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WKB quantisation

$$\oint \mathrm{d}x\, p(x) = 2\pi\hbar\left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, \ldots$$

This is the quantisation condition that determines the energy levels. The energy hides in $p(x) = \sqrt{2m\,(E - V(x))}$. The curve is a closed trajectory in phase space. The energy also comes in when we choose initial conditions in phase space.

For the Harmonic oscillator

$$H = \frac{p^2}{2m} + \frac{k\,x^2}{2} = E$$

$$p(x) = \pm\sqrt{2m\left(E - \frac{k\,x^2}{2}\right)}$$

Call the turning points x_0 and $-x_0$.

$$\frac{k\,x_0^2}{2} = E, \quad x_0^2 = \frac{2\,E}{k}$$

$$\oint p(x)\,\mathrm{d}x = 2\int_{-\sqrt{\frac{2E}{k}}}^{\sqrt{\frac{2E}{k}}} \mathrm{d}x\,\sqrt{2\,m\,E - \frac{k\,x^2}{2}} = 2\sqrt{m\,k}\int_{-x_0}^{x_0}\mathrm{d}x\,\sqrt{x_0^2 - x^2} = 2\sqrt{m\,k}\cdot\frac{\pi}{2}\,x_0^2 =$$

$$= 2\sqrt{m\,k}\cdot\frac{\pi}{2}\cdot\frac{2\,E}{k} = 2\pi\,\hbar\left(n + \frac{1}{2}\right)$$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

We have to add $\pi/2$ when crossing a turning point. In general: $\pi\nu$, where ν is the Maslov index.

$$n = \frac{1}{2\pi\hbar}\oint \mathrm{d}x\,p = \int\frac{\mathrm{d}x\,\mathrm{d}p}{2\pi\hbar}\,\theta(E - H(x,p)) \quad \text{where}\,\theta(z) = \begin{cases} 1 & \text{if } z > 0, \\ 0 & \text{if } z < 0. \end{cases}$$

The area in phase space is $2\pi\hbar\,n$.

This has all been in one dimension, so far. How to do this in several dimensions?

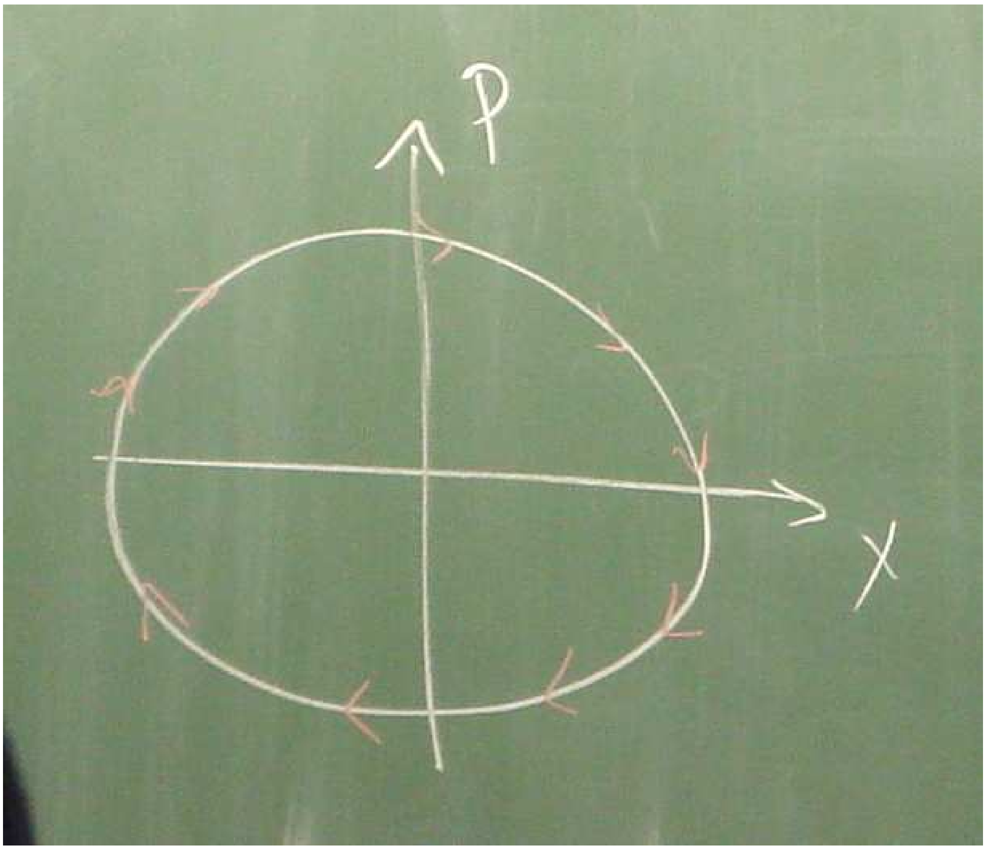

Figure 1. One degree of freedom. The phase-space is two-dimensional.

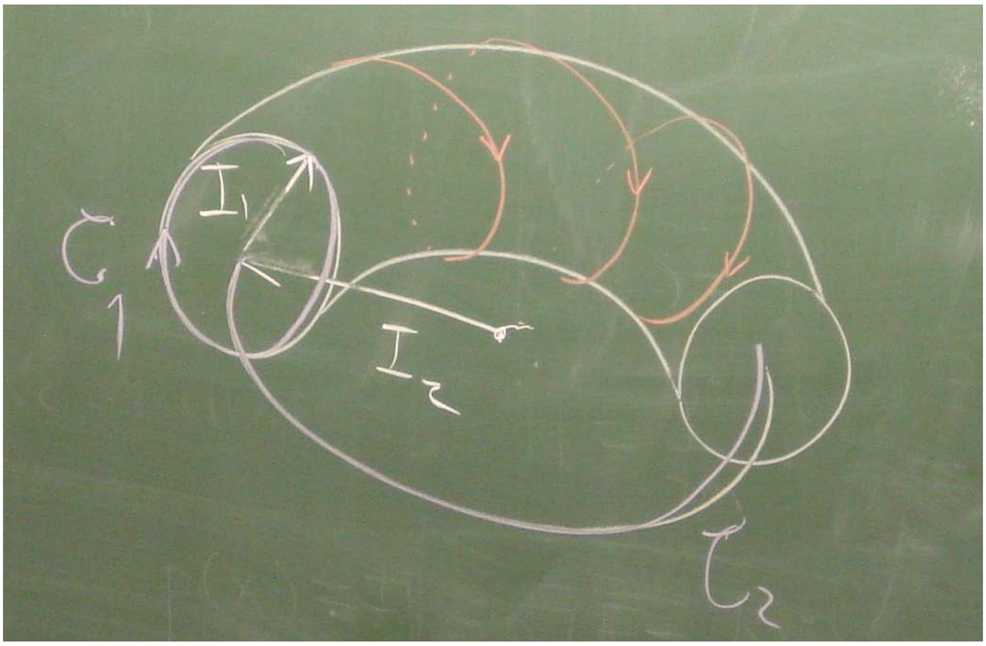

Figure 2. Two degrees of freedom. The phase space is four-dimensional. The trajectory (red) lies on a torus.

$$I_j = \oint_{C_j} \mathrm{d}\boldsymbol{x} \cdot \boldsymbol{p}$$

$H(\theta, I)$. H does not depend on θ. Hamilton's equations.

$$\dot{I} = -\frac{\partial H}{\partial \theta} = 0, \quad \dot{\theta} = \frac{\partial H}{\partial I} = \text{constant}$$

$$\theta = \theta_0 + \frac{\partial H}{\partial I}\, t$$

$$\boldsymbol{x}, \boldsymbol{p} \rightarrow \theta, I \rightarrow \text{solve} \rightarrow \boldsymbol{x}, \boldsymbol{p}$$

Canonical transformation to action, angle coordinates. Problem: this will only work if such tori exists.

$$I_j = \oint_{C_j} \mathrm{d}\boldsymbol{x} \cdot \boldsymbol{p} = 2\,\pi\,\hbar\,(n_j + \nu_j), \quad j = 1, \ldots, \text{number of degrees of freedom}$$

Scattering

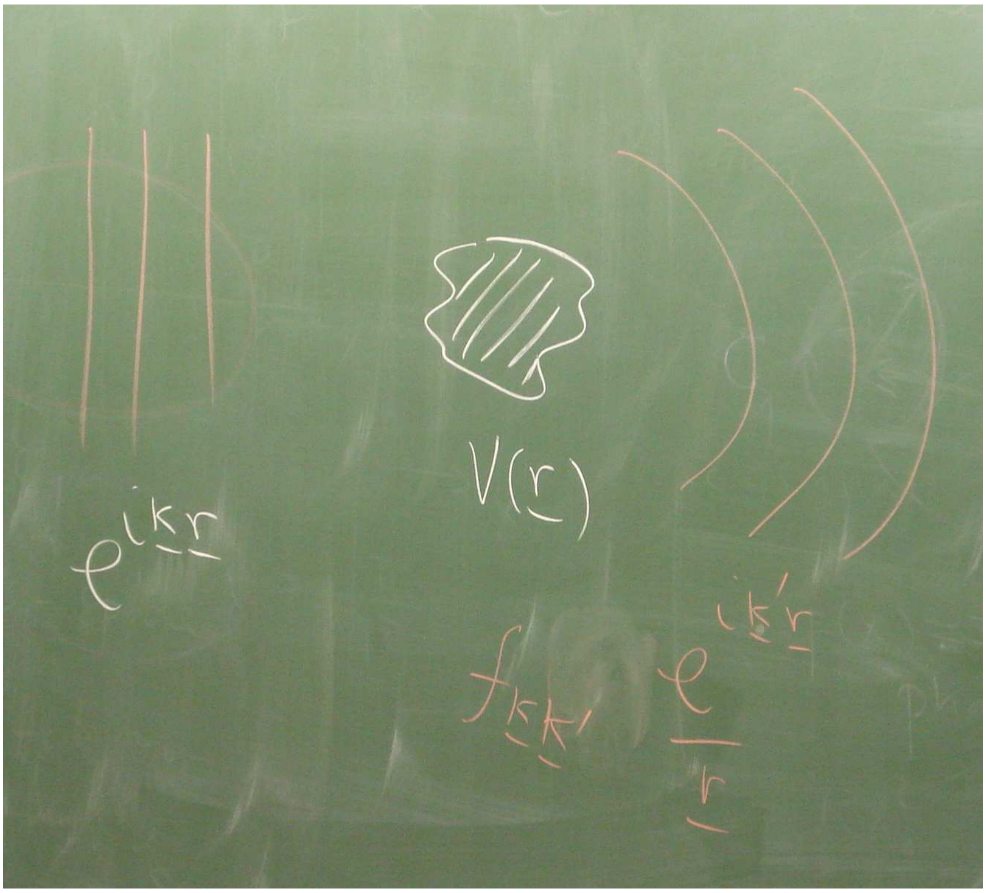

Figure 3. Scattering of a plane wave by a potential $V(r)$ into spherical waves $f_{\boldsymbol{k}}(\theta, \varphi)\, \mathrm{e}^{\mathrm{i}\boldsymbol{k}' \cdot \boldsymbol{r}}/r$.

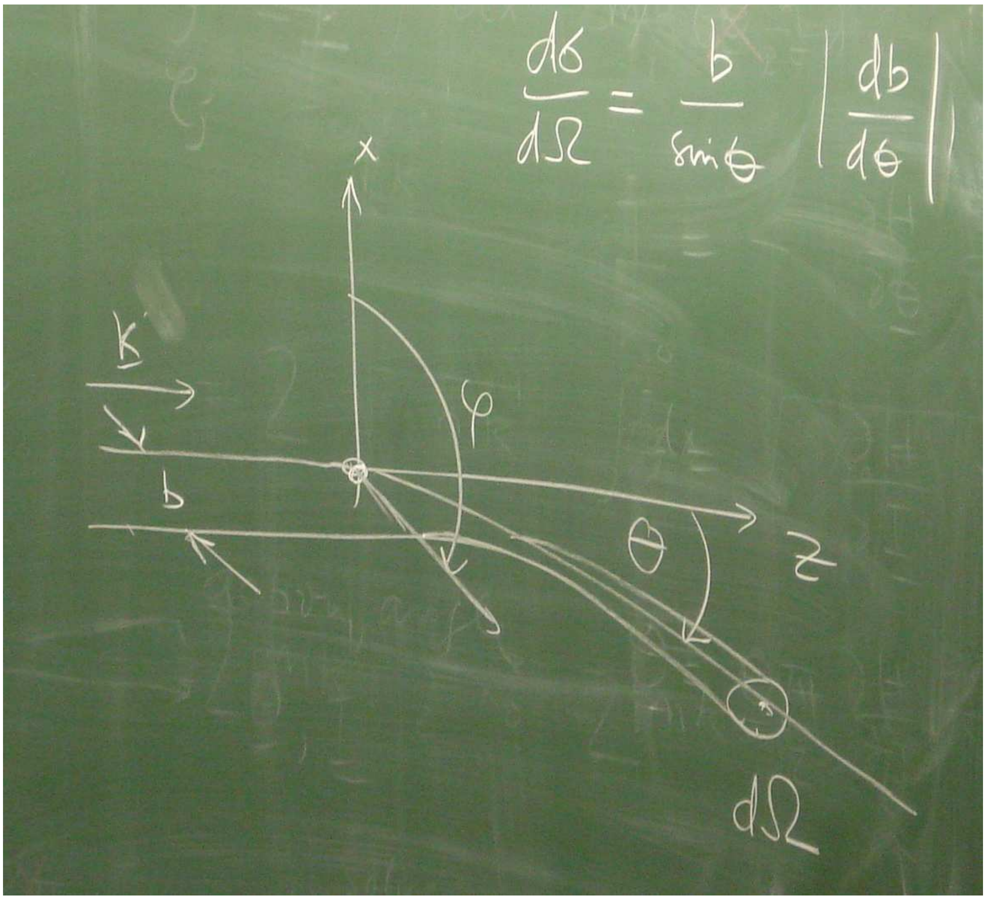

Figure 4. b is the impact parameter.

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{I_{\mathrm{scat}}(\theta, \varphi)}{I_{\mathrm{inc}}}, \quad \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{b}{\sin\theta}\left|\frac{\mathrm{d}b}{\mathrm{d}\theta}\right|$$

Rutherford

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{1}{4}\frac{\left(Z Z' e^2\right)^2}{(2E)^2}\frac{1}{|\sin\frac{\theta}{2}|^4}$$

$$\sigma_{\mathrm{tot}} = \int \mathrm{d}\Omega\, \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}$$

Rutherford: $\sigma_{\mathrm{tot}} = \infty$.

Hard sphere with radius a: $\sigma_{\mathrm{tot}} = \pi a^2$.

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |f_k(\theta, \varphi)|^2$$

$$f_k(\theta, \varphi) = \frac{1}{k}\sum_{l=0} (2l+1)\, \mathrm{e}^{\mathrm{i}\delta_l} \sin\delta_l\, P_l(\cos\theta)$$

This is a formula for radial symmetry. All the information about the scattering is in the scattering phase shifts δ_l.

$$\left[\frac{\partial^2}{\partial r^2} + k^2 - V(r) - \frac{l\,(l+1)}{r^2}\right] u_l(r) = 0$$

$$u_l(r) \sim \sin\!\left(k\,r + \frac{l\pi}{2} + \delta_l\right) \text{ as } r \to \infty, \text{forward direction}$$

For $k\,a \ll 1$, the hard sphere has $\sigma_{\text{tot}} = 4\pi a^2$. For $k\,a \gg 1$ (large energies), you expect to get classical. But we get $\sigma_{\text{tot}} = 2\pi a^2$.

Fraunhofer: Optical scattering from a completely black sphere: $\sigma_{\text{tot}} = \pi\,a^2$. Due to diffraction.

Eikonal approximation

$$\psi_{\boldsymbol{k}}^+ = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} + f_k(\theta, \varphi)\,\frac{\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}}{r}$$

Approximate with $\psi_{\boldsymbol{k}}^+ = \exp\!\left(\frac{\mathrm{i}}{\hbar}S\right)$, where S is the eikonal. We get the Hamilton-Jacobi equation

$$\frac{(\nabla S)^2}{2\,m} + V = E$$

$$S = \int_{\substack{\text{classical}\\ \text{path}}}^{\boldsymbol{r}} \mathrm{d}\boldsymbol{r}' \cdot \boldsymbol{p}$$

Next: approximate the path as a straight line.

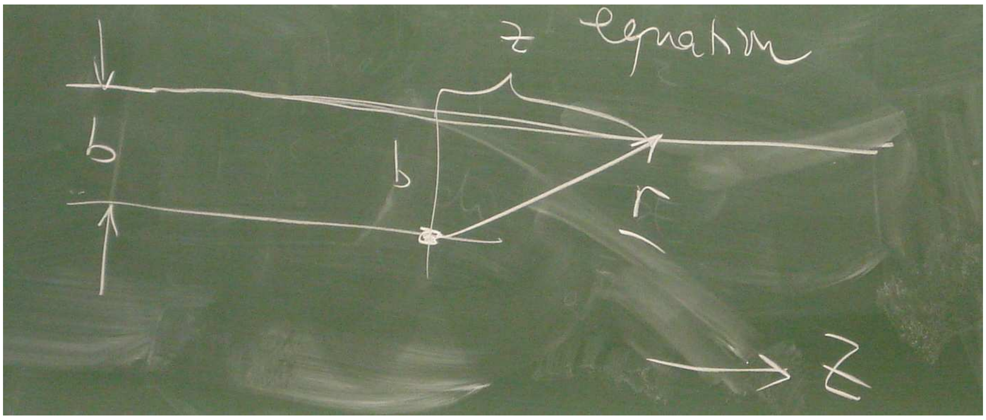

Figure 5.

$$\frac{S}{\hbar} = \int_{-\infty}^{z} \mathrm{d}z' \sqrt{k^2 - \frac{2m}{\hbar} V\!\left(\sqrt{b^2 + z'^2}\right)} + \text{const}$$

The integration constant is chosen so that $S/\hbar \to k\,z$ as $V \to 0$. If we have no potential, we want the plane wave to just go through.

The next approximation is $|V_0| \ll E$. Expand:

$$\frac{S}{\hbar} = k\,z - \frac{m}{\hbar^2 k} \int_{-\infty}^{z} \mathrm{d}z'\, V\left(\sqrt{b^2 + z'^2}\right)$$

$$f_k(\theta, \varphi) = -\frac{(2\pi)^3}{4\pi} \cdot \frac{2\,m}{\hbar^2} \langle \theta, \varphi | V | \psi_{\boldsymbol{k}}^{+} \rangle = -\,\mathrm{i}\,k \int_0^{\infty} \mathrm{d}b\, b\, J_0(k\,b\,\theta) \left[\mathrm{e}^{2\mathrm{i}\chi} - 1\right]$$

$$\chi = -\frac{m}{2\,\hbar^2\,k} \int_{-\infty}^{\infty} \mathrm{d}z\, V\left(\sqrt{b^2 + z^2}\right)$$

$$\frac{|V_0|}{E} \ll 1, \quad k\,a \gg 1, \quad l\,\hbar = b \cdot p = b\,\hbar\,k, \quad l \approx b\,k$$

$$\sum_l \sim k \int \mathrm{d}b$$

$$P_l(\cos\theta) \sim J_0(l\,\theta) = J_0(\theta\,k\,b)$$

$$\delta_l \sim \chi|_{b = l/k}$$

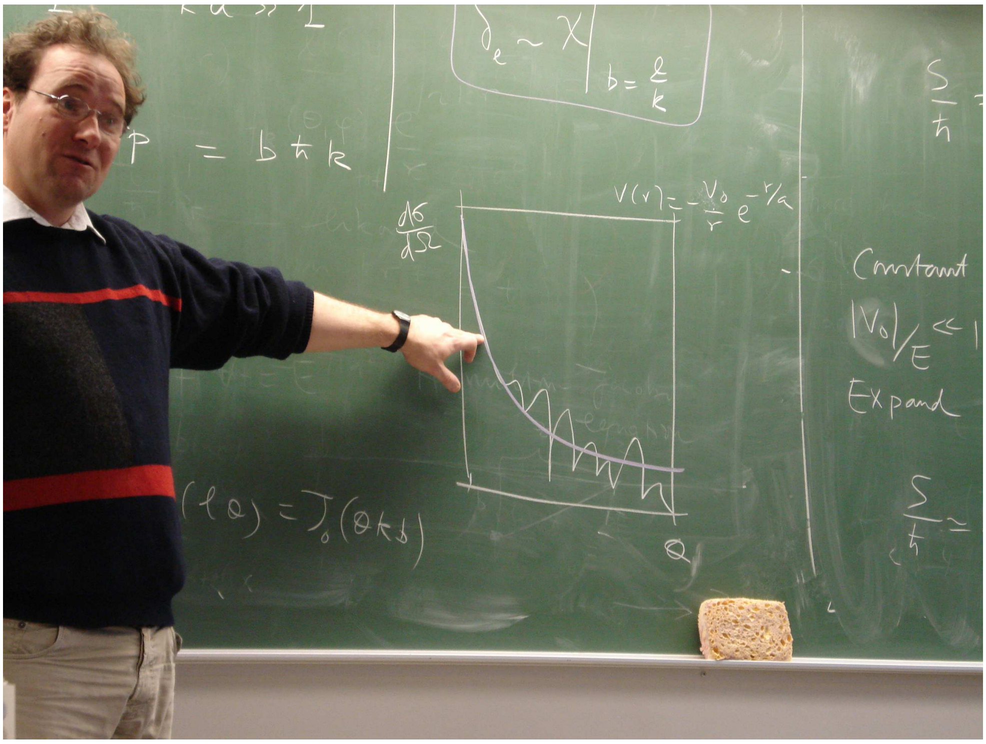

Figure 6. Yukawa: $V(r) = -\frac{V_0}{r}\,\mathrm{e}^{-r/a}$. $V_0 = 250$, $a = 1$, $k = 5$, $m = \frac{1}{2}$, $\hbar = 1$. The approximation is very accurate for small θ.

$$V(r) = \begin{cases} -V_0 & \text{if } r < a \\ 0 & \text{if } r > a \end{cases}$$

$$V_0 = V_0' + \mathrm{i}\,V_0''$$

$$\chi = \begin{cases} 0 & \text{if } b > a \\ \frac{V_0}{4k}\sqrt{a^2 - b^2} & \text{if } b < a \end{cases}$$

$$|\mathrm{e}^{2\mathrm{i}\chi}|^2 = \mathrm{e}^{-4\,\mathrm{Im}\,\chi} = \mathrm{e}^{-\frac{V_0''}{4k}\sqrt{a^2 - b^2}} = \mathrm{e}^{-L/\Lambda}, \quad \Lambda = \frac{k}{V_0''}$$

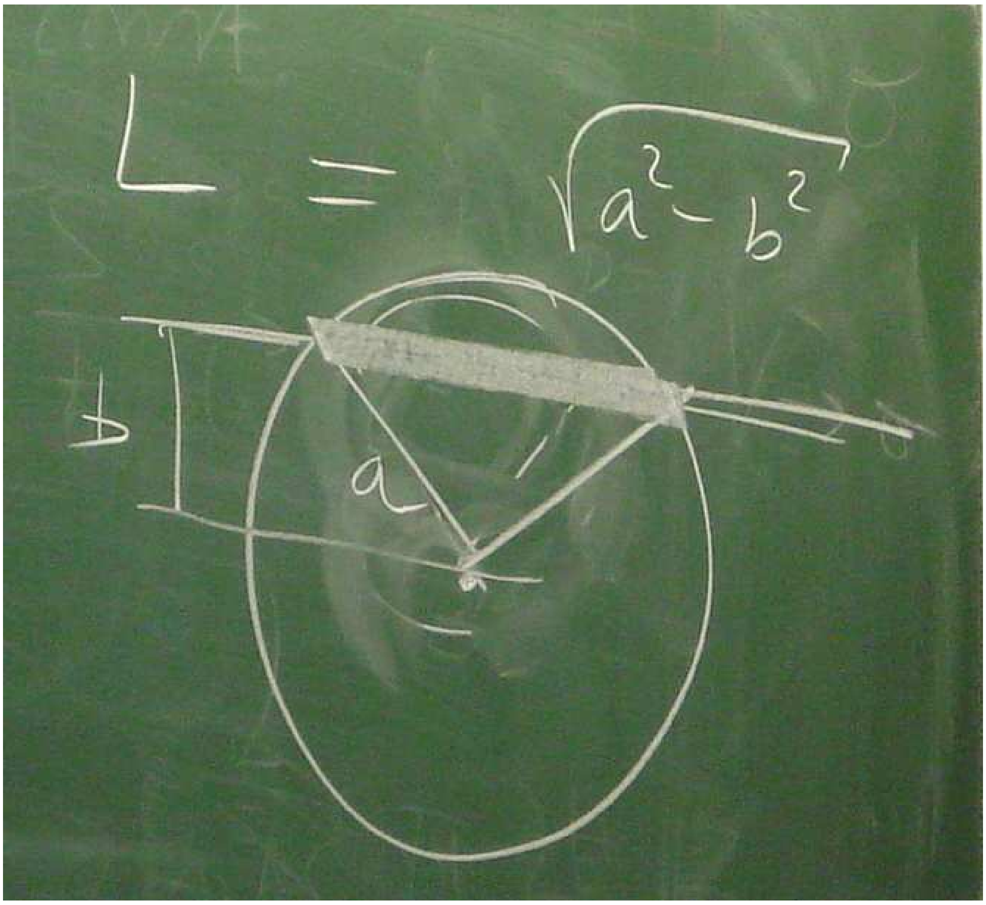

Figure 7.

We get rid of the $\mathrm{e}^{2\mathrm{i}\chi} - 1$ factor if $L \gg \Lambda$.

$$f \sim \mathrm{i}\, k \int_0 \mathrm{d}b\, b\, J_0(k\, b\, \theta) = \mathrm{i}\, a\, \frac{J_1(k\, a\, \theta)}{\theta}$$

The Fraunhofer result has $2\sin\frac{\theta}{2}$ instead of θ. But for small angles, we can say that this is the famous Fraunhofer diffraction from a black sphere.

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |f|^2$$

$$\sigma_{\mathrm{tot}} = \pi\, a^2$$