8. gyakorlat (nov. 12)

1. **Klein-Gordon equation in external electromagnetic field and continuity equation**

Four component vector potential:

$$A^\mu = \begin{pmatrix} \frac{\Phi}{c} \\ A_1 \\ A_2 \\ A_3 \end{pmatrix} \equiv \begin{pmatrix} \frac{\Phi}{c} \\ \mathbf{A} \end{pmatrix} \tag{1}$$

Klein Gordon equation for a free particle:

$$\left(p^\mu p_\mu - m^2c^2\right)\psi(x_\mu) = 0 \tag{2}$$

where $p^\mu = \left(\frac{i\hbar}{c}\frac{\partial}{\partial t}, \mathbf{p}\right)$, $\mathbf{p} = \frac{\hbar}{i}\nabla$. Now in the same way as in the case of magnetic field and 3 dimensional vectorpotential the A_μ enters the equation in the following way:

$$\left((p^\mu - qA^\mu)(p_\mu - qA_\mu) - m^2c^2\right)\psi = 0 \tag{3}$$

In the "usual way" one can take the conjugate equation and multiply it with ψ while the original one with ψ^* and substracting them from each other we obtain a continuity equation. That is, first we write out the derivatives with respect to the spatial and temporal parts and expand the squares:

$$\begin{aligned} &\frac{1}{c^2}\left(i\hbar\partial_t - qV\right)^2\psi = \left((\mathbf{p} - q\mathbf{A})^2 + m^2c^2\right)\psi \\ \Leftrightarrow &\left(-\frac{\hbar^2}{c^2}\partial_t^2 - \frac{2iq\hbar V}{c^2}\partial_t + \frac{q^2V^2}{c^2}\right)\psi = \left(-\hbar^2\nabla^2 + 2iq\hbar\mathbf{A}\nabla + q^2\mathbf{A}^2 + m^2c^2\right)\psi \end{aligned} \tag{4}$$

Now taking the adjungate of this equation, that is just complex conjugating the wave-functions and multiply the original equation with ψ^* and the adjungate with ψ and substracting them from each other the terms without differentiation operators drop trivially and we arrive at:

$$\frac{\hbar^2}{c^2}\left(\psi\partial_t^2\psi^* - \psi^*\partial_t^2\psi\right) - \frac{2i\hbar V}{c^2}\left(\psi\partial_t\psi^* + \psi^*\partial_t\psi\right) = \hbar^2\left(\psi\nabla^2\psi^* - \psi^*\nabla^2\psi\right) + \frac{2i\hbar\mathbf{A}}{c^2}\left(\psi\nabla\psi^* + \psi^*\nabla\psi\right) \tag{5}$$

Now using the identity $\psi\nabla^2\psi^* - \psi^*\nabla^2\psi = \nabla\left(\psi\nabla\psi^* - \psi^*\nabla\psi\right)$ and similarly for the time derivatives $\psi\partial_t^2\psi^* - \psi^*\partial_t^2\psi = \partial_t\left(\psi\partial_t\psi^* - \psi^*\partial_t\psi\right)$ while for the second term on both sides we trivially have $\psi\nabla\psi^* + \psi^*\nabla\psi = \nabla\left(|\psi|^2\right)$ and similarly for the time-derivative! Then we only need to assign the dimensionally properly the constants:

$$\nabla\mathbf{j} + \partial_t\rho = 0 \tag{6}$$

$$\rho = \frac{iqh}{2mc}(\psi^*\partial_t\psi - \psi\partial_t\psi^*) - \frac{qV}{mc}\psi^*\psi \tag{7}$$

$$\mathbf{j} = \frac{qh}{2im}(\psi^*\nabla\psi - \psi\nabla\psi^*) - \frac{q\mathbf{A}}{m}\psi^*\psi \tag{8}$$

Or writing it with the four current, $j^\mu = \left(\rho/c, \mathbf{j}\right) = \frac{iq\hbar}{2m}(\psi^*\partial^\mu\psi - \psi\partial^\mu\psi^*) - \frac{qA^\mu}{m}\psi^*\psi$ we obtain:

$$\partial_\mu j^\mu = 0 \tag{9}$$

which can be derived straightfrowardly from the Klein-Gordon equation with the four component notation, where we again take the adjungate equation and multiply it with ψ, while the original equation is multiplied with ψ^* and again substract them from each other:

$$\psi^* \left((p^\mu - qA^\mu)(p_\mu - qA_\mu) + \frac{m^2c^2}{\hbar^2} \right) \psi - \psi \left((p^\mu - qA^\mu)(p_\mu - qA_\mu) + \frac{m^2c^2}{\hbar^2} \right) \psi^* =$$
$$\psi^* \left(p^\mu p_\mu - 2qA^\mu p_\mu \right) \psi - \psi \left(p^\mu p_\mu - 2qA^\mu p_\mu \right) \psi^* = -q\hbar^2 \partial_\mu (\psi^* \partial^\mu \psi - \psi \partial^\mu \psi^*) - \partial_\mu (i2q\hbar A^\mu \psi^* \psi)$$
$$= -\frac{i}{2m\hbar} \partial_\mu j^\mu = 0 \Leftrightarrow \partial_\mu j^\mu = 0 \tag{10}$$

Next we consider the free particle case with plane wave solutions $\psi(\mathbf{r}, t) = Ae^{\frac{i}{\hbar}\mathbf{pr} - \frac{i}{\hbar}Et}$. In the continuity equation without magnetic and electric field the spatial derivatives can be replaced by $\nabla \leftrightarrow \frac{i}{\hbar}\mathbf{p}$ while the temproal derivatives with $\partial_t \leftrightarrow -\frac{i}{\hbar}E$ with which the current and density become:

$$\mathbf{j} = \frac{qh}{2mi} \frac{2i\mathbf{p}}{\hbar} = q\frac{\mathbf{p}}{m} |\psi(\mathbf{r}, t)|^2 \tag{11}$$
$$\rho = q\frac{E}{mc^2} |\psi(\mathbf{r}, t)|^2 \tag{12}$$

but that is not satisfying the positive definiteness of the particle density as it can take negative values as well, as $E = \pm\sqrt{m^2c^4 + p^2c^2}$. The reason behind it is that we have a second order equation with respect to time, meaning that we have an extra initial condition, namely for $\partial_t \rho(\mathbf{r}, t)$ which has no physical meaning!

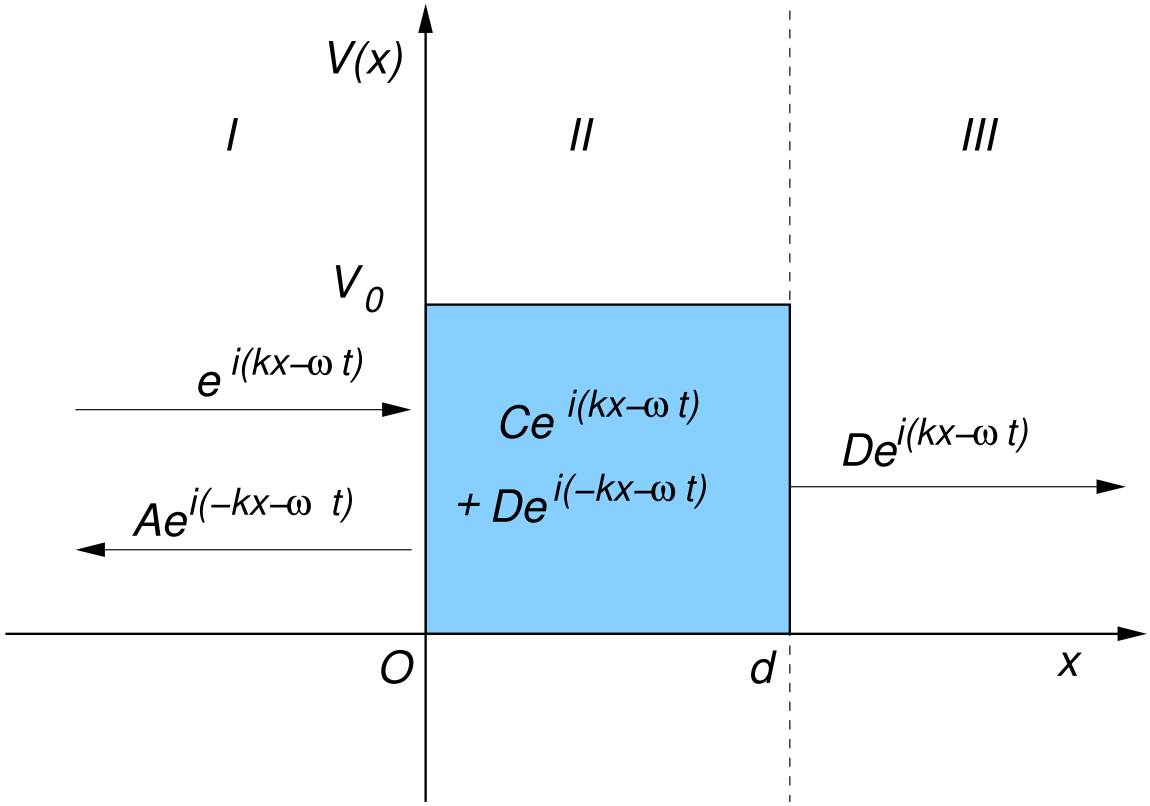
2. **Klein-paradox:**

Consider a potential of height V_0 and width d for which the Klein-Gordon equation reads:

$$\frac{1}{c^2}\left(i\hbar\partial_t - V\right)^2\psi = \left(-\hbar^2\partial_x^2 + m^2c^2\right)\psi$$

$$\psi = e^{i(kx-\omega t)}$$

$$k = \pm\frac{1}{\hbar c}\sqrt{(\hbar\omega - V_0)^2 - m^2c^4}$$



I. domain

$$e^{i(kx-\omega t)} + Ae^{i(-kx-\omega t)}$$

$$ike^{i(kx-\omega t)} - ikAe^{i(-kx-\omega t)}$$

II. domain

$$Be^{i(k'x-\omega t)} + Ce^{i(-k'x-\omega t)}$$

$$ik'Be^{i(k'x-\omega t)} - ik'Ce^{i(-k'x-\omega t)}$$

III. domain

$$De^{i(kx-\omega t)}$$

$$ikDe^{i(kx-\omega t)}$$

I.-II. boudnary

$$\begin{aligned} 1 + A &= B + C \\ ik - ikA &= ik'B - ik'C \end{aligned}\ , \qquad \begin{pmatrix} 1 & 1 \\ ik & -ik \end{pmatrix}\begin{pmatrix} 1 \\ A \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ ik' & -ik' \end{pmatrix}\begin{pmatrix} B \\ C \end{pmatrix}$$

$$\frac{1}{2k'}\begin{pmatrix} k'+k & k'-k \\ k'-k & k'+k \end{pmatrix}\begin{pmatrix} 1 \\ A \end{pmatrix} = \begin{pmatrix} B \\ C \end{pmatrix}$$

II.-III. boundary

$$\begin{array}{c} Be^{ik'd} + Ce^{-ik'd} = De^{ikd} \\ ik'Be^{ik'd} - ik'Ce^{-ik'd} = ikDe^{ikd} \end{array} , \begin{pmatrix} e^{ik'd} & e^{-ik'd} \\ ik'e^{ik'd} & -ik'e^{-ik'd} \end{pmatrix}\begin{pmatrix} B \\ C \end{pmatrix} = e^{ikd}D\begin{pmatrix} 1 \\ ik \end{pmatrix}$$

$$\begin{pmatrix} e^{ik'd} & e^{-ik'd} \\ ik'e^{ik'd} & -ik'e^{-ik'd} \end{pmatrix}\begin{pmatrix} ik'+ik & ik'-ik \\ ik'-ik & ik'+ik \end{pmatrix}\begin{pmatrix} 1 \\ A \end{pmatrix} = \tilde{D}\begin{pmatrix} 1 \\ ik \end{pmatrix} , \ \tilde{D} = 2k'e^{ikd}D$$

$$A = \frac{(k'^2 - k^2)\sin(k'd)}{(k'^2 + k^2)\sin(k'd) + ikk'\cos(k'd)}$$

The reflection coefficient: $R = |A|^2$ and the transition coefficient $T = |D|^2$. If $k'd = n\pi$, then the transition coefficient $T = 1$.

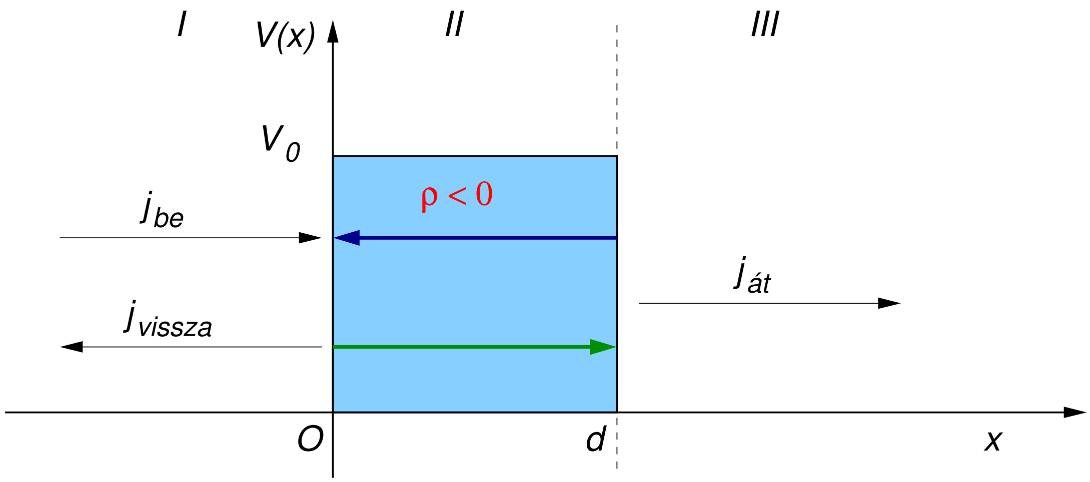
$$k = \pm\frac{1}{\hbar c}\sqrt{\hbar^2\omega^2 - m^2c^4} , \quad k' = \pm\frac{1}{\hbar c}\sqrt{(\hbar\omega - V_0)^2 - m^2c^4} , \quad E = \hbar\omega$$

The wavenumber of the free particle ($x < 0$, $x > d$) is real: $E \geq mc^2$, $\psi = e^{i(kx-\omega t)}$

$$\rho = \frac{iq\hbar}{2mc^2}\left(\psi^*\partial_t\psi - \psi\partial_t\psi^*\right) - \frac{qV}{mc^2}\psi^*\psi = \boxed{q\frac{\hbar\omega - V}{mc^2}}$$

$$\mathbf{j} = \frac{q\hbar}{2im}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right) - \frac{q\mathbf{A}}{m}\psi^*\psi = \boxed{q\frac{\hbar\mathbf{k} - \mathbf{A}}{m}}$$

- $V_0 < E - mc^2$ k' is real, $T = 1$, if $k'd = n\pi$
- $E - mc^2 < V_0 < E + mc^2$ k' is imaginary, inside the well we have decaying solutions, $T < 1$, yielding the familiar tunneling effect.
- $V > E + mc^2$ k' is real again, $T = 1$, if $k'd = n\pi$, we have negative density, $\rho = q\dfrac{E - V}{mc^2} < 0$. Negative particle currents flowing from the right to the left are interpreted as currents of anti-particles going from the left to the right!



$$T = \frac{j_{at}}{j_{be}}$$

$$R = 1 - T = \frac{j_{vissza}}{j_{be}}$$

Klein-Gordon equation in homogenous magnetic field

Klein-Gordon equation:

$$\frac{1}{c^2}\left(i\hbar\partial_t\right)^2\psi = \left((\mathbf{p} - q\mathbf{A})^2 + m^2c^2\right)\psi$$

Let us look for the solution in form of $\psi = e^{-i\omega t}\varphi(\mathbf{r})$ and substitute it into the KG equation:

$$\frac{\hbar^2\omega^2}{c^2}\varphi = \frac{E^2}{c^2}\varphi = \left((\mathbf{p} - q\mathbf{A})^2 + m^2c^2\right)\varphi$$

Reordering the equation and multiplying by $1/2m$:

$$\frac{1}{2m}\left(\frac{E^2}{c^2} - m^2c^2\right)\varphi = \frac{1}{2m}\left(\mathbf{p} - q\mathbf{A}\right)^2\varphi$$

The right hand side is the familiar, classical Hamiltonian of the Schrödinger equation with vector potential $\mathbf{A}$

$$\frac{1}{2m}\left(\mathbf{p} - q\mathbf{A}\right)^2\varphi_{nm} = \tilde{E}_n\varphi_{nm}$$

where $\tilde{E}_n = \hbar\omega_L(n + \frac{1}{2})$ and $\varphi_{nm} = \frac{a_1^{+n}a_2^{+m}}{\sqrt{n!m!}}|0,0\rangle$ eigenstates of the harmonic oscillator , $\omega_L = \frac{qB}{m}$.

Symmetric gauge: $\mathbf{A} = (-By/2, Bx/2, 0)$, $\omega_L = \frac{qB}{m}$

$$H = \frac{1}{2m}\left(\mathbf{p} - q\mathbf{A}\right)^2 = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2}m\left(\frac{\omega_L}{2}\right)^2(x^2 + y^2) - \frac{\omega_L}{2}L_z$$

introducing in the usual way the ladder operators $a_x = \frac{1}{\sqrt{2}}\left(\frac{x}{x_0} + i\frac{p_x}{p_0}\right)$ and $a_y = \frac{1}{\sqrt{2}}\left(\frac{y}{x_0} + i\frac{p_y}{p_0}\right)$:

$$H = \hbar\frac{\omega_L}{2}\left(a_x^+a_x + a_y^+a_y + 1\right) - \frac{\hbar\omega_L}{2i}(a_x^+a_y - a_y^+a_x)$$

$$H = \begin{array}{c}(a_x^+, a_y^+)\end{array} \hbar\frac{\omega_L}{2}\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix}\begin{pmatrix} a_x \\ a_y \end{pmatrix} + \hbar\frac{\omega_L}{2} = \hbar\frac{\omega_L}{2}A^+(\mathbb{I} - \sigma_y)A + \hbar\frac{\omega_L}{2}$$

where we introduced the notation $A = \begin{pmatrix} a_x \\ a_y \end{pmatrix}$, $A^+ = (a_x^+, a_y^+)$.

$$H = \hbar\frac{\omega_L}{2}A^+(\mathbb{I} - \sigma_y)A + \hbar\frac{\omega_L}{2}$$

Diagonalizing the matrix $\mathbb{I} - \sigma_y$ we can separate the ladder operators in the Hamiltonian. The eigenvalues are: 2 and 0. While only the 2 eigenvalue gives contribution to the Hamiltonian the ladder operators corresponding to the 0 eigenvalue only change the degeneratev eigenstates. The energy can be read out from the original operator, given that the relevant eigenvalue is 2:

$$E_n = \hbar\omega_L\left(n + \frac{1}{2}\right) \;, a_1 = \frac{1}{\sqrt{2}}(a_x + ia_y) \;, a_2 = \frac{1}{\sqrt{2}}(a_x - ia_y)$$

$$\varphi_{nm} = \frac{1}{\sqrt{n!m!}}{a_1^+}^n {a_2^+}^m |0, 0\rangle$$

Back to the Klein-Gordon equation:

$$\frac{1}{2m}\left(\frac{E^2}{c^2} - m^2c^2\right) = \hbar\omega_L\left(n + \frac{1}{2}\right)$$

$$E = \pm\sqrt{2mc^2\hbar\omega_L\left(n + \frac{1}{2}\right) + m^2c^4} = \pm mc^2\sqrt{1 + \frac{2\hbar\omega_L}{mc^2}\left(n + \frac{1}{2}\right)}$$

In the low energy limit we get back the classical energies:

$$E - mc^2 \approx \hbar\omega_L\left(n + \frac{1}{2}\right)$$