Superconductivity

levitov@mit.edu

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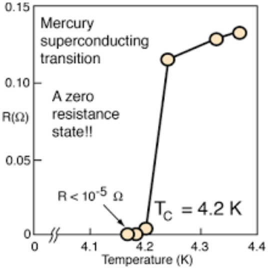
Superconductivity. Historical survey I

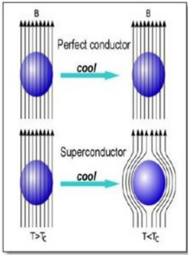
- Kamerlingh Onnes liquified helium in 1908, discovered SC in 1911
- Meissner and Ochsenfeld effect (1933): magnetic field expelled from SC bulk; complete expulsion from SC of type I, incomplete from type II SC
- London F. and H. (1935) phenomenological theory, explained MO effect
- Ginzburg-Landau theory (1950) symmetry-based approach, complex order parameter; provided basis for London eqs, explained type I and II SC
- Quantized vortices (Abrikosov 1957)

Superconductivity and magnetic field expulsion

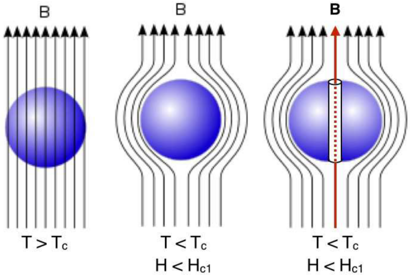


Meissner Effect:

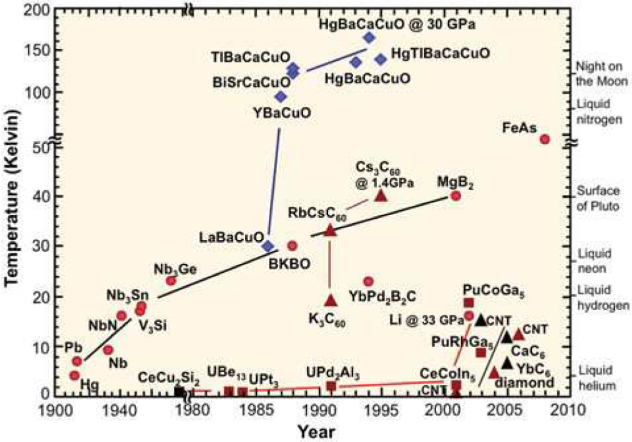
Meissner and Ochsenfeld in 1933 observed—
When a superconducting material at temp. $T > T_c$, is placed in ext. magnetic field, lines of magnetic induction pass through its body, but when it is cooled below the critical temp. i.e., $T < T_c$, these lines of induction are pushed out of the superconducting body.
So, **inside the SC body** **B = 0**
This is known as **Meissner Effect**, which is the characteristic property of a superconductor



Suppose superconductor has a hole drilled in it. Will magnetic field be expelled from it?

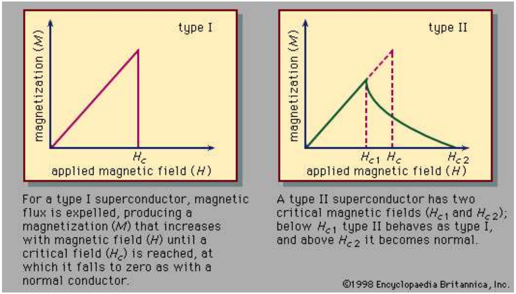


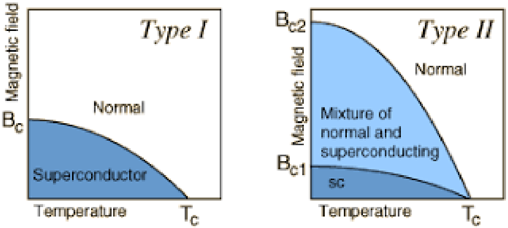
Timeline of superconductors and their transition temperatures (from Wikipedia)



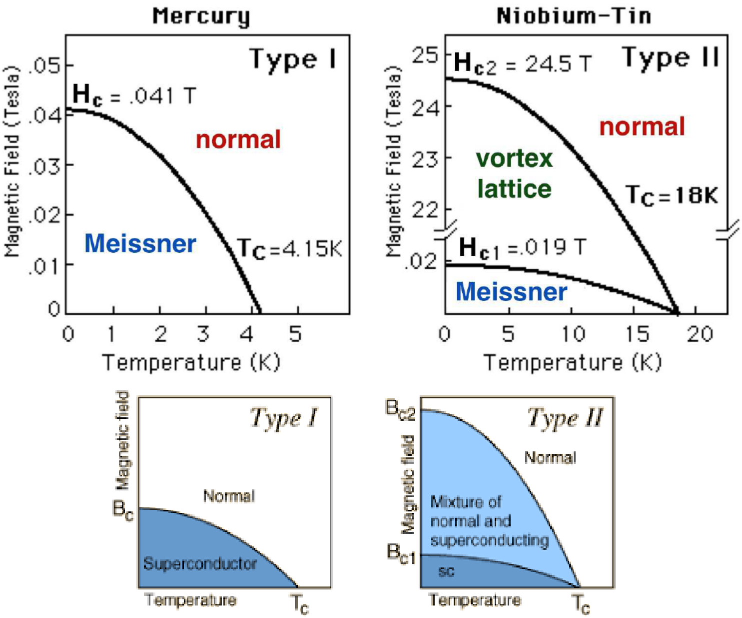
Type I and type II superconductivity

Magnetization curves and phase diagrams

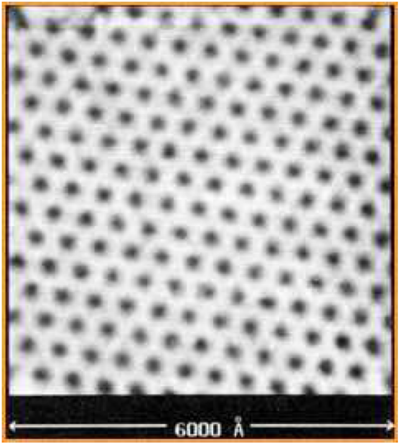




Phase diagrams for type I and type II superconductors

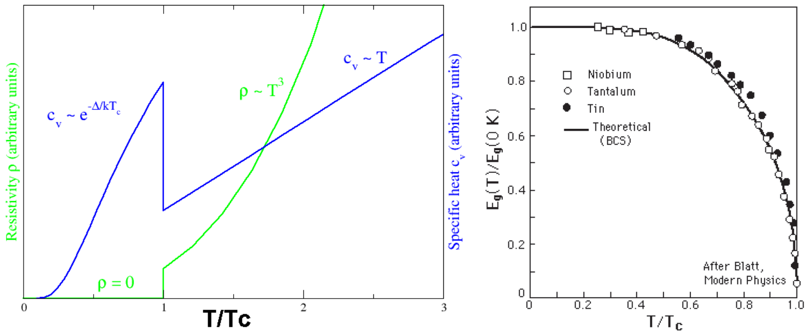


Vortex lattice in a type II superconductor



STM image of a vortex lattice in $\mathrm{NbSe_2}$ at $H = 1$T and $T = 1.8$K. From H. F. Hess et al., Phys. Rev.Lett. 62, 214 (1989).

Specific heat and energy gap



Left: Behavior of heat capacity (C_v, blue) and resistivity (ρ, green) at the superconducting phase transition;

Right: Dimensionless energy gap $\Delta(T)/\Delta_0$ in niobium, tantalum, and tin. The solid curve is the prediction from BCS theory, derived below.

Superconductivity. Historical survey II

- Bardeen-Cooper-Schrieffer, microscopic theory (1957)
- Gor'kov: QFT-based framework, derived GL theory from BCS theory (1959)
- Josephson effect (1962)
- Magnetic flux quantization Little & Parks (1962)
- Exotic superconductivity in 3He (triplet pairing) Osheroff, Richardson & Lee (1971)
- High-T_c superconductivity Bednorz & Muller (1986)
- Superconducting qubits Nakamura, Pashkin & Tsai (1999)
- Majorana states & majorana qubits (stay tuned)

- Phenomenology = the way of reasoning when direct calculation is impossible.

$$\frac{\partial \vec{j}_s}{\partial t} = \frac{n_s e^2}{m}\vec{E}, \quad \nabla \times \vec{j}_s = -\frac{n_s e^2}{mc}\vec{B}$$

1st eqn follows from $\dot{\vec{v}} + \gamma\vec{v} = \frac{e}{m}\vec{E}$ after suppressing dissipation γ; 2nd eqn follows from $\nabla \times \vec{E} = -\frac{1}{c}\frac{\partial \vec{B}}{\partial t}$.
Together they yield $\vec{j} = -\frac{n_s e^2}{mc}(\vec{A} - \nabla\chi)$ with some yet-unspecified function $\chi(r)$.
Gauge invariance???

- Describes field penetration in SC: $\nabla^2\vec{B} = \frac{1}{\lambda^2}\vec{B}$

$$\vec{B}(x) = \vec{B}_0 e^{-x/\lambda}, \quad \lambda = \sqrt{mc^2/(4\pi n_s e^2)}$$

London length typical values: $\lambda \lesssim 10\text{nm}$.

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- free energy functional for $\psi(x)$, complex order parameter (many-body w.f.), in a Mexican hat:

$$F = F_n + \alpha|\psi|^2 + \frac{\beta}{2}|\psi|^4 + \frac{1}{2m}|(-i\hbar\nabla - \frac{2e}{c}\vec{A})\psi|^2 + \frac{\vec{B}^2}{8\pi}$$

- spontaneous symmetry breaking in SC state, $\frac{\delta F}{\delta \psi} = 0$ at $\vec{B} = 0$, $\alpha < 0$, yields $\psi = \sqrt{\frac{|\alpha|}{\beta}} e^{i\theta}$
- Phase transition: $\alpha(T)$ changing sign at $T = T_c$
- Derive London eqn from $\frac{\delta F}{\delta \vec{A}} = \frac{1}{c}\vec{j} - \frac{1}{4\pi}\nabla \times \vec{B} = 0$:

$$\vec{j} = \frac{e}{m}\psi^*(-i\hbar\nabla - \frac{2e}{c}\vec{A})\psi + \mathrm{c.c.} = -\frac{4e^2}{mc}|\psi|^2(\vec{A} - \frac{\hbar c}{2e}\nabla\theta)$$

- Relation between superflow and gradient of θ the phase of ψ (a charged superfluid)
- Gauge invariance restored! $A(r) \to A(r) + \nabla\chi(r)$, $\theta(r) \to \theta(r) + \frac{2e}{\hbar c}\chi(r)$

Why do superconductors superconduct?

- Supercurrent flowing in a ring, no external B field

$$j(r) = |\psi|^2 \frac{e^* \hbar}{m^*} \nabla\theta, \quad \oint dr \cdot \nabla\theta = 2\pi n, \quad n = \pm 1, \pm 2 \ldots$$

- Topological invariant: the winding number. The ring is a circle, the order parameter space $0 \leq \theta \leq 2\pi$ is also a circle. Discrete winding number means that circulation of current is quantized in discrete units
- When a magnetic field is applied, magnetic flux through the ring is quantized (provided that the ring thickness is greater than λ)
- Superconducting flux quantum $\Phi_0 = \frac{hc}{2e} = 2.07 \times 10^{-7}$ gauss cm^2
- Vortices in the mixed phasee of type-II SC: quantized vorticity and magnetic flux

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1) Second-order transition at $T = T_c$. Supefluid density vanishes continuously as T grows: $n_s(T < T_c) = |\psi|^2 \sim T_c - T$, and zero at $T > T_c$. Zero latent heat. Jump in specific heat.

2) Thermodynamic critical field for Meissner effect. Phase transition occurs when condensation energy equals the energy of the expelled field:

$$V\frac{H_c^2}{8\pi} = F_N - F_S = V\frac{\alpha^2(T)}{2\beta}, \;\; (V = \text{system volume})$$

Predicts $H_c = \sqrt{\frac{4\pi}{\beta}}\alpha(T)$ linear near T_c as seen in experiment.

An abrupt (first-order) transition at $H = H_c$.

Later we'll show that $\frac{H_c^2}{8\pi} \approx n_s \frac{\Delta^2}{E_F}$ (at $T \to 0$, from BCS theory)

3) Type-II superconductors. Continuous transition at $H = H_{c2}$, quantized vortices at $H < H_{c2}$. Superconductivity **survives** in the presence of a magnetic field by letting (some of) the field in.

Find the upper critical field?
Simplification: ψ small at transition, can neglect ψ^4
Minimize F in ψ at a finite B field ($\rightarrow$ pset2):

$$-a(T_c - T)\psi(x) - \frac{\hbar^2}{4m}\left(\nabla + \frac{2ei}{\hbar c}\vec{A}\right)^2 \psi(x) = 0, \quad \vec{B} = \nabla \times \vec{A}$$

This eqn is identical to Schroedinger equation for Landau levels. Lowest energy states give $a(T_c - T) = \frac{1}{2}\hbar\tilde{\omega} = \frac{\hbar}{2}\frac{eB}{mc}$, giving $H_{c2} = \frac{2mc}{e\hbar}\alpha(T)$.

Nondimensionalize: $H_{c2} = \sqrt{2}\kappa H_c$, where $\kappa = \frac{mc}{e\hbar}\sqrt{\frac{\beta}{2\pi}}$.

Two distinct regimes:

$\kappa > 1/\sqrt{2}$: type II superconductivity, $H_{c2} > H_c$

$\kappa < 1/\sqrt{2}$ type I superconductivity, $H_{c2} < H_c$

At $\kappa = 1/\sqrt{2}$ a sign change in NS surface tension

Supercurrent in a weak link (see Leggett lecture notes)

Josephson effect(s):

1) $I = I_c \sin \Delta\phi$ dissipationless current $I < I_c$ (with zero voltage across the link)

2) $\frac{d}{dt}\Delta\phi = \frac{2eV}{\hbar}$ where V is voltage across junction

Understand Josephson effects 1 and 2:
Consider current in a massive SC ring with a weak link:
$\vec{j}(r) \sim \nabla\phi(r) - 2e\vec{A}(r)/\hbar$; phase difference across the weak link:

$$\Delta\phi = 2\pi\Phi/\Phi_0, \quad \Phi_0 = h/2e$$

where $\Phi = \oint \vec{A}\cdot dr$ the magnetic flux. Can tune SC phase by a B field!
JE2: Consider a time dependent flux $\Phi(t)$. From Faraday's law:
$\frac{d}{dt}\Delta\phi = \frac{2e}{\hbar}\frac{d\Phi}{dt} = \frac{2eV}{\hbar}$
JE1: Energy of the ring must be a 2π-periodic function of the flux $\phi = \Phi/\Phi_0$, even under $\Phi \to -\Phi$. In general, $F(\Phi) = \sum_m F_m \cos 2\pi m\phi$.
For a weak link the $m = 1$ term dominates: $F(\Phi) = (-I_c\Phi_0/2\pi)\cos\Delta\phi$

Find current from the work done under time-varying flux (and using JE2 relation):
$\frac{dF}{dt} = \frac{\partial F}{\partial \Delta\phi}\frac{\Delta\phi}{dt} = IV = I\frac{\Phi_0}{2\pi}\frac{\Delta\phi}{dt}$
This gives $I(\Delta\phi)\frac{\Phi_0}{2\pi} = \frac{\partial F}{\partial \Delta\phi}$. For $F \sim \cos\Delta\phi$ obtain JE1. QED
Josephson junctions
* control SC phase by magnetic field
* SQUIDs: magnetometry, superconducting electronics
* Josephson interference as probe of superconductivity
* Macroscopic quantum phenomena
* Qubits

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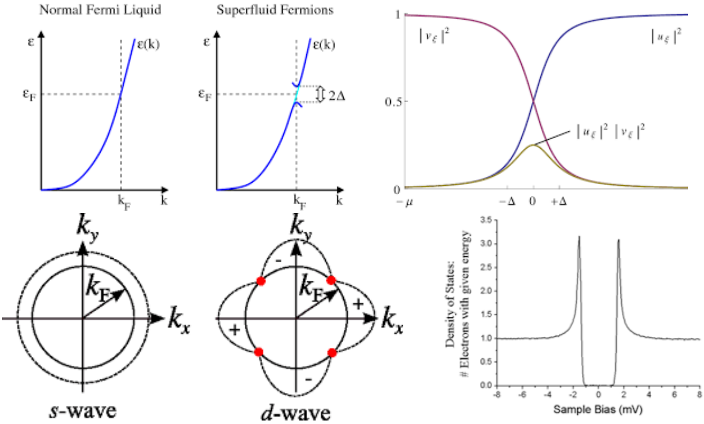
Microscopic picture preview: the pairing gap $\Delta(p)$, the u_p and v_p amplitudes, the gap angular dependence, the density of states of quasiparticles



Microcopic picture: bound pairs in Cooper's toy model

- Two electrons $(\vec{k}\uparrow, -\vec{k}\downarrow)$ scattering near FS between states above the Fermi level, $\epsilon_k, \epsilon_{k'} > 0$, while the states inside FS are Pauli-blocked
- Solve the two-body problem with an attractive interaction:
  $$E\psi(r_1, r_2) = \left[-\frac{\hbar^2\nabla^2_{r_1}}{2m} - \frac{\hbar^2\nabla^2_{r_1}}{2m} + V(r_1 - r_2)\right]\psi(r_1, r_2)$$
- Change variables to the relative displacement $\vec{r} = \vec{r}_1 - \vec{r}_2$ and the center of mass $\vec{R} = \frac{1}{2}(\vec{r}_1 + \vec{r}_2)$, giving ($m_* = 2m$, $\mu = m/2$):
  $$E\psi(r, R) = \left[-\frac{\hbar^2\nabla^2_R}{2m_*} - \frac{\hbar^2\nabla^2_r}{2\mu} + V(r)\right]\psi(r, R)$$
- Since V does not depend on the center of mass coordinate R, we look for the solution $\psi(r, R) = \psi(r)e^{iKR}$ which gives
  $\tilde{E}\psi(r) = \left[-\frac{\hbar^2\nabla^2_r}{2\mu} + V(r)\right]\psi(r)$ with $\tilde{E} = E - \hbar^2K^2/2m_*$
- For a given eigenvalue $\tilde{E}$ the lowest energy E is the one for which $K = 0$
- Depending on the symmetry of the spatial part of the wave-function, even $(\psi(-r) = \psi(r))$ or odd $(\psi(-r) = -\psi(r))$, the spins of the electrons will form either a singlet or a triplet state, respectively, in order to ensure the anti-symmetry of the total wave-function.

Microcopic picture: bound pairs in Cooper's toy model

- Fourier transform: $\psi(r) = \int \frac{d^3k}{(2\pi)^3} \Delta(k) e^{-ikr}$, $r = r_1 - r_2$ and demand that $\Delta(k)$ vanishes when $|\vec{k}| < k_F$
- $\psi(r_1 - r_2) = \sum_{|\vec{k}|>k_F} \Delta(k) e^{i\vec{k}\vec{r}_1} e^{-i\vec{k}\vec{r}_2} (\alpha_1\beta_2 - \beta_1\alpha_2)$
- The condition $|\vec{k}| > k_F$ accounts for Pauli blocking of states inside FS
- plugging it in SE gives: $(E - 2\epsilon_k)\Delta(k) = \sum_{|\vec{k}'|>k_F} V_{kk'} \Delta(k')$
- Bound state exists for any attractive interaction $V_{kk'} = -V$, no matter how weak
- Selfconsistency eqn: $1 = \sum_{|\vec{k}'|>k_F} V/(2\epsilon_k - E)$
- Binding energy is a negative exponential in the coupling strength,

  $$E = 2E_F - 2\omega_c e^{-2/N(0)V}$$

  This dependence explains the widely varying SC temperature values, and why SC is so ubiquitous
- **A more systematic approach is BCS theory that does not single out one pair but treats all electrons on equal footing predicts a similar relation for the gap,** $\Delta \sim e^{-1/N(0)V}$

The origin of superconductivity

- Macroscopic coherent state: spontaneous breaking of gauge symmetry; characterized by a phase similar to QM wavefunction, but a globally phase-synchronized macroscopic state
- Cooper pairs, formed due to attractive interaction, are not particle-like objects
- The origin of attraction? Coulomb repulsion hurts SC: strong but short-ranged because of screening, and relatively short-lived (frequencies $\omega \sim E_F$); can be overwhelmed by H_{el-ph} phonon-mediated attraction: long-lived because of retardation at $\omega \sim \theta_D$, $\to$ larger distances
- Weakly bound "fluffy" pairs: $\xi = \frac{\hbar v_F}{\Delta} > 100$ nm in size (despite short e-e distances $d_{ee} < 1$nm)
- Unique applications: nanodevices that behave as elementary but macrosocpic QM systems (Josephson junctions, qubits, etc)

Review second quantization for fermions

- Two-body interaction Hamiltonian for pair scattering near FS:

$$H_2 = \frac{1}{2V} \sum_{k,k',q} \sum_{\sigma,\sigma'} U(\vec{q}) c^\dagger_{\vec{k}+\vec{q},\sigma} c^\dagger_{\vec{k}'-\vec{q},\sigma'} c_{\vec{k}',\sigma'} c_{\vec{k},\sigma}$$

- Creation and annihilation operators for Cooper pairs. One pair per each electron momentum $\vec{k}$:

$$b^\dagger_k = c^\dagger_{\vec{k},\uparrow} c^\dagger_{-\vec{k},\downarrow}, \quad b_k = c_{-\vec{k},\downarrow} c_{\vec{k},\uparrow} \tag{1}$$

- Apprx 1: contact interaction $U(q) = U < 0$
- Apprx 2: concentrate on pairs with $\vec{k}' = -\vec{k}$, $\sigma = -\sigma'$ (throw away other terms, justify later)
- This yields the BCS interaction Hamiltonian

$$H_2^{BCS} = \frac{U}{2V} \sum_{k,q} \sum_{\sigma} c^\dagger_{\vec{k}+\vec{q},\sigma} c^\dagger_{-\vec{k}-\vec{q},-\sigma} c_{-\vec{k},-\sigma} c_{\vec{k},\sigma}$$

Cooper's toy model: one pair above the Fermi level

- Filled Fermi sea: $|FS\rangle = \prod_{|\vec{k}'|<k_F} c^\dagger_{\vec{k}',\uparrow} c^\dagger_{\vec{k}',\downarrow}|0\rangle$
- Add one pair: $|\psi_{pair}\rangle = \sum_{|\vec{k}|>k_F} g_k c^\dagger_{\vec{k},\uparrow} c^\dagger_{-\vec{k},\downarrow}|FS\rangle$
- $(H_1 + H_2^{BCS})|\psi\rangle = E|\psi\rangle$
- Apply H_2^{BCS} to $|\psi\rangle$, but leave $|FS\rangle$ intact
- $(E - 2\epsilon_k)g_{\vec{k}} = U \sum_{|\vec{k}'|>k_F} g_{\vec{k}'}$
- Selfconsistency eqn: $1 = \sum_{|\vec{k}'|>k_F} \frac{U}{E-2\epsilon_{\vec{k}}}$
- Seek a bound state with energy $E = 2E_F - \Delta$
- Approximate the sum over states as $\sum_{|k'|>k_F} \ldots = N(0)\int_0^W d\xi \ldots$, where W is the band of energies where pairing happens, and we defined $\xi = \epsilon_k - E_F$. Integrating over ξ gives $1 = \frac{1}{2}N(0)|U| \ln \frac{2W+\Delta}{\Delta}$
- Solution for the one-pair bound state energy $\Delta = 2We^{-2/N(0)|U|}$ (good so long as $\Delta \ll W$)

Pairing field and SC order

- 1-pair bound state $\to$ many-body state?
- Can factor H_{BCS} in terms of pair operators (1) as

$$H_{BCS} = \frac{U}{V}\left(\sum_{\vec{k}'} b^\dagger_{\vec{k}'}\right)\left(\sum_{\vec{k}} b_{\vec{k}}\right) \equiv \frac{V}{U}\hat{\Delta}^\dagger\hat{\Delta}$$

with $\hat{\Delta} = \frac{U}{V}\sum_{\vec{k}} b_{\vec{k}}$, $\hat{\Delta}^\dagger = \frac{U}{V}\sum_{\vec{k}} b^\dagger_{\vec{k}}$

- Particle nonconserving, analogous to SHO ladder operators $b^\dagger$, b
- Zero for the Fermi sea $|g\rangle = \prod_{|\vec{k}|<k_F,\sigma} c^\dagger_{k,\sigma}|0\rangle$

$$\langle g|\hat{\Delta}^\dagger|g\rangle = \langle g|\hat{\Delta}|g\rangle = 0$$

- Create a paired state: $\Delta = \langle g_s|\hat{\Delta}|g_s\rangle \neq 0$
- System can gain energy by going to the paired state since $U < 0$, $\langle g_s|H_{BCS}|g_s\rangle < 0$

BCS trial variational state

- $\psi_{BCS} = \prod_{\vec{k}} (u_k + v_k c^\dagger_{-\vec{k},\downarrow} c^\dagger_{\vec{k},\uparrow})|0\rangle$ (intuition: a single pair and no-pair superposition, fermionic coherent states analogous to SHO bosonic coherent states $|\lambda\rangle = e^{-|\lambda|^2/4} \sum_{n=0}^{\infty} \frac{\lambda^n}{\sqrt{n!}}|n\rangle$)
- Arrive at a variational problem $E = \langle \psi_{BCS}|H_1 + H_2^{BCS}|\psi_{BCS}\rangle \rightarrow$ *min* constrained by the normalization condition $|u_k|^2 + |v_k|^2 = 1$
- $E = \sum_k 2\epsilon_k |v_k|^2 + \frac{U}{V} \left(\sum_k u_k \bar{v}_k\right) \left(\sum_{k'} \bar{u}_{k'} v_{k'}\right)$
- $\delta E = \sum_k 4\epsilon_k v_k \delta v_k + 2\Delta(u_k \delta v_k + v_k \delta u_k) = 0$ and $u_k \delta u_k + v_k \delta v_k = 0$, where $\Delta = \frac{U}{V} \sum_k u_k v_k$.
  Without loss of generality we suppressed phases, treating u_k, v_k and Δ as real variables (will generalize later).
- This gives $\frac{\delta E}{\delta v_k} = 4\epsilon_k v_k + 2\Delta(u_k - v_k^2/u_k) = 0$
- Solved by $u_k^2, v_k^2 = \frac{1}{2}\left(1 \pm \frac{\epsilon_k}{\sqrt{\epsilon_k^2 + \Delta^2}}\right)$

The BCS selfconsistency equation

- Energy change per single pair-nopair box:
  $\delta E_k = 2\epsilon_k v_k^2 + 2u_k v_k \Delta = \epsilon_k - \sqrt{\epsilon_k^2 + \Delta^2} < 0$
  (we used $v_k^2 = \frac{1}{2}(1 - \frac{\epsilon_k}{\sqrt{\epsilon_k^2+\Delta^2}})$ and $u_k v_k = -\frac{1}{2}\frac{\Delta}{\sqrt{\epsilon_k^2+\Delta^2}}$)
- Negative $\delta E_k < 0$ means energy is gained through forming a paired state
- The order parameter
  $\Delta = \frac{U}{V}\sum_k u_k v_k = \frac{U}{V}\sum_k (-\frac{1}{2})\frac{\Delta}{\sqrt{\epsilon_k^2+\Delta^2}}$
- The selconsistency equation for Δ:
  $\Delta = \frac{|U|}{2V}\sum_k \frac{\Delta}{\sqrt{\epsilon_k^2+\Delta^2}} = \frac{|U|}{2}\int \frac{d^3k}{(2\pi)^3}\frac{\Delta}{\sqrt{\epsilon_k^2+\Delta^2}}$
  This equation has a nonzero solution (next page)
- A variational solution so far. Later ψ_{BCS} will be found to be an exact ground state.

Solving the selfconsistency equation

- Integrate over energies near the Fermi level: $\int \frac{d^3k}{(2\pi)^3}... = \int \nu(\epsilon) d\epsilon ... \approx \nu_0 \int d\epsilon ...$
- It is convenient to explicitly account for the energy band around Fermi level where pairing happens by replacing U with $U\chi_{\epsilon_k}\chi_{\epsilon_{k'}}$, where $\chi_\epsilon = 1$ for $-W < \epsilon < W$, and zero elsewhere
- $\Delta = \frac{|U|\nu_0}{2} \Delta \int_{-W}^{W} d\epsilon \frac{\Delta}{\sqrt{\epsilon^2 + \Delta^2}} = |U|\nu_0 \Delta \sinh^{-1} \frac{W}{\Delta}$
- At weak coupling we have $\Delta \ll W$, giving

$$\Delta = 2W e^{-1/|U|\nu_0} \tag{2}$$

- The bandwidth W value depends on the pairing mechanism: $W \sim \theta_D$ for phonon-mediated attraction, $W \sim \epsilon_F$ for contact interaction (e.g. in cold atoms), etc.

- SC persists at weak interaction (unlike, e.g. Stoner instability)
- The exponential dependence (2) explains why 1) SC is widespread; 2) occurs at low T
- Ga 1.1 K, Al 1.2 K, In 3.4 K, Sn 3.7 K, Hg 4.2 K, Pb 7.2 K, Nb 9.3 K
- La-Ba-Cu-oxide 17.9 K, Y-Ba-Cu-oxide 92 K, Ti-Ba-Cu-oxide 125 K
- BCS bandgap 2Δ at the Fermi level. Testable!
- Gap vs. critical temperature $2\Delta_{T=0} \approx 3.52 k_B T_c$
- SC correlation length (the Cooper pair size)

$$\xi = \frac{\hbar v_F}{\Delta} \sim 100 - 1000\,\mathrm{nm}$$

Superconductivity: quasiparticles and phase transition

- We have argued that fermion attraction gives rise to a very simple paired ground state – a direct product of pair/no-pair superposition states for all opposite momenta k and $-k$:
  $\Psi_{BCS} = \prod_{\vec{k}}(u_k + v_k c^\dagger_{-k\downarrow} c^\dagger_{k\uparrow})|0\rangle$.
- Next, we want to understand excitations in this state and describe the phase transition. We'll introduce an elegant and intuitive approach – a Bogoliubov transformation – to show that the excitations in the BCS state are superpositions of particles and holes. These quasiparticles are fermions with a gap in the energy spectrum. The energy gap is directly related to, and is in fact equal, the BCS order parameter Δ. Quasiparticle notes
- After introducing the quasiparticles we will discuss superconductivity at $T > 0$. We will describe the pair-breaking effect of a finite temperature in terms of thermally excited quasiparticles. This will lead to a finite-temperature gap equation that predicts the critical temperature T_c at which superconductivity disappears.
- Describe thermodynamics of superconductors: the universal relation between T_c and the gap, the character of the phase transition and heat capacity at $T < T_c$. We will compare the behavior for the BCS and non-BCS (unconventional) superconductivity and identify the differences that help to experimentally determine the superconductivity type. Phase transition notes

The mean field approach

- We'll start with an example from spin physics (ferromagnetic order). The method, however, is completely general and applicable for ordering of any kind.
- Hamiltonian for Ising spin variables on a lattice

$$H = -\frac{1}{2} \sum_{\vec{x} \neq \vec{x}'} J(\vec{x} - \vec{x}') s_{\vec{x}} s_{\vec{x}'} , \quad s_{\vec{x}} = \pm 1$$

  Describe the phase transition?
- The Curie-Weiss ("molecular field") method. Start with a single spin in an external field $H = -hs$. Ensemble-averaged magnetization is found as $m = \langle s \rangle = \frac{e^{\beta h} - e^{-\beta h}}{e^{\beta h} + e^{-\beta h}} = \tanh \beta h$.
- For many spins, consider one spin ($s_{\vec{x}}$) in an effective field of all other spins, $h_{\vec{x}} = \sum_{\vec{x}'} J(\vec{x} - \vec{x}') s_{\vec{x}}$. Replacing spins by their average values, have

$$h = Um, \quad m = \tanh \beta h$$

  where $U = \sum_{\vec{x}'} J(\vec{x} - \vec{x}')$. Ensemble average in partition function.
- The equation $m = \tanh \beta U m$ has zero solution at $\beta U < 1$ and nonzero solutions at $\beta U > 1$. Find critical temperature $T_c = 1/U$.
- Validity: small fluctuations, large number of fluctuating spins coupled to each individual spin.

The mean field approach

- Describe symmetry breaking starting from H?
- The mean field method
- Introduce the mean field: $s_{\vec{x}} = \delta s_{\vec{x}} + m, \;\; \delta s_{\vec{x}} = s_{\vec{x}} - m$

$$H = -\tfrac{1}{2} \sum_{\vec{x} \neq \vec{x}'} J(\vec{x} - \vec{x}')(s_{\vec{x}} - m + m)(s_{\vec{x}'} - m + m)$$

$$= -\tfrac{1}{2} \sum_{\vec{x} \neq \vec{x}'} J(\vec{x} - \vec{x}')(\delta s_{\vec{x}} + m)(\delta s_{\vec{x}'} + m)$$

$$= -\tfrac{1}{2} \sum_{\vec{x} \neq \vec{x}'} J(\vec{x} - \vec{x}') \left[\delta s_{\vec{x}} \delta s_{\vec{x}'} + \delta s_{\vec{x}} m + \delta s_{\vec{x}'} m + m^2\right]$$

$$\approx -\tfrac{1}{2} \sum_{\vec{x} \neq \vec{x}'} J(\vec{x} - \vec{x}') \left[\delta s_{\vec{x}} m + \delta s_{\vec{x}'} m + m^2\right] = \sum_{\vec{x} \neq \vec{x}'} J(\vec{x} - \vec{x}') s_{\vec{x}} m - \tfrac{1}{2} m^2$$

Each spin seeing an effective field $h = Um$ that depends on other spins.

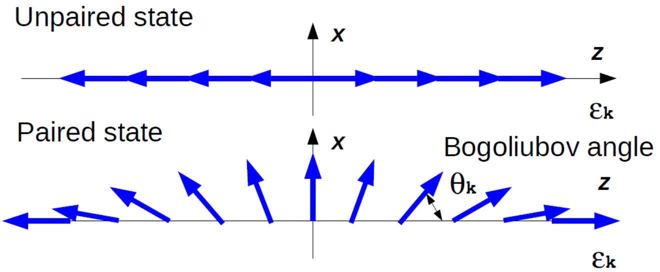
- Find the energy $H(m) = \sum_x -Um \tanh \beta Um + \frac{1}{2} Um^2$
- A double well potential that describes symmetry breaking at $T < T_c$. A state with spontaneously broken Z_2 symmetry!

The mean field approach

- The mean field approach is valid when the number Z of spins interacting with each individual spin is large.
- An Ising magnet in a high-dimensional cubic lattice ($Z = 2d \gg 1$)
- Or, in $d = 3$ with a long-range coupling $J(\vec{x} - \vec{x}') \sim \exp(-|\vec{x} - \vec{x}'|/\xi)$, $\xi \gg a$ the lattice constant
- How does it apply to superconductivity?
- The superconducting coherence length $\xi = \hbar v_F/\Delta$ (the Cooper pair radius) defines the effective range for pairing interaction
- For the mean field approach to work need $\xi \gg \lambda_F$ (typical distance between electrons in a metal)
- This is (almost) always true! Exception: the strong-coupling regime when Cooper pairs are strongy bound and Bose-condense into a superconducting state (in which case, $T_c = T_{BEC}$)
- The BCS theory (within mean field) and the Ginzburg-Landau theory are highly accurate for most superconductors

BCS state as a "magnet" – broken U(1) symmetry

- This BCS interaction Hamiltonian $H = H_1^{kin} + H_2^{el-el}$
- The two-body interaction projected on pair states
  $H_2^{BCS} = \frac{U}{2V} \sum_{k,q} \sum_{\sigma} c^{\dagger}_{\vec{k}+\vec{q},\sigma} c^{\dagger}_{-\vec{k}-\vec{q},-\sigma} c_{-\vec{k},-\sigma} c_{\vec{k},\sigma}$
- Can factor H_2^{BCS} in terms of pair operators $b_k = c_{-k\downarrow} c_{k\uparrow}$,
  $b_k^{\dagger} = c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow}$ as $H_2^{BCS} = \frac{U}{V} \left(\sum_{\vec{k}'} b^{\dagger}_{\vec{k}'} \right) \left(\sum_{\vec{k}} b_{\vec{k}} \right)$
- Identify b_k with spin-1/2 raising and lowering operators. An XY spin model with an external B field $\parallel z$ (the B field varying vs. p)
- A spin-spin coupling of an infinite range (in p space)
- In this case the mean field approach is exact!



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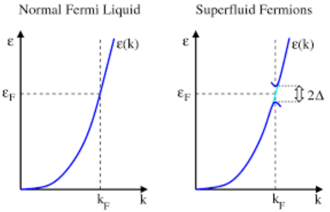
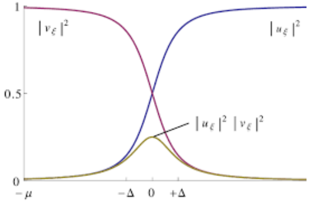
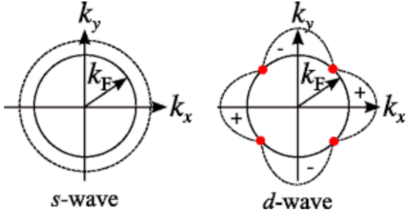
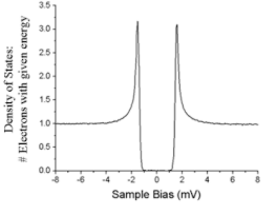
Exotic pairing: the gap function $\Delta(p)$, the u_p and v_p amplitudes, the gap angular dependence, the density of states of quasiparticles









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- Quantum mechanics of identical, indistinguishable particles. Exchange symmetry:

$$\Psi(\ldots,\vec{r}_i,\ldots,\vec{r}_j,\ldots) = +\Psi(\ldots,\vec{r}_j,\ldots,\vec{r}_i,\ldots) \quad \text{(bosons)}$$

$$\Psi(\ldots,\vec{r}_i,\ldots,\vec{r}_j,\ldots) = -\Psi(\ldots,\vec{r}_j,\ldots,\vec{r}_i,\ldots) \quad \text{(fermions)}$$

- Describe $N \gg 1$ (MANY) identical particles?
- First-quantized w.f. a Slater determinant (F), or a permanent (B). Huge $= N!$ number of terms, unmanageable
- Instead, construct w.f. by filling up each single-particle state with a certain number of identical particles (due to Dirac, Fock, Jordan)
- Such as photons, which can be viewed as excitations of EM modes

Many-body QM in Fock space

Hilbert space for identical particles (B or F)

$$F = F_0 \oplus F_1 \oplus F_2 \oplus \ldots = \oplus_{n=0}^{\infty} F_n, \quad F_n = SV^{\otimes n}$$

V_0 vacuum, V_1 one-particle state, V_2 two-particle state (symmetric for B, antisymmetric for F), etc

Hamiltonian in F_N

$$H = -\sum_{i=1\ldots N} -\frac{\hbar^2}{2m}\nabla_i^2 + V(\vec{r}_1 \ldots \vec{r}_N)$$

Eigenfunctions $H\psi_n(\vec{r}_1 \ldots \vec{r}_N) = E_n \psi_n(\vec{r}_1 \ldots \vec{r}_N)$ symm for B, antisymm for F

Basis states: symmetrized products of complete 1-particle ONB states (position eigenstates, momentum eigenstates, noninteracting H eigenstates, etc)

$$\psi_B(\vec{x}_1, \vec{x}_2 \ldots \vec{x}_N) = c \sum_P \phi_1(P\vec{x}_1)\phi_2(P\vec{x}_2)\ldots\phi_N(P\vec{x}_N)$$

ϕ_q occurs n_q times (n_q particles in state ϕ_q), $q = 1 \ldots Q$

$N!$ permutations, $c = \left(N!/(n_1! \ldots n_Q!)\right)^{-1/2}$

Occupation number representation:

$$\psi_B = |n_1, n_2 \ldots n_Q \ldots\rangle, \quad n_q = 0, \ q > Q$$

$$b_q^\dagger |n_1, n_2 ... n_q ... n_Q ...\rangle = \sqrt{n_q + 1} |n_1, n_2 ... n_q{+}1 ... n_Q ...\rangle$$

$$b_q |n_1, n_2 ... n_q ... n_Q ...\rangle = \sqrt{n_q} |n_1, n_2 ... n_q - 1 ... n_Q ...\rangle$$

prefactors $\sqrt{n_q + 1}$ and $\sqrt{n_q}$ motivated by the ladder operators for simple harmonic oscillator.
These operators obey

$$[b_r, b_s^\dagger] = \delta_{rs}, \quad [b_r, b_s] = [b_r^\dagger, b_s^\dagger] = 0$$

Consistent with field quanta (e.g. photons or phonons) defined as excitations in the normal-mode oscillators

Antisymmetrized states, the Slater determinant

$$\psi_F(\vec{x}_1, \vec{x}_2 ... \vec{x}_N) = c \sum_P (-1)^P \phi_1(P\vec{x}_1)\phi_2(P\vec{x}_2)...\phi_N(P\vec{x}_N)$$

all ϕ_i different (equiv Pauli exclusion)
N! permutations, $c = (N!)^{-1/2}$
Occupation number representation:

$$\psi_F = |n_1, n_2, n_3...\rangle, \quad n_i = \begin{cases} 1 \text{ for } \phi_1...\phi_N \\ 0 \text{ else} \end{cases}$$

Note: order matters, affects the $(-1)^P$ sign

One particle: $|1\rangle$ a 1-particle state, $|0\rangle$ vacuum, or no-particle state

$a^\dagger|0\rangle = |1\rangle$, $a^\dagger|1\rangle = 0$, $a|1\rangle = |0\rangle$, $a|0\rangle = 0$

☺: $a^\dagger|1\rangle = 0$ enforces Pauli exclusion principle;

☺: $|0\rangle$ and 0 not the same! (vacuum is a physical state rather than nothing)

Algebra: $[a, a^\dagger]_+ = 1$, $[a, a]_+ = [a^\dagger, a^\dagger]_+ = 0$

Many particles:

$$a_q|n_1, n_2 ... n_q ...\rangle = \begin{cases} (-1)^S|n_1, n_2 ... 0 ...\rangle, & n_q = 1 \\ 0, & n_q = 0 \end{cases}$$

$$a_q^\dagger|n_1, n_2 ... n_q ...\rangle = \begin{cases} 0, & n_q = 1 \\ (-1)^S|n_1, n_2 ... 1 ...\rangle, & n_q = 0 \end{cases}$$

with $S = n_1 + n_2 + ... + n_{q-1}$ to keep track of the ordering condition

Full algebra:

$$[a_r, a_s^\dagger]_+ = \delta_{rs}, \quad [a_r, a_s]_+ = [a_r^\dagger, a_s^\dagger]_+ = 0$$

☺: $a_1^\dagger a_2^\dagger |0, 0, ...\rangle = -a_2^\dagger a_1^\dagger |0, 0, ...\rangle$ consistent with Slater determinant definition

Particle number operators:

$$n_q = \begin{cases} b_q^\dagger b_q, & Bosons, \quad n_q = 0, 1, 2... \\ a_q^\dagger a_q, & Fermions, \quad n_q = 0, 1 \end{cases}$$

- $[n_s, n_r]_- = 0$ simultaneously diagonalizable
- For a general state $\langle\psi|n_q|\psi\rangle$ may be nonintegral

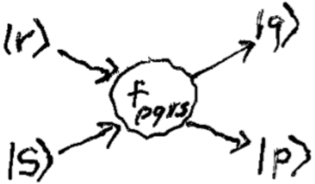
Summing up:

- Complicated many-particle wavefunction
- A more simple occupation number representation
- Algebra for a, $a^\dagger$ operators, states $a_1^\dagger \ldots a_s^\dagger|0\rangle$
- Few-body operators $T = \sum_i -\frac{1}{2m}\nabla_i^2$, $V = \sum_{i<j} u(x_i - x_j)$. Second-quantized?
- Basis dependent? Actually, basis independent (discuss later)

Physical operators

- One-body operators $O_1 = \sum_i f(x_i)$.
  Second-quantized form $O_1 = \sum_{rs} \langle \phi_r | f | \phi_s \rangle c_r^\dagger c_s$
  with matrix elements
  $\langle \phi_r | f | \phi_s \rangle = \int d^3x \phi_r^*(x) f(x) \phi_s(x)$
  c_r repres a_r (fermions) or b_r (bosons)
- Two-body operators $O_2 = \sum_{i<j} f(x_i, x_j)$.
  Second quantized form $O_2 = \sum_{pqrs} f_{pqrs} c_p^\dagger c_q^\dagger c_r c_s$
  with matrix elements
  $f_{pqrs} = \int d^3x d^3x' \phi_p^*(x) \phi_q^*(x') f(x, x') \phi_r(x') \phi_s(x)$
  ☺: $\phi_s(x)$ are mutually orthogonal single-particle orbitals of any kind, e.g. plane waves, localized states, etc.
  ☺: the ordering matters for fermions, does not matter for bosons

Consider a general two-body operator $O_2 = \sum_{i<j} f(x_i, x_j) = \sum_{pqrs} f_{pqrs} c_p^\dagger c_q^\dagger c_r c_s$. This is a sum of terms describing transitions from states r, s to states p, q with transition amplitudes f_{pqrs}.



Transition amplitude is a matrix element of the two-body interaction $f_{pqrs} = \int d^3x d^3x' \phi_p^*(x)\phi_q^*(x') f(x, x')\phi_r(x')\phi_s(x)$. As we will see shortly, for plane-wave states this yields the actual two-body scattering amplitudes.

Prove it for fermions (more difficult). Consider

$$O_1 |\Psi_N\rangle = \left(\sum_i f(x_i) \right) A \left[\phi_1(x_1) \ldots \phi_N(x_N) \right]$$

- move $\sum_i f(x_i)$ inside antisymmetrization A
- Use completeness $f(x_i)\phi_s(x_i) = \sum_r \langle \phi_r | f | \phi_s \rangle \phi_r(x_i)$
- Obtain a sum, with weights $\langle \phi_r | f | \phi_s \rangle$, of antisymm products in which $\phi_s(x_i) \to \phi_r(x_i)$
- But this is the content of 2nd quantization, $c_r^\dagger c_s$ gives just that. QED

Prove for two-particle operators, analogously

$$O_2 = \sum_{i<j} f(x_i, x_j) = \sum_{pqrs} f_{pqrs} c_p^\dagger c_q^\dagger c_r c_s$$

- Consider $O_2|\Psi_N\rangle = \left(\sum_{i<j} f(x_i, x_j)\right) A\left[\phi_1(x_1)\ldots\phi_N(x_N)\right]$
- move $\sum_{i<j} f(x_i, x_j)$ inside A
- Use completeness to replace $\phi_r(x_i)\phi_s(x_j)$ with $\sum_{p,q} f_{pqrs}\phi_p(x_i)\phi_q(x_j)$
- The correct ordering of the operators arises because

$$\left(c_p^\dagger c_q^\dagger c_s c_r\right) c_r^\dagger c_s^\dagger |0\rangle = c_p^\dagger c_q^\dagger |0\rangle$$

agrees with (anti)commutation rules
QED

The Hamiltonian for identical particles with a two-body interaction:

$$H = K + P = \sum_i \frac{p_i^2}{2m} + \sum_{i<j} U(\vec{r}_i - \vec{r}_j), \quad i, j = 1 \ldots N$$

Use plane-wave states as single-particle orbitals,
$\phi_k(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\vec{r}}$, $\vec{k} = \frac{2\pi}{L}(n_1, n_2, n_3)$,
$n_j = 0, \pm 1, \pm 2 \ldots$

Compute matrix elements for kinetic energy:

$$f_{kk'} = \langle \vec{k}' | \frac{\vec{p}^2}{2m} | \vec{k} \rangle = \frac{1}{V} \int d^3 r \frac{\hbar^2 \vec{k}^2}{2m} e^{i(\vec{k}' - \vec{k})\vec{r}} = \frac{\hbar^2 \vec{k}^2}{2m} \delta_{\vec{k}', \vec{k}}.$$

Here we used the identity

$$\int d^3 r e^{i(\vec{k}' - \vec{k})\vec{r}} = V \delta_{\vec{k}', \vec{k}}. \quad (3)$$

Next, we transform the interaction term. Writing the matrix elements $f_{\tilde{k}\tilde{k}'k'k} = \langle \tilde{\vec{k}}\tilde{\vec{k}}' | U(\vec{r} - \vec{r}') | \vec{k}'\vec{k} \rangle = \frac{1}{V^2} \int d^3r d^3r' U(\vec{r} - \vec{r}') e^{i(\vec{k} - \tilde{\vec{k}})\vec{r} + i(\vec{k}' - \tilde{\vec{k}}')\vec{r}'}$, and evaluating integrals in position space gives

$$f_{\tilde{k}\tilde{k}'k'k} = \frac{1}{V} \sum_{\vec{q}} U(\vec{q}) \delta_{\tilde{\vec{k}}', \vec{k}' + \vec{q}} \delta_{\tilde{\vec{k}}, \vec{k} - \vec{q}}.$$

Here we introduced momentum transfer $\vec{q}$ through Fourier transform $U(\vec{r} - \vec{r}') = \int \frac{d^3q}{(2\pi)^3} U(\vec{q}) e^{i\vec{q}(\vec{r} - \vec{r}')}$ and used the identity in Eq.3 to integrate over $\vec{r}$, $\vec{r}'$.

E.g. short-range interaction Fourier transformes as: $\lambda \delta(\vec{r} - \vec{r}') = \lambda \int \frac{d^3q}{(2\pi)^3} e^{i\vec{q}(\vec{r} - \vec{r}')}$, so that $U(\vec{q}) = \lambda$;
Likewise, Coulomb interaction:
$\frac{e^2}{|\vec{r} - \vec{r}'|} = \int \frac{d^3q}{(2\pi)^3} \frac{4\pi e^2}{|\vec{q}|^2} e^{i\vec{q}(\vec{r} - \vec{r}')}$, so $U(\vec{q}) = \frac{4\pi e^2}{|\vec{q}|^2}$;

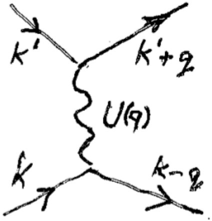
The total Hamiltonian then takes the form

$$H = \sum_k \epsilon_k c_k^\dagger c_k + \frac{1}{2V} \sum_{k,k',q} U(\vec{q}) c^\dagger_{\vec{k}'+\vec{q}} c^\dagger_{\vec{k}-\vec{q}} c_{\vec{k}} c_{\vec{k}'}$$

where $\epsilon_k = \frac{\hbar^2 \vec{k}^2}{2m}$ and the factor $1/2$ is introduced to avoid double counting in pairwise interaction.

☺: Can generalize to particles with spin by adding spin labels to the states as well as creation and annihilation operators.

As discussed earlier, we can interpret the interaction term as a transition amplitude for scattering from $\vec{k}$, $\vec{k}'$ to $\vec{k} - \vec{q}$, $\vec{k}' + \vec{q}$ with momentum transfer $\vec{q}$ and scattering amplitude $U(\vec{q})$. The corresponding Feynman diagram looks like so:



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Physically important systems (superconductors, superfluids, ferromagnets, antiferromagnets) all can be described by a quadratic H (approximately). E.g. $H = \sum_{ij} H_{ij} c_i^\dagger c_j$. Here H_{ij} - hermitian, hence, can be diagonalized by a unitary transformation. **Then**

$$c_j = \sum_l U_{jl} \alpha_l, \quad c_j^\dagger = \sum_l \alpha_l^\dagger \left(U^\dagger\right)_{lj}$$

Use transformed c, $c^\dagger$ operators to transform H:

$$H = \sum_{lm} \alpha_l^\dagger (U^\dagger H U)_{lm} \alpha_m = \sum_m \varepsilon_m \alpha_m^\dagger \alpha_m = \sum_m \varepsilon_m n_m.$$

Note: Operator algebra is basis independent:
$[c_i, c_j^\dagger]_\pm = \delta_{ij}, \ [c_i, c_j]_\pm = [c_i^\dagger, c_j^\dagger]_\pm = 0$
$UB = B, \ UF = F$ (statistics unchanged!)

Mixing c and $c^\dagger$ by Bogoliubov transformations (fermions)

For fermion operators consider the Hamiltonian

$$H = \epsilon(c_1^\dagger c_1 + c_2^\dagger c_2) + \lambda(c_1^\dagger c_2^\dagger + c_2 c_1),$$

which arises in the BCS theory of superconductivity. Note: λ must be real for H to be Hermitian (more generally, with complex λ the second term of H would read $\lambda c_1^\dagger c_2^\dagger + \lambda^* c_2 c_1$). Note also the opposite ordering of labels in the terms $c_1^\dagger c_2^\dagger$ and $c_2 c_1$, which is also a requirement of Hermiticity.

The fermionic Bogoliubov transformation is

$$c_1^\dagger = ud_1^\dagger + vd_2, \quad c_2^\dagger = ud_2^\dagger - vd_1,$$

where u and v are c-numbers, which we can in fact take to be real, because we have restricted ourselves to real λ.

Note: this can be brought to the particle-conserving form by interchanging c_2 and $c_2^\dagger$ (a particle-hole transformation)

The transformation $c_1^\dagger = ud_1^\dagger + vd_2$, $c_2^\dagger = ud_2^\dagger - vd_1$, is useful only if fermionic anticommutation relations apply to both sets of operators. Let us suppose they apply to the operators d and $d^\dagger$, and check the properties of the operators c and $c^\dagger$.

The coefficients of the transformation have been chosen to ensure that $[c_1^\dagger, c_2^\dagger]_+ = 0$, while

$$[c_1^\dagger, c_1]_+ = u^2[d_1^\dagger, d_1]_+ + v^2[d_2^\dagger, d_2]_+$$

and so we must require $u^2 + v^2 = 1$. The transformation matrix $U = \begin{pmatrix} u & v \\ -v & u \end{pmatrix}$ is therefore unitary as expected. This suggests the parameterization $u = \cos\frac{\theta}{2}$, $v = \sin\frac{\theta}{2}$.

Note: we use notation identical to that in the BCS problem. This is intentional. As we will see, the angle θ is nothing but the polar angle introduced in the pseudospin-$1/2$ picture, $\cos\theta = \xi/E$, $E = \sqrt{\xi^2 + \Delta^2}$.

The remaining step is to substitute in H for $c^\dagger$ and c in terms of $d^\dagger$ and d, and pick θ so that terms in $d_1^\dagger d_2^\dagger + d_2 d_1$ have vanishing coefficient.

The calculation is clearest when it is set out using matrix notation:

$$H = \begin{pmatrix} c_1^\dagger & c_2 \end{pmatrix} \begin{pmatrix} \epsilon & \lambda \\ \lambda & -\epsilon \end{pmatrix} \begin{pmatrix} c_1 \\ c_2^\dagger \end{pmatrix} + \epsilon \hat{1}$$

where we have used the anticommutator to make substitutions of the type $c^\dagger c = 1 - cc^\dagger$. Next we write the Bogoliubov transformation

$$\begin{pmatrix} c_1 \\ c_2^\dagger \end{pmatrix} = \begin{pmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2} \\ -\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} d_1 \\ d_2^\dagger \end{pmatrix}$$

We pick angle θ value so that

$$\begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} \epsilon & \lambda \\ \lambda & -\epsilon \end{pmatrix} \begin{pmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2} \\ -\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} = \begin{pmatrix} \tilde{\epsilon} & 0 \\ 0 & -\tilde{\epsilon} \end{pmatrix}$$

where $\tilde{\epsilon} = \sqrt{\epsilon^2 + \lambda^2}$. See next page for details.

To achieve this one can either directly multiply 2×2 matrices or use (pseudo)spin Pauli matrices and spin-$1/2$ rotation as

$$e^{i\theta\sigma_2/2}(\lambda\sigma_1 + \epsilon\sigma_3)e^{-i\theta\sigma_2/2} = \lambda'\sigma_1 + \epsilon'\sigma_3$$

with $\lambda' = \lambda\cos\theta - \epsilon\sin\theta$, $\epsilon' = \epsilon\cos\theta + \lambda\sin\theta$. Choosing θ such that λ' vanishes we obtain

$$H = \tilde{\epsilon}(d_1^\dagger d_1 + d_2^\dagger d_2) + (\epsilon - \tilde{\epsilon})\hat{1}.$$

We have arrived at quasiparticles described by free-fermion operators $d_{1,2}$ and $d_{1,2}^\dagger$. They are noninteracting fermions built out of original fermions, with the energy $\tilde{\epsilon} \neq \epsilon$ that accounts for the interactions in the original Hamiltonian.

Next, consider a boson Hamiltonian

$$H = \varepsilon(c_1^\dagger c_1 + c_2^\dagger c_2) + \lambda(c_1 c_2 + c_2^\dagger c_1^\dagger)$$

Try a linear transformation (with real u, v):

$$c_1 = ud_1 + vd_2^\dagger, \qquad c_1^\dagger = ud_1^\dagger + vd_2,$$
$$c_2 = ud_2 + vd_1^\dagger, \qquad c_2^\dagger = ud_2^\dagger + vd_1.$$

Bosonic algebra? 1) $[c_1^\dagger, c_2^\dagger] = 0$ for any u and v.
2) $[c_1, c_1^\dagger] = u^2[d_1, d_2] - v^2[d_2, d_2^\dagger] = 1$, giving

$$u^2 - v^2 = 1$$

Hence we make a *Minkowski* parametrization

$$u^2 - v^2 = 1: \qquad \begin{aligned} u &= \cosh\theta, \\ v &= \sinh\theta. \end{aligned}$$

The matrix form of our transformation reads

$$\begin{pmatrix} c_1 \\ c_2^\dagger \end{pmatrix} = \begin{pmatrix} u & v \\ v & u \end{pmatrix} \begin{pmatrix} d_1 \\ d_2^\dagger \end{pmatrix}$$

Diagonalize H? change order, $c_2^\dagger c_2 = c_2 c_2^\dagger - \hat{1}$,

$$H = (c_1^\dagger \; c_2) \begin{pmatrix} \varepsilon & \lambda \\ \lambda & \varepsilon \end{pmatrix} \begin{pmatrix} c_1 \\ c_2^\dagger \end{pmatrix} - \underbrace{\varepsilon \hat{1}}_{\text{const (ignore)}}$$

Write in terms of d, $d^\dagger$:

$$H = (d_1^\dagger \; d_2) \begin{pmatrix} u & v \\ v & u \end{pmatrix} \begin{pmatrix} \varepsilon & \lambda \\ \lambda & \varepsilon \end{pmatrix} \begin{pmatrix} u & v \\ v & u \end{pmatrix} \begin{pmatrix} d_1 \\ d_2^\dagger \end{pmatrix}$$

Can use 2×2 Pauli matrices $H = d_i^\dagger H'_{ij} d_j$

$\tilde{H} = (u\hat{1} + v\sigma_1)(\epsilon\hat{1} + \lambda\sigma_1)(u\hat{1} + v\sigma_1)$

$$\tilde{H} = \hat{1}(\varepsilon(u^2 + v^2) + \lambda uv) + \sigma_1(2\varepsilon uv + \lambda[u^2 + v^2]).$$

Setting $\tanh 2\theta = -\lambda/\varepsilon$ obtain

$$\tilde{H} = \tilde{\varepsilon}\hat{1} + \tilde{\lambda}\sigma_1, \quad \tilde{\varepsilon} = \sqrt{\varepsilon^2 - \lambda^2}, \quad \tilde{\lambda} = 0.$$

giving two decoupled bosons:

$$H = \tilde{\varepsilon}(d_1^\dagger d_1 + d_2^\dagger d_2) - \varepsilon + \tilde{\varepsilon}$$

☺: required $\varepsilon > |\lambda|$ for stability

Particle nonconserving transformations: Meaning?

Recall a, $a^\dagger$ for 1D harmonic oscillator

$$H = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2} = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right),$$

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(q + \frac{i}{m\omega}p\right), \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(q - \frac{i}{m\omega}p\right)$$

Squeezed states: Take $\tilde{a}$, $\tilde{a}^\dagger$ with a 'wrong' value $\omega' \neq \omega$. 'Wrong' vacuum, 'wrong' excitations. H is hermitian, but particle-nonconserving!

$$H_\omega = H_{\omega'} + \left(\frac{m\omega^2}{2} - \frac{m\omega'^2}{2}\right)q^2 = \hbar\omega'\left(a^\dagger a + \frac{1}{2}\right) + \frac{m\Delta(\omega^2)}{2}\frac{\hbar}{2m\omega'}\left(\tilde{a} + \tilde{a}^\dagger\right)^2$$

$$= \hbar\frac{\omega^2 + \omega'^2}{2\omega'}\tilde{a}^\dagger\tilde{a} + \frac{m\Delta(\omega^2)}{4\omega'}\left(\tilde{a}\tilde{a} + \tilde{a}^\dagger\tilde{a}^\dagger\right).$$

1. *Natural generalization to many modes*
2. Works for B & F

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$$\psi(\vec{r}) = \sum_i \varphi_i(\vec{r}) c_i, \quad \psi^\dagger(\vec{r}) = \sum_i \varphi_i^*(\vec{r}) c_i^\dagger.$$

for any orthonormal set of one-particle modes $\langle\varphi_i|\varphi_j\rangle = \delta_{ij}$ and associated Bose or Fermi operators, $[c_i, c_j^\dagger]_\pm = \delta_{ij}$, $[c_i, c_j]_\pm = [c_i^\dagger, c_j^\dagger]_\pm = 0$. In appearance, the field operators $\psi(\vec{r})$, $\psi^\dagger(\vec{r})$ are basis dependent. Is this really so? To prove that they aren't, go to a new basis by a unitary transformation and change c and $c^\dagger$'s accordingly, $\phi_i = \sum_{i'} U_{ii'} \tilde{\phi}_{i'}$, $c_i = \sum_{i'} U_{ii'} \tilde{c}_{i'}$, $c_i^\dagger = \sum_{i'} U_{ii'}^* \tilde{c}_{i'}^\dagger$. We see that $\tilde{\psi}(\vec{r}) = \sum_i \tilde{\phi}_i \tilde{c}_i = \sum_{i'} \phi_{i'} c_{i'} = \psi(\vec{r})$, $\tilde{\psi}^\dagger(\vec{r}) = \ldots = \psi^\dagger(\vec{r})$. Therefore the quantities $\psi(\vec{r})$ and $\psi^\dagger(\vec{r})$ are basis independent, as expected. QED

One-particle operators:

$O_1 = \sum_{i=1}^{N} f(\vec{r}_i) \ \rightarrow O_1 = \sum_{rs} f_{rs} c_r^\dagger c_s$ with matrix elements $f_{rs} = \int d^3 r \varphi_r^*(\vec{r}) f(\vec{r}) \varphi_s(\vec{r})$. Here $f(\vec{r})$, say, a 1-particle kinetic or potential energy operator: $f(\vec{r}) = -\frac{\hbar^2 \nabla^2}{2m}$ or $f(\vec{r}) = U(\vec{r})$. Two-particle operators are constructed in a similar manner:

$$O_2 = \sum_{i<j} g(\vec{r}_i, \vec{r}_j) \rightarrow O_2 = \frac{1}{2} \sum_{rspq} g_{rspq} c_r^\dagger c_s^\dagger c_p c_q$$

with matrix elements

$g_{rspq} = \int \int d^3 r d^3 r' g(\vec{r}, \vec{r}\,') \phi_r^*(\vec{r}) \phi_s^*(\vec{r}\,') \phi_p(\vec{r}\,') \phi_q(\vec{r})$.

The meaning of field operators: $\psi(\vec{r})$ annihilates particle at $\vec{r}$, $\psi^\dagger(\vec{r}')$ creates particle at $\vec{r}'$. Algebra:

$$[\psi(\vec{r}), \psi^\dagger(\vec{r}')]_\pm = \delta^{(3)}(\vec{r} - \vec{r}'), \quad [\psi(\vec{r}), \psi(\vec{r}')]_\pm = 0$$

Notation: $[A, B]_\pm = AB \pm BA$

one-particle/many-particle correspondence:

$$O_1 = \int d^3r \psi^\dagger(\vec{r}) f(\vec{r}) \psi(\vec{r})$$

two-particle/many-particle correspondence:

$$O_2 = \frac{1}{2} \int d^3r_1 d^3r_2 \psi^\dagger(\vec{r}_1) \psi^\dagger(\vec{r}_2) g(\vec{r}_1, \vec{r}_2) \psi(\vec{r}_2) \psi(\vec{r}_1)$$

Resembles one-particle and two-particle H's with wavefunctions replaced by field operators.

For $H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i<j} V(\vec{r}_i - \vec{r}_j)$ we arrive at **a quantum field picture:**

$$H = \int d^3r\, \psi^\dagger(\vec{r}) \frac{p^2}{2m} \psi(\vec{r})$$

$$+\frac{1}{2} \int d^3r d^3r' \psi^\dagger(\vec{r}) \psi^\dagger(\vec{r}') V(\vec{r} - \vec{r}') \psi(\vec{r}') \psi(\vec{r})$$

The result looks, tantalizingly, a lot like a single particle Hamiltonian but of course $\psi(\vec{r})$ and $\psi^\dagger(\vec{r})$ are operators not wavefunctions! More precisely, they are many-body operators paired together with single-particle orbitals — i.e. a quantum field.

☺: a macroscopic system of $N \sim 10^{23}$ particles is described by H comprising only two terms!

Particle number operator N and its properties:

- Define $N = \int d^3r \psi^\dagger(\vec{r})\psi(\vec{r})$. N obeys:

  $[N, H] = 0,\ [\psi(\vec{r}), N] = \psi(\vec{r})],\ [\psi^\dagger(\vec{r}), N] = -\psi^\dagger(\vec{r})$

  with commutators rather than anticommutators, identical for B and F!
- Interpretation: action of ψ ($\psi^\dagger$) on eigenstate of N is to decrease (increase) eigenvalue by 1
- Define grand-canonical Hamiltonian, useful in problems w fluctuating particle $\#$: $H' = H - \mu N$
- Eigenstates of N: The vacuum state $\psi(\vec{r})|0\rangle = 0$ (for any $\vec{r}$) where $|0\rangle$ is a (nonzero) vacuum vector state and 0 is the null vector
- $\psi^\dagger(\vec{r}_1)\psi^\dagger(\vec{r}_2)...\psi^\dagger(\vec{r}_m)|0\rangle$ w/ eigenvalue $= m$