PHYS-E055101 Low Temperature Physics: Nanoelectronics

Lecture 1: Survival kit

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I. INTRODUCTION

In this lecture you will learn about various systems and devices that are classified, from the point of view of their dimensions, as *mesoscopic*. Another widely-used terminology is that of *nanostructure*. It refers to structures with dimensions ranging from about 1 nm (10^{-9} m) up to typically hundreds of nm. These systems are in-between the atomic scale and that of macroscopic solids. Like the solids, they are made of many atoms, however their dimensions are below that of the length scales that characterize the properties of macroscopic solid. This means that one cannot make the approximation that the volume is large with respect to these length scales, as we usually do in solid state physics. Given the fact that the usual approximations from both solid-state physics and atomic physics are not applicable, you might worry that the physics in the mesoscopic world is going to be very complicated, with transport properties very sensitive to the shape and composition of the materials. As you will see in this course, this is not the case. New energy scales (*e.g.* single-electron charging energy, Thouless energy) and time and length scales will appear, but the physics will be rather robust against imperfections from fabrication, etc.

For example, in solids the collisions of electrons with impurities and phonons are characterized by a length scale called mean free path. In a macroscopic metal, these collisions decrease the conductivity. This results in a so-called Ohmic resistivity, where the resistance R of the sample is

$$R = \rho \frac{L}{S}, \tag{1}$$

where $\rho = \sigma^{-1}$ is the resistivity (the inverse of conductivity σ), L is the length of the resistor, and S is the transverse area. Ohmic samples are well-described by the semiclassical Boltzmann approach, which we will study in the next lecture. However, with modern lithographic techniques, one cane make devices with size below the mean free path, and in this case the electrons do not encounter anything to scatter on: the transport, in this case, is said to be ballistic, and Eq. (1) does not hold. In this case, a new quantity that characterizes transport in so-called conduction channels appears - called the conductance quantum - defined as

$$G_Q = \frac{2e^2}{h}. \tag{2}$$

It is indeed possible nowadays to fabricate a large variety of structures and devices of dimensionality in the nano/meso range, with properties that are dramatically different from the

corresponding bulk materials. Examples of such nanostructures are: fullerenes, nanotubes, quantum wires, quantum dots, graphene, single-electron transistors, *etc.* The search for new materials and devices for the electronics industry is of tremendous economic importance. The well-known Moore's law has held in the semiconductor industry for many decades (the doubling of the number of transistors fabricated on the same-size chip every two years) but currently the dimensions have reached 32 nm. At such distances, heating and tunneling of electrons become important effects.

Moreover, with current cryogenic technology it is possible to cool the samples to temperatures typically close to 10 mK (using dilution refrigerators). This is important from a scientific point of view, as new phenomena appear at low temperatures (*e.g.* superconductivity), and also because the length scales mentioned above change with temperature (for example, the electron-phonon scattering length). These low-temperature phenomena have already resulted in new applications (detectors, thermometry, etc.).

II. ELEMENTARY QUANTUM MECHANICS

The evolution of a quantum state is given by the Schrödinger equation,

$$i\hbar\frac{d}{dt}|\Psi(t)\rangle = \hat{H}(t)|\Psi(t)\rangle, \tag{3}$$

where $\hat{H}(t)$ is the Hamiltonian operator that can be in general time-dependent. We will briefly review the main three representations of time-evolution in quantum physics - namely the Schrödinger (we add a subscript S for clarity), Heisenberg (we add a subscript H for clarity), and the interaction picture (we add a subscript I for clarity).

a. Schrödinger picture In the Schrödinger picture we have

$$i\hbar\frac{d}{dt}|\Psi(t)\rangle_S = \hat{H}_S(t)|\Psi(t)\rangle_S. \tag{4}$$

Formally one can solve the above equation as

$$|\Psi(t)\rangle_S = \hat{U}(t)|\Psi(0)\rangle_S, \tag{5}$$

where $\hat{U}(t)$ is the time-evolution operator that propagates the state from time 0 to time t,

$$\hat{U}(t) = \mathcal{T}e^{-\frac{i}{\hbar}\int_0^t d\tau \hat{H}(\tau)}, \tag{6}$$

where $\mathcal{T}$ represents time-ordering. If the Hamitonian is time-independent, *i.e.* $\hat{H}(t) = \hat{H}$, then $\hat{U}(t)$ becomes

$$\hat{U}(t) = e^{-\frac{i}{\hbar}\hat{H}t}. \tag{7}$$

If you now use Eqs. (5) and (7) you can immediately check that this fulfills the Schrödinger equation Eq. (4).

b. Heisenberg picture In the Heisenberg picture the state remains constant but the operators become time-dependent. We denote the state in the Heisenberg picture by $|\Psi(t)\rangle_H$,

$$|\Psi(t)\rangle_{\mathrm{H}} = |\Psi(0)\rangle_{\mathrm{S}} =: |\Psi\rangle_{\mathrm{H}}. \tag{8}$$

This implies

$$|\Psi(t)\rangle_{\mathrm{H}} = \hat{U}(t)^{-1}|\Psi(t)\rangle_{\mathrm{S}}, \tag{9}$$

where we used the inverse of the time evolution operator, $\hat{U}(t)^{-1}$, which as we know from the Schrödinger picture yields $|\Psi(0)\rangle_{\mathrm{S}} = \hat{U}(t)^{-1}|\Psi(t)\rangle_{\mathrm{S}}$.

Since the states are time-independent, the evolution is transferred into the operators (and observables)

$$\hat{\mathcal{O}}_{\mathrm{H}}(t) = \hat{U}(t)^{-1}\hat{\mathcal{O}}_{\mathrm{S}}\hat{U}(t), \tag{10}$$

where $\hat{\mathcal{O}}_{\mathrm{S}}$ is the observable $\hat{\mathcal{O}}$ in the Schrödinger representation. One can immediately check that the operators satisfy the Heisenberg equation of motion

$$i\hbar\frac{d\hat{\mathcal{O}}_{\mathrm{H}}(t)}{dt} = [\hat{\mathcal{O}}_{\mathrm{H}}(t), \hat{H}]. \tag{11}$$

c. Interaction picture It is sometimes the case that the Hamiltonian $\hat{H}(t)$ has two parts: one corresponding to a system that we know how to solve, let us denote it $\hat{H}_0$ (usually a noninteracting Hamiltonian), and the part $\hat{V}(t)$ (usually an interaction Hamiltonian) which is difficult to solve analytically,

$$\hat{H}(t) = \hat{H}_0 + \hat{V}(t). \tag{12}$$

In general one can regard $\hat{H}_0$ as the system of interest and $\hat{V}$ a small perturbation used for probing it. We then treat $\hat{H}_0$ as in the Heisenberg picture and $\hat{V}$ as in the Schrödinger picture. This approach is known as the interaction picture.

So we define a time-evolution operator $\hat{U}_0$ for the $\hat{H}_0$ part of the Hamiltonian:

$$\hat{U}_0(t) = \mathcal{T}e^{-\frac{i}{\hbar}\int_0^t d\tau\, \hat{H}_0(\tau)}. \tag{13}$$

where $\mathcal{T}$ represents time-ordering (operators evaluated at different times do not in general commute with each other).

Often $\hat{H}_0(t)$ is time-independent ($\hat{H}_0(t) = \hat{H}_0$) and the time-dependence appears only in the perturbation $\hat{V}(t)$. In this case, we can write for the operators in the interaction picture

$$\hat{\mathcal{O}}_{\mathrm{I}}(t) = e^{i\hat{H}_0 t/\hbar}\hat{\mathcal{O}}_{\mathrm{S}}e^{-i\hat{H}_0 t/\hbar}, \tag{14}$$

which shows that the time-dependence of operators is given only by $\hat{H}_0$ (Heisenberg picture w.r.t. $\hat{H}_0$), and we have initially $|\psi_0\rangle_I = |\psi_0\rangle_S$. For the states, we use again the interaction picture w.r.t. $\hat{H}_0$ as in Eq. (9) to find

$$\begin{aligned} |\psi(t)\rangle_{\mathrm{I}} &= e^{i\hat{H}_0 t/\hbar}|\psi(t)\rangle_{\mathrm{S}} \\ &= e^{i\hat{H}_0 t/\hbar}\mathcal{T}e^{-\frac{i}{\hbar}\int_0^t d\tau\, \hat{H}(\tau)}|\psi(0)\rangle_{\mathrm{S}} \\ &= e^{i\hat{H}_0 t/\hbar}\mathcal{T}e^{-\frac{i}{\hbar}\int_0^t d\tau\, \hat{H}(\tau)}|\psi(0)\rangle_{\mathrm{I}}. \end{aligned} \tag{15}$$

This immediately yields an elegant evolution law, expressed only in terms of the interaction

$$\begin{aligned} i\hbar\frac{d}{dt}|\psi(t)\rangle_{\mathrm{I}} &= i\hbar\frac{d}{dt}\left(e^{i\hat{H}_0 t/\hbar}\mathcal{T}e^{-\frac{i}{\hbar}\int_0^t d\tau\, \hat{H}(\tau)}|\psi(0)\rangle_{\mathrm{I}}\right) \\ &= -\hat{H}_0 e^{i\hat{H}_0 t/\hbar}\mathcal{T}e^{-\frac{i}{\hbar}\int_0^t d\tau\, \hat{H}(\tau)}|\psi(0)\rangle_{\mathrm{I}} + e^{i\hat{H}_0 t/\hbar}\hat{H}(t)\mathcal{T}e^{-\frac{i}{\hbar}\int_0^t d\tau\, \hat{H}(\tau)}|\psi(0)\rangle_{\mathrm{I}} \\ &= -\hat{H}_0|\psi(t)\rangle_{\mathrm{I}} + \hat{H}_{\mathrm{I}}(t)|\psi(t)\rangle_{\mathrm{I}} \\ &= \hat{V}_{\mathrm{I}}(t)|\psi(t)\rangle_{\mathrm{I}}, \end{aligned} \tag{16}$$

where $\hat{H}_{\mathrm{I}}$ and $\hat{V}_{\mathrm{I}}$ are the operators $\hat{H}$ and $\hat{V}$ in the interaction picture.

III. FERMI GOLDEN RULE

Fermi's Golden rule is based on first-order time-dependent perturbation theory. It gives transition rates in case the perturbation couples a state into a continuum, or a band, of states.

The total Hamiltonian is

$$\hat{H}(t) = \hat{H}_0 + \hat{H}' e^{\eta t}. \tag{17}$$

Here the factor η is meant to show that the small perturbation H' is turned on adiabatically. Then one solves the Schrödinger equation using first-order perturbation theory and

calculates the transition rates from an initial state $|i\rangle$ to the final state $|f\rangle$, both eigenstates of the unperturbed Hamiltonian $\hat{H}_0$, $\hat{H}_0|i\rangle = \epsilon_i|i\rangle$, $\hat{H}_0|f\rangle = \epsilon_f|f\rangle$, and $\hat{H}'_{fi} = \langle f|H'|i\rangle$.

The **transition rate** $\Gamma_{i\to f} = dP_{i\to f}/dt$ is

$$\Gamma_{i\to f} = \frac{2\pi}{\hbar}|\hat{H}'_{fi}|^2\delta(\epsilon_f - \epsilon_i). \tag{18}$$

Note the units: the units of the delta function are 1/energy, and the matrix element has units of energy; this means that $\Gamma_{i\to f}$ is measured in 1/time, as it should be.

To obtain the total rate one has to integrate Eq. (18) over energies. If the state $|f\rangle$ belongs to a continuum with density of states $\mathcal{N}(\epsilon)$, then the total rate per unit sample volume is

$$\bar{\Gamma}_{i\to f} = \int d\epsilon_f \mathcal{N}(\epsilon_f)\Gamma_{i\to f} = \frac{2\pi}{\hbar}\mathcal{N}(\epsilon_f = \epsilon_i)|\hat{H}'_{fi}|^2. \tag{19}$$

Later in this lecture we will go a bit more in-depth on how to calculate the density of states.

IV. SECOND QUANTIZATION

Second quantization is an elegant way of formulating quantum physics and it is an essential tool for quantum many-body systems and fields. The idea is to bypass the cumbersome procedure of symmetrization (for bosons) and anti-symmetrization (for fermions) by using an already symmetrized/antisymmetrized space called Fock space - defined by the eigenvectors of the occupation numbers. The name "second quantization" is used for historical reasons for this procedure and can be misleading (it is not the case that we quantize the system once and then again for the second time; it is only a single quantization procedure involved).

Fock space

The Fock space is a space where the basis vectors are defined by the occupation numbers. The states that span this space satisfy the following properties:

1. Orthogonality:

$$\langle n_1, n_2, \ldots | n'_1, n'_2, \ldots\rangle = \delta_{n_1 n'_1}\delta_{n_2 n'_2}\ldots \tag{20}$$

2. Completeness:

$$\sum_{n_1,n_2,\ldots} |n_1, n_2, \ldots\rangle \langle n_1, n_2, \ldots| = \hat{I}, \tag{21}$$

where $\hat{I}$ is the identity operator.

Some operators, for example $\hat{x}$, $\hat{p}$, and the number of particle operator $\hat{N}$, when acting on an N-particle state they leave it as an N-particle state. Other operators change the occupation number, for example the creation and annihilation operators.

The main idea in second quantization is: use the states $|n_1, n_2, \ldots\rangle$, which have already the correct wavefunction symmetry and write all the operators in terms of creation/annihilation operators acting on these states, including the Hamiltonian.

Bosons

The creation operator is:

$$\hat{a}_i^\dagger \left|\ldots, n_i, \ldots\right\rangle = \sqrt{n_i + 1} \left|\ldots, n_i + 1, \ldots\right\rangle . \tag{22}$$

The adjoint (annihilation) operator is then

$$\left\langle\ldots, n'_i, \ldots\right| \hat{a}_i = \sqrt{n'_i + 1} \left\langle\ldots, n'_i + 1, \ldots\right| , \tag{23}$$

therefore

$$\left\langle\ldots, n'_i, \ldots\right| \hat{a}_i \left|\ldots, n_i, \ldots\right\rangle = \sqrt{n_i} \delta_{n'_i+1, n_i}, \tag{24}$$

and so

$$\hat{a}_i \left|\ldots, n_i, \ldots\right\rangle = \sqrt{n_i} \left|\ldots, n_i - 1, \ldots\right\rangle , \qquad for \quad n_i \geq 1, \tag{25}$$

and

$$\hat{a}_i \left|\ldots, n_i = 0, \ldots\right\rangle = 0 \tag{26}$$

These relations together with the completeness relation imply that the operators fulfill the Bose commutation relations:

$$[\hat{a}_i, \hat{a}_j] = 0, \qquad \left[\hat{a}_i^\dagger, \hat{a}_j^\dagger\right] = 0, \qquad \left[\hat{a}_i, \hat{a}_j^\dagger\right] = \delta_{ij}. \tag{27}$$

Now, we can construct all states by using the annihilation and creation operators and starting from the ground state (vacuum state).

Ground (vacuum) state:

$$|0\rangle \equiv |0, 0, \ldots\rangle . \tag{28}$$

Single-particle states:

$$\hat{a}_i^\dagger |0\rangle , \qquad \ldots . \tag{29}$$

Two-particle states:

$$\frac{1}{\sqrt{2}}\left(\hat{a}_i^\dagger\right)^2|0\rangle\,, \qquad a_i^\dagger a_j^\dagger|0\rangle\,, \qquad \ldots \tag{30}$$

N-particle states:

$$|n_1, n_2, \ldots\rangle = \frac{1}{\sqrt{n_1! n_2! \ldots}}\left(\hat{a}_1^\dagger\right)^{n_1}\left(\hat{a}_2^\dagger\right)^{n_2}\ldots|0\rangle\,, \ldots \tag{31}$$

Normalization:

$$\left\|\hat{a}^\dagger|n-1\rangle\right\| = \sqrt{n}. \tag{32}$$

Useful relations:

$$\hat{a}^\dagger|n-1\rangle = \sqrt{n}\,|n\rangle\,, \tag{33}$$

$$|n\rangle = \frac{1}{\sqrt{n}}\hat{a}^\dagger|n-1\rangle\,. \tag{34}$$

Occupation number in state $|i\rangle$:

$$\hat{n}_i = \hat{a}_i^\dagger\hat{a}_i. \tag{35}$$

Total number of particles:

$$\hat{N} = \sum_i \hat{n}_i, \tag{36}$$

$$\hat{N}|n_1, n_2, \ldots\rangle = N|n_1, n_2, \ldots\rangle\,. \tag{37}$$

Fermions

For fermions the wavefunction is antisymmetric and fermionic operators anticommute:

$$\left\{\hat{a}_i^\dagger, \hat{a}_j^\dagger\right\} = 0, \qquad \hat{a}_i^\dagger\hat{a}_j^\dagger = -\hat{a}_j^\dagger\hat{a}_i^\dagger. \tag{38}$$

This implies also that two fermions cannot occupy the same state,

$$\hat{a}_i^\dagger\hat{a}_j^\dagger = -\hat{a}_j^\dagger\hat{a}_i^\dagger \Rightarrow \left(\hat{a}_i^\dagger\right)^2 = 0. \tag{39}$$

In order to have a simple, unified notation for the commutator/anticommutator we could introduce the notation

$$[A, B]_+ \equiv \{A, B\} = AB + BA, \tag{40}$$

$$[A, B]_- \equiv [A, B] = AB - BA. \tag{41}$$

Then we occupy states one by one (compare also with Equation (31) for bosons)

$$|n_1, n_2, \ldots\rangle = \left(\hat{a}_1^\dagger\right)^{n_1}\left(\hat{a}_2^\dagger\right)^{n_2}\ldots|0\rangle\,, \qquad n_i = 0, 1. \tag{42}$$

The creation operator $\hat{a}_i^\dagger$ must be (compare with Equation (22) for bosons):

$$\hat{a}_i^\dagger \left|\ldots, n_i, \ldots\right\rangle = (1-n_i)\,(-1)^{\sum_{j<i} n_j} \left|\ldots, n_i+1, \ldots\right\rangle. \tag{43}$$

The term $(-1)^{\sum_{j<i} n_j}$ appears because the operator $\hat{a}_i^\dagger$ has to be brought to the position i and along the way commuted with the other operators $\hat{a}_j^\dagger$. Note that if $n_i = 1$ the result of applying $\hat{a}_i^\dagger$ is zero, reflecting the Pauli exclusion principle. The adjoint (annihilation) operator is

$$\left\langle\ldots, n_i, \ldots\right| \hat{a}_i = (1-n_i)\,(-1)^{\sum_{j<i} n_j} \left\langle\ldots, n_i+1, \ldots\right|, \tag{44}$$

therefore

$$\left\langle\ldots, n_i, \ldots\right| \hat{a}_i \left|\ldots, n'_i, \ldots\right\rangle = (1-n_i)\,(-1)^{\sum_{j<i} n_j}\, \delta_{n_i+1, n'_i}, \tag{45}$$

$$\hat{a}_i \left|\ldots, n'_i, \ldots\right\rangle = \sum_{n_i} \left|n_i\right\rangle \left\langle n_i\right| \hat{a}_i \left|n'_i\right\rangle = n'_i\,(-1)^{\sum_{j<i} n_j} \left|\ldots, n'_i - 1, \ldots\right\rangle. \tag{46}$$

We then obtain

$$\begin{aligned} \hat{a}_i \hat{a}_i^\dagger \left|\ldots, n_i, \ldots\right\rangle &= \hat{a}_i\,(1-n_i)\,(-1)^{\sum_{j<i} n_j} \left|\ldots, n_i+1, \ldots\right\rangle \\ &= (1-n_i)\,(n_i+1) \left|\ldots, n_i, \ldots\right\rangle \\ &= (1-n_i) \left|\ldots, n_i, \ldots\right\rangle, \end{aligned} \tag{47}$$

$$\hat{a}_i^\dagger \hat{a}_i \left|\ldots, n_i, \ldots\right\rangle = n_i \left|\ldots, n_i, \ldots\right\rangle. \tag{48}$$

($n_i^2 = n_i$ for $n_i = 0, 1$). From here, one obtains the anticommutation rules for fermions (take sums of Equations (47) and (48), compare with (27) for bosons):

$$\left[\hat{a}_i, \hat{a}_j\right]_+ = 0, \qquad \left[\hat{a}_i^\dagger, \hat{a}_j^\dagger\right]_+ = 0, \qquad \left[\hat{a}_i, \hat{a}_j^\dagger\right]_+ = \delta_{ij}. \tag{49}$$

Quite often fermionic annihilation and creation operators are denoted by the $\hat{c}$: $\hat{c}_i$, $\hat{c}_i^\dagger$, and the bosonic ones by $\hat{a}$ (or $\hat{b}$): $\hat{a}_i$, $\hat{a}_i^\dagger$ ($\hat{b}_i$, $\hat{b}_i^\dagger$).

A. Field quantization

The distinction between particles and fields exists only in classical mechanics. In quantum physics, particles are the quanta of a certain field. Thus, given a particular field (say the electromagnetic field) one follows a rather standard procedure of quantizing the field. A

field is defined at every point $\vec{r}$ in space, but the quanta are defined typically with another observable (momentum, energy, *etc.*). Therefore it is important to understand how to make this kind of change of basis.

Take now a single-particle basis set $\{|i\rangle\}$ with the corresponding annihilation and creation operators, $\hat{a}_i$ and $\hat{a}_i^\dagger$. Changing to a new basis $\{|\lambda\rangle\}$ with new annihilation and creation operators $\hat{b}_\lambda$, $\hat{b}_\lambda^\dagger$ is done in the following steps. First, note that now we talk about basis of single particles, therefore creating one particle in a state $|\lambda\rangle$ means $|1\rangle_\lambda = |\lambda\rangle = \hat{b}_\lambda^\dagger|0\rangle$, and similarly for $\hat{a}$, $|1\rangle_i = |i\rangle = \hat{a}_i^\dagger|0\rangle$. We first expand the eigenvectors of the new basis,

$$|\lambda\rangle = \sum_i |i\rangle\langle i|\lambda\rangle. \tag{50}$$

Let us assume that the vacuum state in both bases is the same; we find from $|\lambda\rangle = \sum_i \langle i|\lambda\rangle|i\rangle$ that

$$\hat{b}_\lambda^\dagger|0\rangle = \sum_i \langle i|\lambda\rangle \hat{a}_i^\dagger|0\rangle, \tag{51}$$

which gives the relation between the creation/annihilation operators in the two basis,

$$\hat{b}_\lambda^\dagger = \sum_i \langle i|\lambda\rangle \hat{a}_i^\dagger, \tag{52}$$

$$\hat{b}_\lambda = \sum_i \langle \lambda|i\rangle \hat{a}_i. \tag{53}$$

An important basis is the position basis $\{|\vec{r}\rangle\}$. This defines the so-called **field operators**:

$$\hat{\psi}^\dagger(\vec{r}) = \sum_i \langle i|\vec{r}\rangle \hat{a}_i^\dagger = \sum_i \varphi_i^*(\vec{r})\hat{a}_i^\dagger, \tag{54}$$

where $\varphi_i(\vec{r})$ is the wave function corresponding to the single-particle state $|i\rangle$, by definition $\varphi_i(\vec{r}) = \langle \vec{r}|i\rangle$.

You can immediately verify that the field operators satisfy the commutation/anticommutation relations

$$\left[\hat{\psi}(\vec{r}), \hat{\psi}(\vec{r}')\right]_\pm = \sum_{ij} \varphi_i(\vec{r})\varphi_j(\vec{r}') \left[\hat{a}_i, \hat{a}_j\right]_\pm = 0, \tag{55}$$

$$\left[\hat{\psi}^\dagger(\vec{r}), \hat{\psi}^\dagger(\vec{r}')\right]_\pm = \sum_{ij} \varphi_i^*(\vec{r})\varphi_j^*(\vec{r}') \left[\hat{a}_i^\dagger, \hat{a}_j^\dagger\right]_\pm = 0, \tag{56}$$

and

$$\left[\hat{\psi}(\vec{r}), \hat{\psi}^\dagger(\vec{r}')\right]_\pm = \sum_{ij} \varphi_i(\vec{r})\varphi_j^*(\vec{r}') \left[\hat{a}_i, \hat{a}_j^\dagger\right]_\pm = \sum_i \varphi_i(\vec{r})\varphi_i^*(\vec{r}') = \delta^{(3)}(\vec{r} - \vec{r}'). \tag{57}$$

Example: momentum representation

For free particles the most encountered basis is the plane wave basis $\varphi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}/\sqrt{V}$, where now the index i is replaced by the momentum $\vec{k}$,

$$\hat{\psi}(\vec{r}) = \sum_{\vec{k}} \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}} \hat{a}_{\vec{k}}, \tag{58}$$

where $V = L_x L_y L_z$ is the volume and $\vec{k}$ is the momentum.

With periodic boundary conditions, the quantized momentum eigenstates are

$$\vec{k} = 2\pi \left(\frac{n_x}{L_x}, \frac{n_y}{L_y}, \frac{n_z}{L_z} \right). \tag{59}$$

where $n_i \in \mathcal{Z}$, and with corresponding eigenfunctions

$$\varphi_{\vec{k}}(\vec{r}) = \langle \vec{r} | \varphi \rangle_{\vec{r}} = \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}}. \tag{60}$$

The annihilation and creation operators for a particle with a wave vector $\vec{r}$ (i.e. in the state $|\varphi\rangle_{\vec{r}}$) satisfy the usual commutation relations:

$$\left[\hat{a}_{\vec{k}}, \hat{a}_{\vec{k'}}\right]_{\pm} = 0, \tag{61}$$

$$\left[\hat{a}^{\dagger}_{\vec{k}}, \hat{a}_{\vec{k'}}\dagger\right]_{\pm} = 0, \tag{62}$$

$$\left[\hat{a}_{\vec{k}}, \hat{a}^{\dagger}_{\vec{k'}}\right]_{\pm} = \delta_{\vec{k}\vec{k'}}. \tag{63}$$

Any observable can be written in the second-quantization representation. For example, the free-electron Hamiltonian can be written conveniently in the momentum basis as

$$\hat{H} = \sum_{\vec{k},\sigma=\uparrow,\downarrow} \frac{\hbar^2 k^2}{2m} \hat{c}^{\dagger}_{\vec{k},\sigma} \hat{c}_{\vec{k},\sigma}, \tag{64}$$

where σ is the spin index and $c_{\vec{k},\sigma}$ and $c^{\dagger}_{\vec{k},\sigma}$ are fermionic annihilation and creation operators (the notation $\hat{c}$ instead of $\hat{a}$ is often used for electrons). You can recognize the operator $\hat{c}^{\dagger}_{\vec{k},\sigma}\hat{c}_{\vec{k},\sigma}$ as the number operator of the electrons with spin σ and momentum $\vec{k}$. Note also that this Hamiltonian is already diagonal in the number of particle (Fock) basis, see Eq. (45-49).

V. ELEMENTS OF SOLID STATE PHYSICS

Most of the time in mesoscopic physics we deal with energies close to the Fermi level and as a result many quantities that depend on energy can be considered constant, and at the Fermi energy value E_F.

A. Momentum representation

To explain this representation, let us consider first the case $T = 0$ and the three-dimensional case. Due to the Pauli exclusion principle, the electrons fill in all the available levels up to the Fermi level with energy E_F. In k-space the result is the Fermi surface. If the energy is independent on the direction of the momentum, this surface is a sphere S_F, and we can calculate in 3D the particle number density as follows

$$n(T=0) = 2 \times \frac{1}{V} \sum_{\vec{k} \in S_F} 1 \approx 2 \frac{1}{(2\pi)^3} \int_{\vec{k} \in S_F} d\vec{k} \tag{65}$$

$$= \frac{1}{4\pi^3} \int_0^{k_F} k^2 dk \int_0^{2\pi} d\varphi \int_0^{\pi} \sin(\phi) d\phi \tag{66}$$

$$= \frac{1}{3\pi^2} k_F^3, \tag{67}$$

where the factor of 2 in front comes from the spin and we used the usual discrete-to-continuum transformation which follows immediately from $dk_{x,y,z} = (2\pi/L) dn_{x,y,z}$,

$$\frac{1}{V} \sum_{\vec{k}} \to \frac{1}{(2\pi)^3} \int d^3\vec{k}. \tag{68}$$

The total energy density is then

$$E_{\text{tot}} = 2 \frac{1}{V} \sum_{\vec{k}} \epsilon_k = \frac{1}{\pi^2} \int_0^{k_F} dk k^2 \epsilon(k), \tag{69}$$

where ϵ_k is the energy of a momentum state k. The chemical potential is then defined as the energy needed to add one extra particle (electron) in the system,

$$\mu = \frac{dE_{\text{tot}}}{dn} = \frac{dE_{\text{tot}}}{dk_F} \frac{dk_F}{dn} = \epsilon(k_F) = \epsilon_F. \tag{70}$$

B. Energy representation - the concept of density of states

When calculating, as above, the number of carriers, it is usually the case that there is no angle-dependence and instead of integration over momentum it is more convenient to integrate over energies. This apparently simple change of variables gives rise to a very useful concept - that of density of states, denoted usually by $\mathcal{D}(E)$ or $\mathcal{N}(E)$. In general, the density of states depends on dimensionality and on the bandstructure, and in the case of simple dependence $E(k)$ it is possible to find analytical results. We will look in the following at the simplest case, namely a quadratic dispersion relation $E(k) = \hbar^2 k^2/(2m)$.

As usual, we impose periodic boundary conditions on the wavefunctions of the electrons, which are assumed noninteracting and moving in a null potential (free electron gas). Therefore the electron wavefunction is an eigenvalue of the momentum operator,

$$\psi(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}, \tag{71}$$

where we assume periodic boundary conditions in all directions over a length L, and $V = L^3$. This imposes the momentum quantization

$$k_x = \frac{2\pi n_x}{L}, \quad k_y = \frac{2\pi n_y}{L}, \quad k_z = \frac{2\pi n_z}{L}, \tag{72}$$

where n_x, n_y, n_z are integers.

Density of states in 3D

The volume element in the momentum space in 3D is then

$$V_{3D} = \left(\frac{2\pi}{L}\right)^3. \tag{73}$$

Consider now in $\vec{k}$-space a shell between the radiuses k and $k + dk$. The volume of this shell is the area of the sphere of radius k, which is $4\pi k^2$, multiplied by dk, that is

$$4\pi k^2 dk. \tag{74}$$

The number of states in the shell is

$$2 \times \frac{4\pi k^2 dk}{V_{3D}} = \frac{k^2 dk}{\pi^2} L^3, \tag{75}$$

where the factor of 2 is the spin degeneracy. For the energy let us assume the quadratic dispersion

$$\epsilon(k) = \frac{\hbar^2 k^2}{2m}, \tag{76}$$

therefore

$$dk = \left(\frac{2m\epsilon}{\hbar^2}\right)^{-1/2} \frac{m}{\hbar^2} d\epsilon. \tag{77}$$

The density of states is the number of states per unit volume within an interval of energy $(\epsilon, \epsilon + d\epsilon)$,

$$\mathcal{N}_{3D}(\epsilon) d\epsilon = \frac{k^2 dk}{\pi^2} = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \epsilon^{1/2} d\epsilon. \tag{78}$$

Density of states in 2D

The calculation is similar to the one in 3D. The volume element in 2D (the area of a square) is now

$$V_{2D} = \left(\frac{2\pi}{L}\right)^2. \tag{79}$$

Consider now in k-space an anulus between the radiuses k and $k + dk$. The volume of this annulus is the perimeter of the circle of radius k, which is $2\pi k$, multiplied by dk, that is

$$2\pi k dk. \tag{80}$$

The number of states in the shell is

$$2 \times \frac{2\pi k dk}{V_{2D}} = \frac{k dk}{\pi} L^2, \tag{81}$$

where the factor of 2 in front is again the spin degeneracy. For the energy let us assume the quadratic dispersion

$$\epsilon(k) = \frac{\hbar^2 k^2}{2m}, \tag{82}$$

therefore exactly as before

$$dk = \left(\frac{2m\epsilon}{\hbar^2}\right)^{-1/2} \frac{m}{\hbar^2} d\epsilon \tag{83}$$

The density of states is the number of states per unit 2D volume (*i.e.* area) within an interval of energy $(E, E + dE)$,

$$\mathcal{N}_{2D}(\epsilon) d\epsilon = \frac{k dk}{\pi} = \frac{m}{\pi \hbar^2} d\epsilon. \tag{84}$$

The remarkable fact about the density of states in 2D is that it does not depend on energy!

Density of states in 1D

The volume element in 1D is

$$V_{1D} = \frac{2\pi}{L}. \tag{85}$$

Consider now in k-space a length between k and $k + dk$. The corresponding 1D-volume of this length is

$$2dk. \tag{86}$$

The number of states in this length is

$$2 \times \frac{2dk}{V_{1D}} = 2\frac{dk}{\pi} L, \tag{87}$$

where the factor of 2 in front is the spin degeneracy. For the energy the quadratic dispersion

$$\epsilon(k) = \frac{\hbar^2 k^2}{2m}, \tag{88}$$

gives again

$$dk = \left(\frac{2m\epsilon}{\hbar^2}\right)^{-1/2} \frac{m}{\hbar^2} d\epsilon \tag{89}$$

The density of states is the number of states per unit volume in 1D (*i.e. length*) within an interval of energy $(\epsilon, \epsilon + d\epsilon)$,

$$\mathcal{N}_{1D}(\epsilon) d\epsilon = \frac{2dk}{\pi} = \frac{1}{\pi}\sqrt{\frac{2m}{\hbar^2}} \frac{1}{\epsilon^{1/2}} d\epsilon \tag{90}$$

Note that now the energy dependence of the density of states is $\approx \epsilon^{-1/2}$.

Density of states in 0D

In zero-dimensional systems (e.g. quantum dots) the available states exist only at discrete values of the energy, thus the density of states can be represented by delta functions $\delta(\epsilon - \epsilon_i)$. In reality, several effects result in the broadening of these δ-functions.

VI. APPENDIX: USEFUL FERMI INTEGRALS

In many problems in nanoelectronics some rather complicated-looking integrals of Fermi functions may appear, especially when finite temperature is involved. Surprisingly, some of these integrals yield simple, analytical results. One example is shown below.

The Fermi functions are given by

$$f(\epsilon) = \frac{1}{\exp(\epsilon/k_B T) + 1}. \tag{91}$$

We now introduce [1] the function

$$g(x) = \int_{-\infty}^{\infty} d\epsilon \left[f(\epsilon) - f(\epsilon + x) \right]. \tag{92}$$

Obviously $g(0) = 0$. The first derivative of g gives

$$\frac{dg(x)}{dx} = -\int_{-\infty}^{\infty} d(\epsilon + x) \frac{df(\epsilon + x)}{d(\epsilon + x)} = -f(\infty) + f(-\infty) = 1. \tag{93}$$

This means that $g(x) = x$, so we have the result

$$\int_{-\infty}^{\infty} d\epsilon \left[f(\epsilon) - f(\epsilon + x) \right] = x\,. \tag{94}$$

Now, integrals over expressions of the type $f(E)[1 - f(E + x)]$, which appear in the theory of tunneling due to Pauli exclusion principle, can be solved by noticing that

$$f(\epsilon)[1 - f(\epsilon + x)] = \frac{f(\epsilon) - f(\epsilon + x)}{1 - \exp(-\beta x)}, \tag{95}$$

where $\beta = 1/k_B T$. Now, using Eq. (94) we get immediately

$$\int_{-\infty}^{\infty} d\epsilon f(\epsilon)[1 - f(\epsilon + x)] = \frac{x}{1 - \exp(-\beta x)}. \tag{96}$$

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[1] G.-L. Ingold and Yu.V. Nazarov, "Charge tunneling rates in ultrasmall junctions", in *Single Charge Tunneling*, edited by H. Grabert and M. H. Devoret (Plenum, New York, 1992), pp. 21-108.