Basic Equations

This side just serves as a *reminder* since nobody (extrapolating from myself) can remember *all* the basic equations (and some secondary stuff) with their most important connotations *in detail*.

- You should, however, be rather familiar with all of them.

- Some equations are just briefly mentioned, some are dealt with in more detail - as the occasion demands.

Basics

Schrödinger Equation

The Schrödinger equation is one of the most celebrated equations in physics, not least because it is a *differential equation* that was much more "understandable" to the contemporaries of the **20 th** century giants of physics who invented - or discovered? - quantum theory than the more abstract matrix formulation of **Heisenberg** .

- In the context of the fully developed formalized quantum theory of today, the Schrödinger equation has lost some of its clamor - it just happens to be the Eigenwert equation for the energy operator (also called **Hamilton operator**), but since the energy eigenvalues are of course of prime importance, the Schrödinger equation is still a major equation in quantum theory.

- Here is the general Schrödinger equation

$$-\frac{\hbar^2}{2m} \cdot \Delta \psi'(\underline{r},t) + U(\underline{r},t) \cdot \psi'(\underline{r},t) \;=\; \frac{\hbar}{i} \cdot \frac{\partial \psi'(\underline{r},t)}{\partial t}$$

- $U = U(x,y,z)$ = *potential energy*, and all other symbols have their usual meaning. The Δ operator is written large and in blue to avoird confusion with the regular Δ denoting small differences.

- It is hard to imagine retrospectively how revolutionary an equation must have been that *intrinsically included* **i**, the unit of *imaginary numbers*, in a relation purporting to describe *physical reality*. **Pythagoras**, it is claimed, had one of his students executed because the poor guy claimed that *irrational* numbers actually existed. Fortunately the tolerance level in science has gone up since then (though I'm not so sure about religion, politics, and so on).

Stationary states with sharp values of the total energy that do not change in time can be described by

$$\psi'(\underline{r},t) \;=\; \psi(\underline{r}) \cdot \exp(i\,\omega\,t)$$

- Insertion in the general Schrödinger equation gives the well-known *time independent form*

$$-\frac{\hbar^2}{2m} \cdot \Delta \psi(\underline{r},t) + \left(U(\underline{r}) - E_{total} \right) \cdot \psi(\underline{r},t) \;=\; 0$$

- With $E_{total} = \hbar \cdot \omega$.

For some given potential, the problem is thus reduced to solving a *second order partial differential equation*, which is usually not easy, but essentially a mathematical problem.

- Physics only comes in again by

  - Finding some particular *symmetries* of the problem that must have a direct bearing for the symmetries of the solution, and thus make the math somewhat easier. That is what the Bloch theorem does, for example.
  - Finding some *physical approximations* that allow to write down a simplified equation that still makes some sense. The free electron gas approximation is an example.

Combining the Schrödiner equation with the special theory of relativity yields the **Dirac equation** .

- Another wonderul thing happens at that level: The math involved now cannot be satisfied by describing things with complex numbers, it actually demands matrices.

- As a consequence, spin and antiparticles emerge naturally.

Nobody so far has managed to combine the Schrödinger equation with the general theory of relativity; the two even appear to be antoagonistic. This is in fact one of the biggest unsoveld problems in fundamental physics.

de Broglie Equation

The de Broglie equation, coupling the momentum p of a particle with its wavelength λ - an absolutely revolutionary concept when it was introduced - is very simple

$$\lambda = \frac{h}{p}$$

It is not a fundamental equation but follows from the axioms of quantum mechanics. de Broglie, however, arrived at it in a completely different way (there was no quantum theory then): By coupling the most famous equation of all ($E = mc^2$ from **Einsteins** special theory of relativity) and $E = h\nu$ from **Planck** and Einstein in a rather ingenious way.

Mass Action Law

The mass action law, while simple in appearance, is one of the trickier laws of thermodynamics.

It follows from considering equilibrium in a system where the number of particles may change, but in a connected fashion: Any disappearance of some kind of particle from the ensemble must lead to the appearance of some other kind. In other words: We are looking at chemical reactions and everything else that follows this very general restriction.

The reaction equation describing the connection between the particles A_i can always be expressed as

$$\sum_i \nu_i \cdot A_i = 0$$

and the ν_i are the stoichiometric constants. The mass action law gives a relation between the equilibrium concentrations of the particles, $[A_i]$, that takes the general form

$$\prod_i [A_i]^\nu = \left(\sum [A_i]^{\Sigma \nu} \right) \cdot \exp - \frac{\Sigma_i \, g_i \cdot \nu}{RT}$$

With g_i = free enthalpy of component **i** *and the concentrations measured in mols!*.

In this form, written with with the gas constant **R**, it is obviously formulated for *mols* as a measure of concentrations. Note that the formula may change significantly if you switch to other measures of concentrations, e.g. to particle numbers or densities.

Working with the mass action law is difficult - there are a number of pitfalls. Consult the links to the Hyperscript "Defects" for these topics:

- The chemical potential as the starting point for the mass action law
- The mass action law derived from chemical potentials
- The mass action law derived in a direct "physical" way
- Pitfalls and extension of the mass ation law
- Working with the mass action law in general
- Working with the mass action law for defects; in particular electrons and holes

Einstein Relation

The Einstein relation, or as it should be properly called, the Einstein-**Smoluchowski** relation, couples the **mobility μ** and the **diffusion coefficient** D via

$$D = \frac{kT}{e} \cdot \mu$$

- The mobility **μ**, before only defined as some kind of specific constant relating the average *drift velocity* of *carriers* in an *electrical field*, now is a *general parameter* for all diffusing particles, even without any driving force, it is essentially the diffusion D somewhat disguised.
- The atomistic theory of diffusion correlates the diffusion coefficient to atomistic properties via

$$D = g \cdot a^2 \cdot \nu_0 \cdot \exp -\frac{H_M}{kT}$$

- With g = lattice factor in the order of **1**, a = lattice constant, ν_0 = vibration frequency of the diffusing particle (rougly 10^{13} **Hz**), H_M = activation energy of migration (about **0,5 - 5 eV** for particles (= atoms) in "common" crystals.

This is, of course, only valid for diffusion where all individual jumps occur withthe same mechanism.

- If several mechanisms act otgether (e.g. a particle is jumping around in a lattice, but every now and then gets trapped at a defect. The jumping away from the defect the is a different mechanism then the jumps in the lattice), the total diffusion coefficient will be some mixture of the mechanisms.

In any case, the mobility can now be seen as a *material constant* coming directly from atomic mechanisms.

Fick's laws

Fick's laws are purely phenomenological laws relating the particle current j of diffusing particles to the concentration gradient ∇c as the driving force.

- Fick's *first* law is quite simple

$$j = -D \cdot \nabla \cdot c$$

- With the continuity assumption, i.e. no particles are generated or lost, the change of the particle concentration in some volume element at (x,y,z) is easily derived and called Fick's *second* law.

$$\frac{\partial c}{\partial t} = -\text{div}(j) = D \cdot \nabla^2 \cdot c = D \cdot \Delta c$$

While these differential equations look deceptively simple, their solutions generally are not. Even simple cases usually involve statistical functions - as well they should, considering that diffusion is a statistical phenomenon.

Fick's empirical laws are easily derived from a consideration of simple atomic mechanisms.

- The basic underlying statistical concept is *random walk*, as encountered in simple diffusion mechanisms, e.g. vacancy or interstitial diffusion. For more complicated mechanisms, Fick's laws can not be applied anymore without proper corrections. Note that diffusion in semiconductors is amost always such a "more complicated" case.
- If there are other driving forces besides the concentration gradients, and if particles are generated and/or disappear with certain ((x,y,z) dependent) rates (consider i.e. carriers generated by light and disappearing by recombination), additional terms must be added.

Poisson Equation

The Poisson equation is not a basic equation, but follows directly from the *Maxwell equations* if all time derivatives are zero, i.e. for electrostatic conditions. The first Maxwell equation for the electrical field **E** under these conditions is **div D = ρ** or, for spatially homogeneous dielectric properties,

$$\nabla \cdot \underline{E} \; = \; \frac{\rho}{\epsilon \cdot \epsilon_0}$$

Using the potential **V**, **E** can be expressed as

$$\underline{E} \; = \; - \; \nabla \cdot V$$

Insertion in the first Maxwell equation yields the *Poisson equation*!

$$- \, (\, \nabla \cdot \nabla \,) \cdot V \; = \; \frac{\rho_0}{\epsilon \cdot \epsilon_0}$$

$\nabla \cdot \nabla \cdot$ **V**, of course, can be written as

$$(\nabla \cdot \nabla) \cdot V \; = \nabla^2 \cdot V = \frac{\partial^2 \, V}{\partial \, x^2} \; + \; \frac{\partial^2 \, V}{\partial \, y^2} \; + \; \frac{\partial^2 \, V}{\partial \, z^2}$$

This gives the Poisson equation in its usual form

$$- \, \Delta \, V \; = \; \frac{\rho}{\epsilon \cdot \epsilon_0}$$

We have used the definition of the electrical field **E** as the (negative) gradient of the potential; $E = - \, \nabla V$.

Since the *second* derivative of the electrical potential times $\epsilon \cdot \epsilon_0$ is just the charge density as asserted by Poisson's equation, integrating the charge density *once* essentially yields the electrical *field strength*, integrating it *twice* the *potential*. We will use this feature quite often.

A few words to the signs:

The *negative sign* comes from the general definition of a potential, which applies to the electrostatic potential **V**, too. The existence of a potential demands that the work done **to** a unit charge moving in the gradient of the potential is independent of the path.

In other words, moving a charge **q** in an electrical field from **A** to **B**, the work **W** done is

$$W \; = \; - \, q \int_A^B \underline{E} \cdot \mathrm{d}\underline{s} \; = \; q \int_A^B \nabla \, V \cdot \mathrm{d}\underline{s} \; = \; q \left(V(B) - V(A) \right)$$

So if **q** is *negative*, moving it to a point with a higher potential (assuming that **V(B) > V(A)**), gives a *negative* sign of the work – i.e. work is coming out of the system. For a *positive* charge, **W** is positive and work needs to be done to the system – everything is as it should be.

Newton's Laws

Newton's laws are all too familiar; we will therefore just look at the first one, stating that

$$F = m \cdot a$$

- i.e. a mass m accelerates with the rate $a = dv/dt$ (v = velocity) if a force F acts on it.

Written in three dimensions and with the force expressed as the gradient of an appropriate potential by $F = - \nabla V(r)$, we have

$$m \cdot \frac{d^2 \underline{r}}{dt^2} + \nabla \cdot V(\underline{r}) = 0$$

- which looks a lot less simple.

The formulation most appropriate for this lecture is to express Newton's law via the momentum $p = m \cdot v$ by substituting $a = dv/dt = (1/m) \cdot dp/dt$ and obtaining

$$\frac{d \underline{p}}{dt} + \nabla \cdot V(\underline{r}) = 0$$

Continuity Equation

The continuity equation is simply a balance equation, stating that the change in density n (of whatever) that you will find at a time t in a given volume element at (x,y,z), is determined by how much flows in per time unit minus how much flows out.

- Think of your bank account. The amount of money in it will change depending on how much is deposited minus how much is withdrawn.

While this is elementary, the statement contains two not so obvious topics that are also easily understood thinking about your money in the bank

- No statement whatsoever is made considering the *absolute* amount of money in your account. If you deposit **$ 1,000** a day and withdraw **$ 500**, you are finding **$ 500** *more* in your account and your new balance now might be **$ 1,000,500** instead of **$ 1,000,000** , or **$ 250** instead of **–$ 250**, or whatever – only *you* know because you know the *initial condition* .

- No statement whatsoever is made considering the *absolute* amount of deposits and withdrawal either. You would have obtained the same result for the example above if you would have deposited **$ 500,000** and withdrawn **$ 499,500** – only the *difference* counts.

In mathematical terms, the continuity equation writes

$$\frac{\partial n}{\partial t} = - \nabla \cdot j_{\text{part}}(x,y,z)$$

- and j_{part} is the *particle current* of whatever particles you are considering,

- If j is an *electrical current* while ρ is the *charge density*, you may express it as

$$\frac{\partial \rho}{\partial t} = - \nabla \cdot j(x,y,z)$$

In this version of the continuity equation it is assumed that the particle number is conserved, i.e. no particles are generated or annihilated. So, integrating n (or ρ) over the total volume where particles (or charges) might be, always gives the same total number of particles (or the same total charge). This is the **continuity assumption**.

- This is a perfectly good assumption for *classical* particles and always applicable to, e.g., the flow of water or air.

It is not necessarily, however, a good assumption for electrons and holes in semiconductors.

- First of all, electrons and holes disappear all the time by recombination and appear by generation. However, since in equilibrium the generation rate **G** and the recombination rate **R** are identical, there is a constant particle number *on average* and we can use the continuity equation in its simple form.
- But if we now illuminate a *defined* part of a semiconductor, we have some *defined localized* additional generation and some enhanced recombination *somewhere*, too. The "somewhere" comes from the fact that the recombination does not have to take place wherever the generation took place – the carrier diffuse away before the eventually disappear.

The continuity equation now must be written as follows:

$$\frac{\partial n}{\partial t} = G(x,y,z) - R(x,y,z) - \nabla \cdot j_{\text{part}}(x,y,z)$$

- While we may know **G(x,y,z)** for an illuminated semiconductor, **R(x,y,z)** is not known a priori, and solving the continuity equation together with the two other equations (Ohm's law and Fick's law), making statements about currents may not be easy.
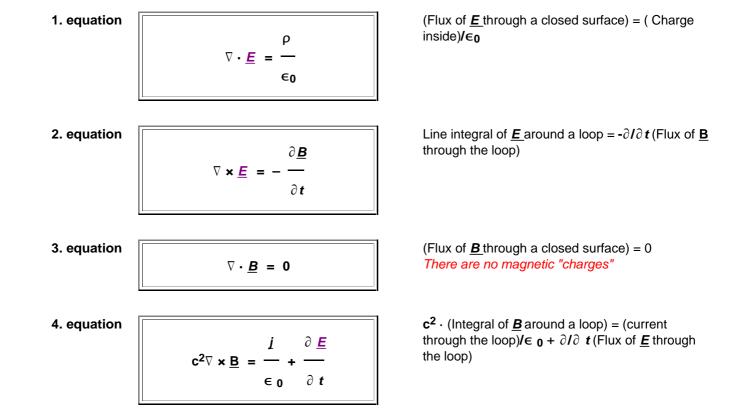
Maxwell's Equations

Maxwell's equations contain all there is to know about electromagnetic phenomena in a classical world (including the special theory of relativity). They essentially link the abstract quantities *electric field*, *magnetic field*, *charge* and *electrical current*.

- Note that the Maxwell equations contain (or demand, as you like it) the *special theory of relativity*, because the velocity of charges is involved. Which velocity? The number you get depends on the frame of reference you chose.
- The paradigmatic "experiment" to that is to look at two electrons, moving with some velocity in parallel. They will attract each other magnetically. What happens if you chose a frame of reference that is tied to the electrons? They are now at rest - no more magnetic attraction?

This is a very difficult question. Look up the answer in any good textbook, e.g. in the Feynman lectures II; chapter 13-6.

Here is an overview, giving the common vector formulation and the integral formulation in prose. Some more laws either following form the Maxwell equation, or needed in the general context, are also given

1. equation

$$\nabla \cdot \underline{E} = \frac{\rho}{\epsilon_0}$$

(Flux of $\underline{E}$ through a closed surface) = (Charge inside)/ϵ_0

2. equation

$$\nabla \times \underline{E} = -\frac{\partial \underline{B}}{\partial t}$$

Line integral of $\underline{E}$ around a loop = $-\partial/\partial t$ (Flux of $\underline{B}$ through the loop)

3. equation

$$\nabla \cdot \underline{B} = 0$$

(Flux of $\underline{B}$ through a closed surface) = 0
There are no magnetic "charges"

4. equation

$$c^2 \nabla \times \underline{B} = \frac{j}{\epsilon_0} + \frac{\partial \underline{E}}{\partial t}$$

$c^2 \cdot$ (Integral of $\underline{B}$ around a loop) = (current through the loop)/ϵ_0 + $\partial/\partial t$ (Flux of $\underline{E}$ through the loop)
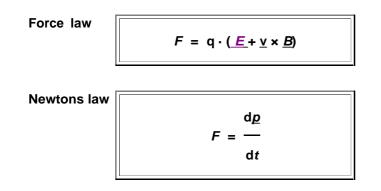
These are the Maxwell equations. Note that they are not only valid for vacuum, but also for materials if the correct charge density is included (we do not really need the *electrical "displacement"* **D**. We also use what is often called "*magnetic induction* **B** " as the primary quantity calling it "magnetic field", and not the outdated secondary quantity **H** .

🔵 The conservation of total charge (essentially the continuity equation "falling out" of the Maxwell equations) gives us.

Charge Conservation

$$\nabla \cdot \underline{j} = - \frac{\partial \rho}{\partial t}$$

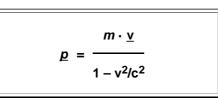Flux of current through a closed surface) = $-\delta \rho/\delta t$(Charge inside)

The coupling to classical mechanics is achieved by introducing the force **F** via the force law and Newtons law expressed for the momentum **p**

Force law

$$F = q \cdot (\underline{E} + \underline{v} \times \underline{B})$$

Also known as Lorentz law.

Newtons law

$$F = \frac{d\underline{p}}{dt}$$

And the special theory of relativity is included by using the relativistic momentum

Special relativity

$$\underline{p} = \frac{m \cdot \underline{v}}{1 - v^2/c^2}$$

If we throw in the (classical) law of gravitation, we have almost *all* basic equations of classical physics as it was known up to about **1905**, in just half a page!

Gravitation

$$F = - G_r \cdot \frac{m_1 \cdot m_2}{r^2}$$

G_r is the gravitational constant