}\frac{e^2}{4\pi\epsilon_0\,|\mathbf{r}_i-\mathbf{r}_j|}$$

$$\hat{U}_{nn} = \frac{1}{2}\sum_i\sum_{j\neq i}\frac{Z_iZ_je^2}{4\pi\epsilon_0\,|\mathbf{R}_i-\mathbf{R}_j|} = \sum_i\sum_{j>i}\frac{Z_iZ_je^2}{4\pi\epsilon_0\,|\mathbf{R}_i-\mathbf{R}_j|}. \quad \hat{U}_{en} = -\sum_i\sum_j\frac{Z_ie^2}{4\pi\epsilon_0\,|\mathbf{R}_i-\mathbf{r}_j|}$$

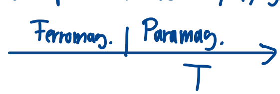
⇝ What are the possible phases of matter?
⇝ What are the universal properties?
⇝ Interplay between quantum fluctuations and interactions?

Examples: - Water:

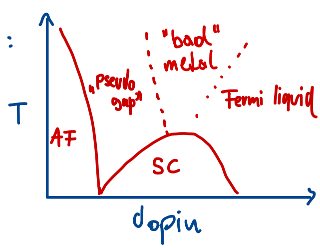


Solid phase(s) vs. liquid/gas phase

- Ferromagnet: (magnetite)



- Superconductor: (cuprates)



Phase transitions

- As we tune any parameter $(p, T, \dots)$, the free energy $F = U - TS$ is continuous
- Classify phase transitions according to singularities of the derivatives of F (First- or second order)

1.1 Mean-field theory of phase transitions for classical phase transitions

(Later we will see deep connections between quantum and classical phase transitions)

Different phases of matter are distinguished by spontaneous symmetry breaking, i.e., the state has a lower symmetry than the Hamiltonian.

Example: Ising model $\uparrow \downarrow \downarrow \downarrow$ with spins $+1 \; -1 \; -1 \; -1$

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - B \cdot \sum_i \sigma_i \qquad , \; \sigma_i = \pm 1 \, , \; J > 0$$

For now $B = 0$ with $\mathbb{Z}_2$ symmetry : H invariant under global spinflip

$T = 0$: Ground state $\uparrow\uparrow\uparrow\uparrow$, $\downarrow\downarrow\downarrow\downarrow$ $\rightsquigarrow$ breaks $\mathbb{Z}_2$ symmetry ! $m = \langle \sigma_i \rangle \neq 0$

magnetization

$T = \infty$: Entropy dominates : no preferred direction $\rightsquigarrow$ no symmetry breaking $m = \langle \sigma_i \rangle = 0$

Reminder : Canonical Ensemble

$$P(\{\sigma_i\}) = \frac{1}{Z} \cdot \exp\left[-\beta H(\{\sigma_i\})\right] , \; \beta = \frac{1}{k_B T}$$

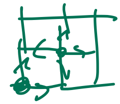
$$Z = \sum_{\{\sigma_i\}} \exp\left[-\beta H(\{\sigma_i\})\right]$$

$$\langle X \rangle = \sum_{\{\sigma_i\}} P(\{\sigma_i\}) \cdot X(\{\sigma_i\}) , \quad F = -\frac{1}{\beta} \ln Z \qquad (Z = e^{-\beta F})$$

Assume that fluctuations around m are small $\qquad m = \frac{1}{N}\sum_i \langle\sigma_i\rangle$

$$\overbrace{(\sigma_i - m)}^{\delta\sigma_i}\,\overbrace{(\sigma_j - m)}^{\delta\sigma_j} \approx 0$$

$$\sigma_i\sigma_j = m(\sigma_i + \sigma_j) - m^2$$



$N\cdot 2$

$\frac{1}{2}N\cdot q$

Mean-field Hamiltonian: $H = -J\sum_{\langle i,j\rangle}\left[m(\sigma_i+\sigma_j) - m^2\right] - B\sum \sigma_i$

$$= \frac{1}{2}J\cdot N\cdot \underset{\text{coordination number}}{q}\cdot m^2 - \overbrace{(Jqm + B)}^{B_{eff}}\cdot\sum_i \sigma_i$$

Partition function: $\mathrm{tr}\, e^{-\beta H_1} = e^{-\beta\left[\frac{1}{2}Jqm^2\right]}\left(e^{+\beta B_{eff}} + e^{-\beta B_{eff}}\right)$

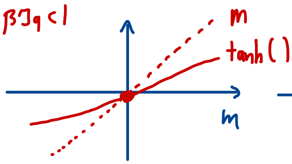
$$Z = (Z_1)^N = \exp\left[-\frac{1}{2}\beta JNqm^2\right]\cdot 2^N\cdot\cosh^N\left[\beta B_{eff}\right]$$

Free energy:

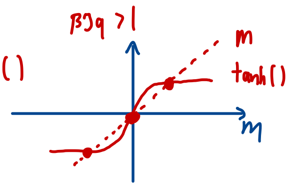
$$F = -\frac{1}{\beta}\ln Z = \frac{1}{2}JNqm^2 - \frac{N}{\beta}\cdot\ln\left[2\cdot\cosh\left[\beta(Jqm + B)\right]\right]$$

Minimize F: $\frac{\partial F}{\partial m} = 0 \rightsquigarrow m = \tanh\left[\beta(qJm + B)\right]$

$B = 0$:



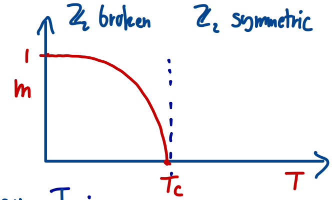
$\rightsquigarrow m = 0$



$\rightsquigarrow m = \pm m_0$ ($m = 0$ not stable)

Local orderparameter m: $\begin{cases} m = 0 : \text{disordered phase} \\ m \neq 0 : \text{ordered phase}\end{cases}$

Phase diagram:



Asymptotic dependence near T_c:

$$m_0 = \beta q J m_0 - \frac{1}{3}(\beta q J)^3 \cdot m_0^3 + \cdots \rightsquigarrow m_0(T) \propto \left(\frac{T_c}{T} - 1\right)^{1/2}$$

$1/2$ mean field exp. $\neq$ exact!

$$\propto \left(\frac{T_c - T}{T}\right)^{1/2}$$

Comment 1: Mean field approach exact for infinite dimensions and fails for low dimensions (e.g., there is no phase transition for the Ising model in 1D)
Scaling differs from exact results for $D < D_c$ (critical dimension)

Comment 2: There is a lot of exciting stuff missed! Topological classification!

1.2 Landau theory

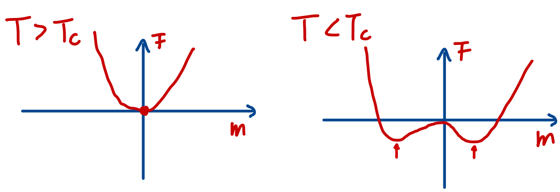
① Identify the symmetry group G of the Ham. and order parameter m that transforms under this symmetry (e.g., Ising $m \to -m$)

② Assume a free energy functional $F = F_0(T) + F_1(T, m)$ which obeys all symmetries G. Typically we consider a polynomial expansion (e.g. $F = F_0(T) + a(T) \cdot m^2 + b(T) \cdot m^4 + \cdots$; where $a(T) \propto (T - T_c)$)

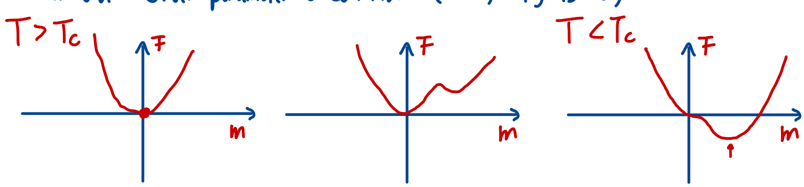
analytic function

Temperature dependence

③ Find minima of F



Second order: Order parameter is continuous (e.g., Ising $B=0$)



First order: Jump in order parameter (e.g. melting of a crystal)

Landau theory can be extendet to include spatial fluctuations

$$m \to \phi(x)$$

the free energy is a functional of $\phi(x)$: $F[\phi(x)]$

expand $F[\phi(x)]$ near a critical point in terms of $\phi(x)$ and its gradient $\nabla\phi(x)$

$$F = F_0 + \int d^d x \left\{ \frac{1}{2} [c (\nabla\phi)^2 + a(\phi(x))^2 + \frac{b}{4!} (\phi(x))^4 \right\}$$

From this functional, spatially dependent correlations can be extracted.

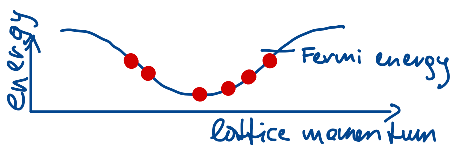
1.3 Quantum phases

Quantum matter can be in various distinct phases.

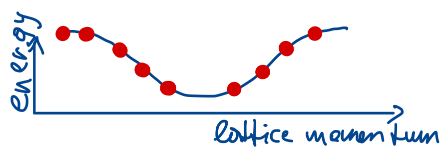
Metals and Band insulators

Described by independent electrons obeying Fermi-Dirac statistics.
Theory developed by Sommerfeld in 1928.

Metal



Band insulator



Symmetry broken states:

Superconductors, Antiferromagnets, Charge density waves, ...

The goal of this lecture will be to understand these types of states and to develop a theoretical tool box that allows us to characterize them

Entangled Quantum Matter

States cannot be adiabatically connected to independent electron states (or single-particle states).

Topological order is important for understanding these states. Defined by quantum entanglement.

Quantum phase transitions

Further reading: Sachdev, Cam. Uni. Press, '11

Quantum many-body systems can undergo zero temperature phase transitions between quantum phases of matter driven by quantum fluctuations.

Phase transitions driven by quantum fluctuations at zero temperature.

Suppose we have a many-body system at $T=0$ (No thermal fluctuations).

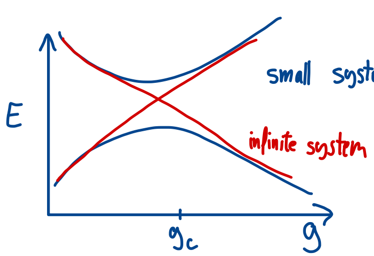
Hamiltonian $\hat{H} = \hat{H}_0 + g\,\hat{H}_1$ depends on parameter g.

Ground state (GS): $\hat{H}|\Psi_0\rangle = E_0|\Psi_0\rangle$

Singularities in $|\Psi_0(g)\rangle$: QPT

These singularities might involve a sudden change of $|\Psi_0\rangle$ or a diverging correlation length.

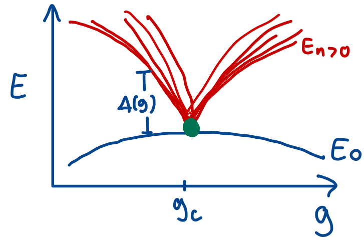
First order

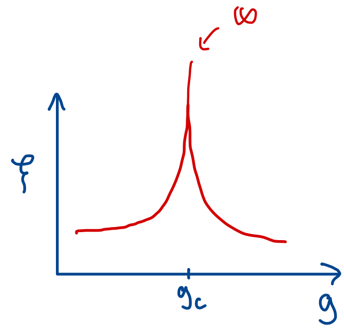


⇝ GS energy non-analytic at g_c.

⇝ In presence of symmetries, level crossing also possible in finite systems.

Second order





⇝ diverging correlation length ξ and closing of gap Δ at quantum critical point (QCP).

QCP have universal scaling properties, e.g., $\frac{1}{\xi} \sim |g-g_c|^{\nu}$ with correlation length exponent ν.

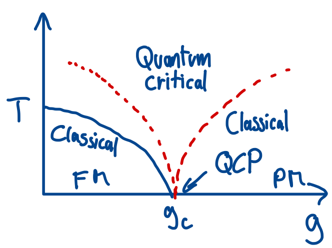
Gap Δ (between GS and continuum): $\Delta \sim \frac{1}{\xi^z} = |g-g_c|^{z\nu}$ with dynamical critical exponent z.

Finite T crossover

$\hat{=}$ zero entropy

A QCP is a property of 'pure' quantum states (usually the GS) and thus it only occurs at $T=0$!

Still useful to derive properties of a system over range of parameters.



Example: 2D Ising transition between FM and PM has 2+1 D Ising universality at $T=0$ and 2D Ising at finite T.

Quantum critical regime: Universal properties inheritated from QCP at finite T
⇝ experimentally relevant.

1.4 Second quantization

Second quantization is a technique that we will use extensively to formulate quantum many-body theories.

Further reading: Altland & Simons Ch. 2

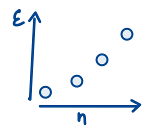
Particle statistics

N indistiguishable particles $\rightsquigarrow$ Wave function is symmetric (antisymmetric) with respect to the exchange of two bosons (fermions).

$$\Psi(x_1,\dots,x_i,\dots x_j,\dots,x_N) = \eta\,\Psi(x_1,\dots,x_j,\dots x_i,\dots,x_N) \quad \text{with } \eta = \begin{cases} +1 & \text{bosons} \\ -1 & \text{fermions} \end{cases}$$

While in 3D, these are the only options, more exotic cases exist in 2D (anyons).

Example: Consider a single particle Hamiltonian with $\hat{h}|\lambda_n\rangle = \varepsilon_n|\lambda_n\rangle$



Normalized and symmetrized wave functions for two particles are:

Fermions: $\Psi_-(x_1,x_2) = \frac{1}{\sqrt{2}}\left(\langle x_1|\lambda_1\rangle\langle x_2|\lambda_2\rangle - \langle x_1|\lambda_2\rangle\langle x_2|\lambda_1\rangle\right)$
(Slater determinant)

eigenstates of $\hat{h}$
eigenstates of $\hat{x}$

Bosons: $\Psi_+(x_1,x_2) = \frac{1}{\sqrt{2}}\left(\langle x_1|\lambda_1\rangle\langle x_2|\lambda_2\rangle + \langle x_1|\lambda_2\rangle\langle x_2|\lambda_1\rangle\right)$
(Permanent)

Using Dirac notation, this can be written independently of the basis $|\Psi\rangle_{-/+} = \frac{1}{\sqrt{2}}\Big(\underbrace{|\lambda_1\rangle|\lambda_2\rangle}_{\hat{=}\,|\lambda_1\rangle\otimes|\lambda_2\rangle} -/+ |\lambda_2\rangle|\lambda_1\rangle\Big)$.

tensor product

For N particles we find

$\eta = \begin{matrix} +1 & \text{Bosons} \\ -1 & \text{Fermion} \end{matrix}$

sgn P is +1 (-1) for even (odd) permutations.

$$|\Psi)_{+/-} = \frac{1}{\sqrt{N! \prod_\lambda (n_\lambda !)}} \cdot \sum_P \eta^{(1-\operatorname{sgn} P)/2} |\lambda_{P_1}) |\lambda_{P_2}) \cdots |\lambda_{P_N})$$

Sum over all $N!$ permutations.

P	sgn P
123	1
132	-1
312	1
231	1
213	-1

with n_λ being the number of particles in state λ.

For Fermions we have $n_\lambda \leq 1$ (Pauli exclusion).

Note: Explicit symmetrization of the wave function is necessitated by the indistinguishability of the particles.

Second Quantization

Basic idea: Introduce an occupation number n_i of state $|\lambda_i)$ to avoid redundancies in the description of the many-body state.

Encode the state by the number of particles occupying a single particle state $|\lambda_i)$:

$$|n_1 n_2 \cdots\cdots) \quad \text{with} \quad n_i = \begin{cases} 0,1 & \text{Fermions} \\ 0,1,2,\ldots & \text{Bosons} \end{cases}$$

⇝ Total number $N = \sum n_i$

⇝ Fock space $\mathcal{F} = \bigoplus_{N=0}^{\infty} \mathcal{F}^N$, $\mathcal{F}^N$ is a Hilbert space with N particles. ($\mathcal{F}^0$ is the vacuum)

Let us now introduce operators acting on the Fock space, $\hat{a}^+ : \underline{\mathcal{F}} \to \underline{\mathcal{F}}$

$$\hat{a}_i^+ |n_1, n_2, \cdots, n_i, \ldots) = \sqrt{n_i + 1}\, \eta^{s_i} |n_1, n_2, \cdots, n_i + 1, \cdots),$$

where $s_i = \sum_{j=1}^{i-1} n_j$. For Fermions, the n_i are defined mod 2 $(1+1=0)$.

Specifically, we find:

Bosons: $\hat{b}^{+}_{\alpha} \,|\ldots, n_{\alpha}, \ldots\rangle = \sqrt{n_{\alpha}+1}\; |\ldots, n_{\alpha}+1, \ldots\rangle$ (creation operator)

$\hat{b}_{\alpha} \,|\ldots, n_{\alpha}, \ldots\rangle = \sqrt{n_{\alpha}}\; |\ldots, n_{\alpha}-1, \ldots\rangle$ (annihilation operator)

$$\underbrace{\hat{b}^{+}_{\alpha}\hat{b}_{\alpha}}_{:=\hat{n}_{\alpha}} |\ldots, n_{\alpha}, \ldots\rangle = n_{\alpha} |\ldots, n_{\alpha}, \ldots\rangle$$

$$[\hat{b}^{+}_{\alpha}, \hat{b}^{+}_{\beta}] = [\hat{b}_{\alpha}, \hat{b}_{\beta}] = 0, \quad [\hat{b}_{\alpha}, \hat{b}^{+}_{\beta}] = \hat{b}_{\alpha}\hat{b}^{+}_{\beta} - b^{+}_{\beta} b_{\alpha} = \delta_{\alpha\beta}$$

Fermions: $\hat{c}^{+}_{\alpha} |\ldots, n_{\alpha}, \ldots\rangle = (-1)^{\sum_{\beta<\alpha} n_{\beta}} (1-n_{\alpha}) |\ldots, n_{\alpha}+1, \ldots\rangle$

$$\hat{c}_{\alpha} |\ldots, n_{\alpha}, \ldots\rangle = (-1)^{\sum_{\beta<\alpha} n_{\beta}} n_{\alpha} |\ldots, n_{\alpha}-1, \ldots\rangle$$

$$\underbrace{\hat{c}^{+}_{\alpha}\hat{c}_{\alpha}}_{:\hat{n}_{\alpha}} |\ldots, n_{\alpha}, \ldots\rangle = n_{\alpha} |\ldots, n_{\alpha}, \ldots\rangle$$

$$\{\hat{c}^{+}_{\alpha}, \hat{c}^{+}_{\beta}\} = \{\hat{c}_{\alpha}, \hat{c}_{\beta}\} = 0, \quad \{\hat{c}_{\alpha}, \hat{c}^{+}_{\beta}\} = \hat{c}_{\alpha}\hat{c}^{+}_{\beta} + \hat{c}^{+}_{\beta}\hat{c}_{\alpha} = \delta_{\alpha\beta}$$

↑ anti commutator

$$\begin{tikzcd}
\boxed{\mathcal{F}^0} \arrow[r, bend left, "\hat{a}^{+}"] & \boxed{\mathcal{F}^1} \arrow[l, bend left, "\hat{a}"] \arrow[r, bend left, "\hat{a}^{+}"] & \boxed{\mathcal{F}^2} \arrow[l, bend left, "\hat{a}"]
\end{tikzcd}$$

Generate an arbitrary number state:

$$|n_1\, n_2 \ldots\rangle = \prod_i \frac{1}{\sqrt{n_i!}} (a^{+}_i)^{n_i} \;|0\rangle$$

↑ empty vaccum state

Basis transformations

Creation operators $\hat{b}^{+}_{\lambda_i}$ ($\hat{c}^{+}_{\lambda_i}$) are defined with respect to a single particle state $|\lambda_i\rangle$.

Perform a basis transformation : $|\mu_j\rangle = \underbrace{\sum_{\lambda_i} |\lambda_i\rangle\langle\lambda_i|}_{\text{Identity}}\mu_j\rangle$

$$|\lambda_i\rangle = a^{+}_{\lambda_i}|0\rangle \qquad |\mu_j\rangle = a^{+}_{\mu_j}|0\rangle$$

$$\rightsquigarrow \hat{a}^{+}_{\mu_j} = \sum_{\lambda_i} \hat{a}^{+}_{\lambda_i}\langle\lambda_i|\mu_j\rangle \; , \; \hat{a}_{\mu_j} = \sum_{\lambda_i} \hat{a}_{\lambda_i}\langle\mu_j|\lambda_i\rangle .$$

Example : real to momentum space

$$|k\rangle = \int d^D x \; |x\rangle \underbrace{\langle x|k\rangle}_{\frac{1}{L^{D/2}} \cdot e^{ikx}} \rightsquigarrow \hat{a}^{+}_{k} = \frac{1}{L^{D/2}} \int d^D x \; e^{ikx} \, \hat{a}^{+}_{x}$$

Representation of one-body operators

$$\hat{V}^{(1)}(r) = \underbrace{\sum_{i=1}^{N} \hat{v}^{(1)}(r_i)}_{=:\,\hat{V}_i^{(1)}} \qquad \text{(e.g., density operators).}$$

These one-body operators act on a particle at position r_i.

Choose a single-particle basis of eigenstates of $\hat{v}_i^{(1)}$ with

$$\hat{v}_i^{(1)}|\lambda_i) = v_i^{(1)}|\lambda_i) \rightsquigarrow \hat{V}^{(1)}|\lambda_1\lambda_2\cdots\lambda_N) = \Big(\sum_i v_i^{(1)}\Big)|\lambda_1,\lambda_2,\ldots,\lambda_N).$$

This can now be directly rewritten in terms of the occupation basis

$$\hat{V}^{(1)}|n_1,n_2,\ldots) = \Big(\sum_i v_i^{(1)} n_i\Big)|n_1,n_2,\ldots)$$

$$\rightsquigarrow \hat{V}^{(1)} = \sum_i v_i^{(1)} \underbrace{\hat{a}_i^{+}\hat{a}_i}_{=\hat{n}_i} = \sum_i (\lambda_i|\hat{V}_i^{(1)}|\lambda_i)\,\hat{a}_i^{+}\hat{a}_i .$$

For a generic basis, we find $\boxed{\hat{V}^{(1)} = \sum_{\mu,\nu} \hat{a}_\mu^{+} V_{\mu\nu}\hat{a}_\nu}$ with $V_{\mu\nu} = (\mu|\hat{V}^{(1)}|\nu)$.

Examples:

	1st quantization	2nd quantization
Density operator	$\hat{\varrho}(x) = \sum_{i=1}^{N}\delta(x-\hat{x}_i)$	$\hat{\varrho}(x) = \hat{a}^{+}(x)\,\hat{a}(x)$
on-site potential	$\hat{U} = \sum_{i=1}^{N} U(\hat{x}_i) = \int d^Dx\, U(x)\,\hat{\varrho}(x)$	$\hat{U} = \int d^Dx\, U(x)\,\hat{a}^{+}(x)\hat{a}(x)$
kinetic energy	$\hat{T} = \sum_i \frac{\hat{p}_i^2}{2m}$	$\hat{T} = \int_k \frac{\hbar^2k^2}{2m}\,\hat{a}_k^{+}\hat{a}_k$

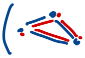
Representation of two-body operators

Choose a basis in which the interaction is diagonal:

$$\hat{V}^{(2)}|\alpha\gamma\rangle = V_{\alpha\gamma}\;|\alpha\gamma\rangle$$

with $V_{\alpha\gamma} = \langle\alpha\gamma|\hat{V}|\alpha\gamma\rangle \rightsquigarrow$ Proceed as in one body case.

We write $\hat{V} = \frac{1}{2}\sum_{\alpha\gamma} V_{\alpha\gamma}\hat{P}_{\alpha\gamma}$, where $\hat{P}_{\alpha\gamma}$ counts the number of pairs of particles in the states $|\alpha\rangle$ and $|\gamma\rangle$.

$|\alpha\rangle = |\gamma\rangle \rightsquigarrow \hat{n}_\alpha(\hat{n}_\alpha - 1)$ pairs ()

$|\alpha\rangle \neq |\gamma\rangle \rightsquigarrow \hat{n}_\alpha \cdot \hat{n}_\gamma$ pairs ()

Thus we find using the commutation relations: $\hat{P}_{\alpha\gamma} = \hat{a}^+_\alpha \hat{a}^+_\gamma \hat{a}_\gamma \hat{a}_\alpha$

and consequently $\hat{V}^{(2)} = \frac{1}{2}\sum_{\alpha\gamma} V^{(2)}_{\alpha\gamma}\hat{a}^+_\alpha \hat{a}^+_\gamma \hat{a}_\gamma \hat{a}_\alpha = \frac{1}{2}\sum_{\alpha\gamma}\langle\alpha\gamma|\hat{V}^{(2)}|\alpha\gamma\rangle \hat{a}^+_\alpha \hat{a}^+_\gamma \hat{a}_\gamma \hat{a}_\alpha$.

Next we transform this expression into an arbitrary basis $|\mu\rangle = \sum_\alpha |\alpha\rangle\langle\alpha|\mu\rangle$ and it follows

$$\hat{V}^{(2)} = \frac{1}{2}\sum_{\alpha\gamma,\lambda\mu\varsigma\nu}\langle\lambda|\alpha\rangle\langle\mu|\gamma\rangle\langle\alpha\gamma|\hat{V}^{(2)}|\alpha\gamma\rangle\langle\alpha|\varsigma\rangle\langle\gamma|\nu\rangle\,\hat{a}^+_\lambda \hat{a}^+_\mu \hat{a}_\nu \hat{a}_\varsigma$$

Simplifying this expression yields

$$\boxed{\hat{V}^{(2)} = \frac{1}{2}\sum_{\lambda\mu\varsigma\nu}\langle\lambda\mu|\hat{V}^{(2)}|\varsigma\nu\rangle\,\hat{a}^+_\lambda \hat{a}^+_\mu \hat{a}_\nu \hat{a}_\varsigma}$$

important for Fermi sign

A general Hamiltonian with two-body interactions

$$\hat{H} = \sum_{i=1}^{N} -\frac{\hbar^2 \hat{\nabla}_i^2}{2m} + \frac{1}{2}\sum_{i \neq j} V(\hat{x}_i - \hat{x}_j)$$

reads in 2nd quantized form:

Real space

$$\hat{H} = \sum_{\sigma = \{\uparrow, \downarrow\}} \int d^D x \; \hat{\psi}^\dagger_{x\sigma} \left(-\frac{\hbar^2 \nabla^2}{2m}\right) \hat{\psi}_{x\sigma}$$

Spin of the electron

$$+ \frac{1}{2}\sum_{\sigma,\sigma'} \int d^D_x \, d^D_{x'} \; V(x - x') \; \hat{\psi}^\dagger_{x\sigma} \; \hat{\psi}^\dagger_{x'\sigma'} \; \hat{\psi}_{x'\sigma'} \; \hat{\psi}_{x\sigma}$$

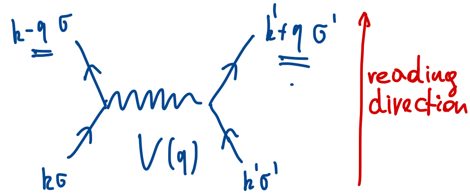
Reciprocal space

$$\hat{H} = \sum_{\sigma,k} \hat{c}^\dagger_{k\sigma} \frac{\hbar^2 k^2}{2m} \hat{c}_{k\sigma} + \frac{1}{2L^D} \sum_{\sigma\sigma'} \sum_{kk'q} V(q) \; \hat{c}^\dagger_{k-q\,\sigma} \, \hat{c}^\dagger_{k'+q,\sigma'} \, \hat{c}_{k'\sigma'} \, \hat{c}_{k\sigma}$$

Volume

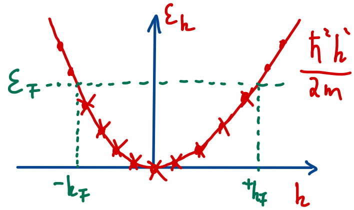
Note: total momentum is conserved!

Diagramatic representation of scattering:



Free fermions and the Fermi sea

Consider the free Fermion Hamiltonian



$$\hat{H} = \sum_{k,\sigma} \frac{\hbar^2 k^2}{2m} \underbrace{\hat{c}^+_{k\sigma} \hat{c}_{k\sigma}}_{= \hat{n}_{k\sigma}}$$

Ground state $(T=0)$: Fermi sea $|\phi_0\rangle = \prod_{|k|<k_F} \prod_{\sigma} \hat{c}^+_{k\sigma} |0\rangle$

All single particle states up to the Fermi energy $\varepsilon_F = \frac{\hbar^2 k_F^2}{2m}$ are occupied.

$\frac{1}{V}\sum_k = \frac{1}{(2\pi)^3}\int d^3k$

Total number of particles: $N = \sum_{k,\sigma} \langle \phi_0 | \hat{n}_{\sigma\vec{k}} | \phi_0 \rangle = \sum_{|\vec{k}|<k_F,\sigma} 1$
$(D=3)$

$$= 2 \frac{V}{(2\pi)^3} \int_0^{k_F} d^3k = 2 \frac{V}{(2\pi)^3} \cdot \underbrace{\frac{4\pi}{3} \cdot k_F^3} = \frac{V k_F^3}{3\pi^2}$$

volume, spin

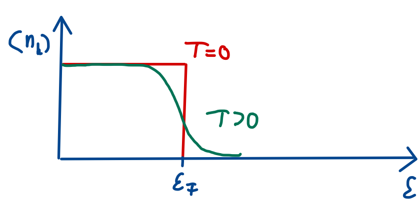
$$\leadsto k_F = \sqrt[3]{3\pi^2 \frac{N}{V}} = (3\pi^2 n)^{1/3} \quad \left(n = \frac{N}{V}\right)$$

Excitations of the Fermi sea:
particle-hole excitations

Finite T: Modes are occupied according to the Fermi-Dirac distribution

$$\langle \hat{n}_k \rangle_\beta = \frac{1}{e^{\beta \cdot (\varepsilon_k - \mu)} + 1}$$

Thermal expectation value



One-body correlation functions in D=3 at T=0:

$$C_\sigma(\vec{x}-\vec{x}') = \langle \phi_0 | \hat{\psi}^{+}_{\vec{x}'\sigma} \hat{\psi}_{\vec{x}\sigma} | \phi_0 \rangle, \quad \hat{\psi}_{\vec{x}\sigma} = \frac{1}{\sqrt{V}} \sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{x}} \cdot \hat{c}_{\vec{k}\sigma}$$

$$= \frac{1}{V} \cdot \sum_{\vec{q},\vec{k}} e^{-i\vec{k}\cdot\vec{x} + i\vec{q}\cdot\vec{x}'} \underbrace{\langle \phi_0 | \hat{c}^{+}_{\vec{q}\sigma'} \hat{c}_{\vec{k}\sigma} | \phi_0 \rangle}_{= \underbrace{\Theta(|\vec{k}|-k_F)}_{\begin{cases} =0 & |\vec{k}| > k_F \\ =1 & |\vec{k}| < k_F \end{cases}} \cdot \delta_{\vec{k},\vec{q}} \cdot \delta_{\sigma\sigma'}}$$

$$= \frac{1}{(2\pi)^3} \cdot \int_0^{k_F} d^3k \; e^{-i\vec{k}(\vec{x}-\vec{x}')} \cdot \Theta(|\vec{k}|-k_F)$$

Spherical coordinates $k=|\vec{k}|$, $x=|\vec{x}|$

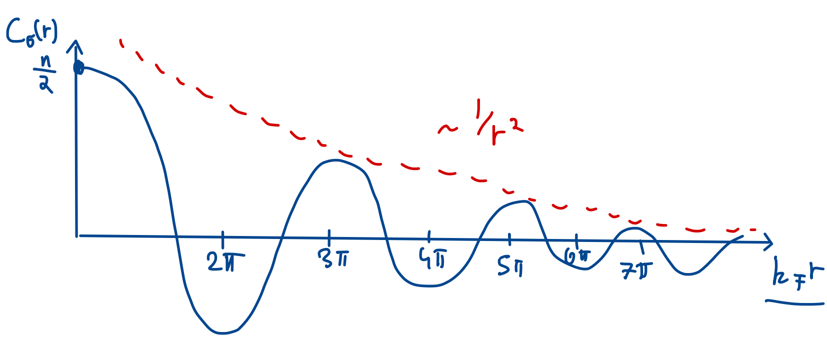
$$= \frac{1}{(2\pi)^2} \int_0^{k_F} dk \, k^2 \cdot \underbrace{\int_{-1}^{1} d\cos\Theta \; e^{ik\cdot|\vec{x}-\vec{x}'|\cdot\cos\Theta}}$$

$r=|\vec{x}-\vec{x}'|$

$$= \frac{e^{ikr} - e^{-ikr}}{i\cdot k\cdot r} = \frac{2\cdot\sin kr}{k\cdot r}$$

$$\rightsquigarrow C_\sigma(r) = \frac{1}{2\pi^2 r} \int_0^{k_F} dk \, k \cdot \sin(kr)$$

$$= \frac{1}{2\pi^2 r^3}\left[\sin(k_F r) - k_F r\cos(k_F r)\right] = \frac{3}{2} \overset{\frac{N}{V}}{\overset{\shortparallel}{n}} \left[\frac{\sin(k_F r) - k_F r\cos(k_F r)}{(k_F r)^3}\right]$$



Pair correlation functions in $D=3$ at $T=0$:

Due to the Pauli exclusion, even non-interacting Fermions of the same spin are correlated with each other! There are different options to characterize such correlations. One of them is the so-called pair correlation function:

$$G_{\sigma\sigma'}(r) = \langle \phi_0 | \hat{\psi}^+_{r\sigma} \hat{\psi}^+_{0\sigma'} \hat{\psi}_{0\sigma'} \hat{\psi}_{r\sigma} | \phi_0 \rangle$$

Wicks theorem (more about this later)

$$= \frac{1}{V^2} \sum_{kk'qq'} e^{-i(k-q)r} \langle \phi_0 | \hat{c}^+_{q\sigma} \hat{c}^+_{q'\sigma'} \hat{c}_{k'\sigma'} \hat{c}_{k\sigma} | \phi_0 \rangle$$

$$= \frac{1}{V^2} \sum_{kk'qq'} e^{-i(k-q)r} \langle \hat{n}_{q\sigma} \rangle \langle \hat{n}_{q'\sigma'} \rangle \left(\delta_{qk} \delta_{q'k'} - \delta_{qk'} \delta_{q'k} \cdot \delta_{\sigma\sigma'} \right)$$

One body correlation function

$$= C_\sigma(0) \cdot C_{\sigma'}(0) - |C_\sigma(r)|^2 \cdot \delta_{\sigma\sigma'}$$

$$= \left(\frac{n}{2}\right)^2 - \delta_{\sigma\sigma'} |C_\sigma(r)|^2$$

⇝ Particles of opposite spin are uncorrelated

⇝ Particles of the same spin have a smaller probability to be close to each other due to the Pauli principle