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Quantenmechanik II
— Theoretische Physik V —

Carsten Henkel

Lecture Keywords

Chapter 1

Many-body physics, second quantisation

1.1 Fri 15 Nov 2019: Paired States

Relevant for

- superconductivity (Cooper pairs, BCS theory)
- Bose-Einstein condensation (BEC, collective excitations)

1.1.1 Key concepts

Cooper pairs

Simple picture: bound state of two electrons, on the "background" of a filled Fermi sphere (sketch with two opposite k-vectors).

Important:

– the filled states of the Fermi sphere stabilise the bound state

– the (repulsive) Coulomb interaction is "screened" (reduced in intensity) by other charges. Re-arrangement of electrons around an additional charge ("impurity"), leading to an excess positive background, total charge of the impurity plus the surrounding charge cloud is much smaller

– effective, short-range, attractive interaction from the deformation of the lattice of background ions. (Experimental evidence: "isotope shift" = the critical temperature for superconductivity depends on the mass of the lattice ions.)

Pairing term in interaction Hamiltonian

Operator form of binary interaction in Fourier space (one summation was missing in the lecture)

$$\hat{W} = \frac{1}{2} \sum_{q,k,k'} a^{\dagger}_{k+q} a^{\dagger}_{k'-q} W_q a_k a_{k'} \tag{1.1}$$

the operators $a_k a_{k'}$ "destroy" two particles (not physically, for the moment just an element of the second quantised formalism). In so-called paired states, this yields a quantum-mechnical amplitude ("pairing field") which can be used to lower the interaction energy and stabilise a system (e.g., in the ground-state of a BCS superconductor).

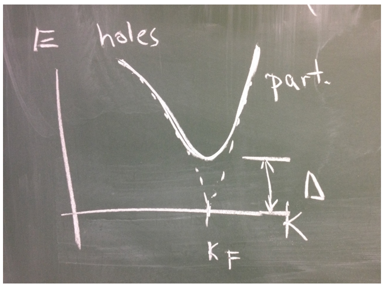
$\rightarrow$ nonzero average $\langle \mathrm{BCS} | a_{k\uparrow} a_{-k\downarrow} | \mathrm{BCS} \rangle$. Total momentum $\hbar k - \hbar k = 0$, total spin = 0 ("singlet pair").

Of course, there is also a nonzero average population, for example in BEC: $\langle \mathrm{BEC} | a^{\dagger}_k a_k | \mathrm{BEC} \rangle \neq 0$ even if $k \neq 0$ does not correspond to the "condensate mode" (typically one-particle state with the lowest energy). This describes the creation of "non-condensate particles" via the interaction. The cost in (kinetic) energy is more than compensated by a lowering of the interaction energy.

Quasi-particle

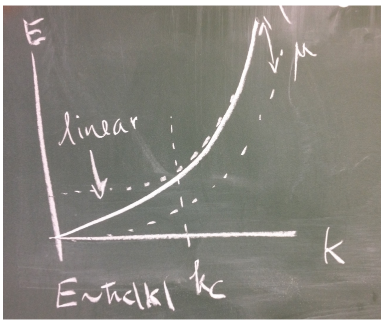
An "excitation" that can be identified by a well-defined momentum $\hbar k$ and an energy $E = E(k)$ (dispersion relation). To be distinguished from a "particle" because its properties depend on the other particles (the "background") and the interactions.

Example: dispersion relation of single-particle excitation in a metal and in a BCS-superconductor.



Concept of “particle” excitations for $k > k_F$ and “holes” for $k < k_F$. In a superconductor, there is a minimum value $\Delta =$ “gap” for $k \approx k_F$. Plays a key role to explain the zero resistance in the superconducting state: the electric current is carried by the ground state. Due to the finite value of the gap, this state is stable with respect to scattering (from impurities or phonons), the dissipation by exciting quasi-particles is suppressed. (If one measures the resistance at finite frequencies, also a superconductor shows losses, for example when $\hbar\omega > 2\Delta$. The vanishing resistance is a “DC phenomenon”.)

Example: dispersion relation of elementary excitations in a BEC – shifted relative to the parabola of non-interacting massive particles.



And for small momentum (large wavelengths) $k \lesssim k_c$, a linear behaviour: $E \approx \hbar c|k|$. This is also called an “acoustic” dispersion, and c (units: velocity) is called the “speed of sound”. It is determined by the interactions between particles in the Bose condensate.

Quasi-particles are sometimes described by a (unitary) transformation

S of the single-particle operators, e.g.

$$a_k \mapsto b_k = S^\dagger a_k S \tag{1.2}$$

This transformation also determines the ground state of the many-body system, e.g., $|\mathrm{BCS}\rangle = S|\mathrm{Fermi\,sea}\rangle$ where the "Fermi sea" is the filled Fermi sea of otherwise non-interacting Fermions. In a Bose condensate, the non-interacting state with N particles in the ground state can be written $|N, 0\ldots\rangle$ (a list of occupation numbers with zeros for all excited modes). The "true" condensate (including interactions) is then approximated by $|\mathrm{BEC}\rangle = S|N, 0\ldots\rangle$.

Example of such a transformation

$$b_k = S^\dagger a_k S = \mu a_k + \nu a^\dagger_{-k} \tag{1.3}$$

(called Bogoliubov transformation for a BEC, Bogoliubov-Valatin in BCS theory). The distinction between "creating" and "destroying" a particle gets blurred. In addition, quantum-mechanical superpositions of both processes appear (!). Note the opposite momentum in the creating operator $a^\dagger_{-k}$.

Compute the expectation values: non-condensate occupation number

$$\langle\mathrm{BEC}|a^\dagger_k a_k|\mathrm{BEC}\rangle = \langle N, 0\ldots|S^\dagger a^\dagger_k S S^\dagger a_k S|N, 0\ldots\rangle = \ldots = |\nu|^2 \tag{1.4}$$

Hence the meaning of the amplitude ν: also excited modes are occupied with some probability. (This has nothing to do with nonzero temperature!)

And the "pairing field"

$$\langle\mathrm{BEC}|a_k a_{-k}|\mathrm{BEC}\rangle = \langle N, 0\ldots|(\mu a_k + \nu a^\dagger_{-k})(\mu a_{-k} + \nu a^\dagger_k)|N, 0\ldots\rangle = \mu\nu \tag{1.5}$$

in general a complex quantity, can be used to lower ("optimise") the interaction energy.

1.1.2 Interaction Hamiltonian in k-space

Start with field-operator formulation

$$\hat{W} = \frac{1}{2}\int \mathrm{d}x\,\mathrm{d}x'\,\psi^\dagger(x)\psi^\dagger(x')W_2(x-x')\psi(x')\psi(x) \tag{1.6}$$

Two-body (binary) interaction potential $W_2(x - x')$ only depends on the distance, as expected for a spatially homogeneous system. Apply Fourier expansion of field operator

$$\psi(x) = \sum_k \frac{\mathrm{e}^{\mathrm{i}kx}}{\sqrt{L^3}} a_k \tag{1.7}$$

Remark on discrete k-vectors in finite "quantisation box" of volume L^3. Completely artificial (or related to crystal unit cell), provides a "countable" basis in the one-particle Hilbert space. It makes the Hilbert space and also the Fock space "separable" (avoiding mathematical problems with topology and convergence).

One gets a four-fold sum

$$\hat{W} = \frac{1}{2\,L^6} \sum_{k,k',p',p} a_k^\dagger a_{k'}^\dagger a_{p'} a_p \int \mathrm{d}x\, \mathrm{d}x'\, W_2(x-x') \exp\left[\mathrm{i}\left(-kx - k'x' + p'x' + px\right)\right] \tag{1.8}$$

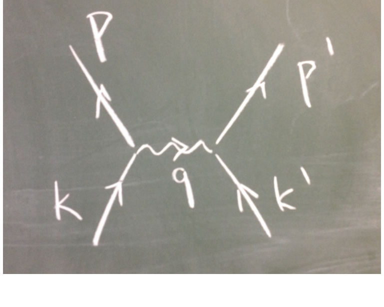
Do the x-integral first and substitute $s = x - x'$ for fixed x'. One gets the Fourier transform of the interaction potential:

$$\int \mathrm{d}s\, W_2(s) \exp\left[-\mathrm{i}(k-p)s\right] = \tilde{W}_2(k-p) \tag{1.9}$$

Collect all phases for the remaining integral and restrict the integration over the finite volume L^3

$$\int_{L^3} \mathrm{d}x' \, \exp\left[\mathrm{i}\left(-kx' - k'x' + p'x' + px'\right)\right] = L^3\, \delta_{p+p'-k-k',0} \tag{1.10}$$

This expresses the conservation of total momentum: in-going particles have total momentum $k + k'$, out-going particles $p + p' = k + k'$. Pictorial representation as a Feynman graph:



lines with arrows for in-going particles, wavy line for the "interaction potential" that connects to "vertices" where three lines meet. Label the lines with momenta in such a way that at each vertex, momentum conservation holds, e.g.: $p' = k' + q$ and $p = k - q$.

Insight: the amplitude (matrix element) for a scattering process

$$A_{\text{out}\leftarrow\text{in}} = \langle \text{out}|\hat{W}|\text{in}\rangle \tag{1.11}$$

is proportional to the *Fourier transform* of the interaction potential $W_2(x - x')$, taken at the momentum transfer $q = p' - k'$. The scattering cross-section is proportional to the square $|\tilde{W}_2(q)|^2$. Example: a short-ranged potential (small water droplets in a cloud) give large momentum transfer = large scattering angles because its Fourier transform contains large q. Long-range potential (bubbles in boiling water) give mainly "forward scattering" = the medium still appears transparent.

Resulting expression for the interaction potential

$$\hat{W} = \frac{1}{2\,L^3} \sum_{k,k',q} a^\dagger_{k-q} a^\dagger_{k'+q} \tilde{W}_2(q) a_{k'} a_k \tag{1.12}$$

1.2 Bogoliubov transformation

Ansatz: exponential form with a "generator" that is quadratic in the field operators

$$S = \bigotimes_k \exp\left[\mathrm{i}\,\theta_k (a^\dagger_k a^\dagger_{-k} + a_{-k} a_k)\right] \tag{1.13}$$

Operators for different k's commute, hence the tensor product (often written as ordinary product).

This operator is unitary, $S^\dagger = S^{-1}$, by taking the adjoint in the exponent. (This ignores mathematical details related to the domain on which the operator is defined, not trivial because the a_k's are not bounded.)

Work out the "conjugation" $S^\dagger a_k S = b_k$: all terms in the product with $k' \neq k$ commute with a_k, hence only one factor remains. Drop the index k for the moment ($a_- = a_{-k}$) and take the derivative :

$$\frac{\mathrm{d}b}{\mathrm{d}\theta} = S^\dagger \left[-\mathrm{i}(a^\dagger a^\dagger_- + a_- a)a + \mathrm{i}a(a^\dagger a^\dagger_- + a_- a)\right] S = \mathrm{i}S^\dagger \left[a,\, (a^\dagger a^\dagger_- + a_- a)\right] S \tag{1.14}$$

See a commutator emerge and work it out with the usual relations (for discrete k-vectors). This gives

$$\frac{\mathrm{d}b}{\mathrm{d}\theta} = \mathrm{i}S^\dagger a_-^\dagger S = \mathrm{i}\, b_-^\dagger \tag{1.15}$$

A similar calculation gives for this adjoint operator

$$\frac{\mathrm{d}b_-^\dagger}{\mathrm{d}\theta} = \mathrm{i}\, b \tag{1.16}$$

And the solution of this linear system of coupled equations is

$$b = a\cosh\theta + \mathrm{i}\, a_-^\dagger \sinh\theta \tag{1.17}$$

using the initial conditions for $\theta = 0$. Hence we identify $\mu = \cosh\theta$, $\nu = \mathrm{i}\sinh\theta$ for Eq.(1.3). Note the "hyperbolic" relation $|\mu|^2 - |\nu|^2 = 1$. Despite this strange form, the Bogoliubov transformation of the operators is achieved with the unitary operator S.

We can get an idea about the paired states in the BCS (or BEC) state when we act with S on the non-interacting ground state. Let us take the BEC case where one typically takes only $k \neq 0$ in the infinite product (generation of pairs of non-condensate particles by interactions between condensate particles). We expand the exponential and find a series with the structure

$$\begin{aligned}
&S|N, 0\ldots\rangle \\
&= (\cdots)|N, 0\ldots\rangle + \sum_k (\cdots)|N, 1_k,\, 1_{-k}\ldots\rangle + \sum_k (\cdots)|N, 2_k,\, 2_{-k}\ldots\rangle \\
&\quad + \sum_{k,k'} (\cdots)|N, 1_k,\, 1_{-k}, 1_{k'},\, 1_{-k'}\ldots\rangle + \ldots
\end{aligned} \tag{1.18}$$

We see states where a pair of particles appears in the modes k and $-k$, a double pair etc. In general, many paired modes are involved, and the state is not simply a statistical mixtures of the pairs (as it would happen in a gas of molecules). Note also the "coherence" between the vacuum state $|N, 0\ldots\rangle$ (for non-condensate particles) and the paired state. This coherence is essential to get a nonzero expectation value for the operator product $a_k a_{-k}$. In the BCS state, there are of course no doubly occupied modes. This means that the higher powers in the exponential generates pairs for more and more modes. The BCS ground state thus contains an infinite-dimensional superposition of Cooper pairs in all momenta.

These series can (for one pair of modes) be re-summed and give an exponential of $a_k^\dagger a_{-k}^\dagger$ times a function of the parameter θ_k, for example $\mathrm{i}\tanh\theta_k$. Note also that the prefactor in front of the vacuum state is not simply unity – this comes by re-arranging the creation and annihilation operators from higher terms in the operator exponential. Such a form is often called the "normally ordered form" of a unitary operator.

In typical many-body systems, the parameter $\theta = \theta_k$ varies in k-space. In a BEC, only modes with $k \lesssim k_c$ have values $\theta_k \gg 1$, while for the "short-wavelength" quasi-particles, we have $b_k \approx a_k$ because $\theta_k \ll 1$. In a BSC superconductor, the transformation "mixes" particles and holes most strongly near $k \sim k_F$. This smears out the Fermi-Dirac distribution, but different from the way that particles are excited at nonzero temperature (statistical mixture). Far from the Fermi level, particle and hole states stay essentially the same as in the normal metal.