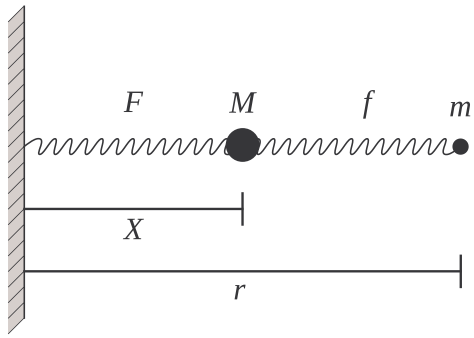
Problem 1: Dynamics of two coupled masses (4 points)

Consider the Hamilton function of two particles in one dimension:



$$H = \frac{P^2}{2\,M} + \frac{p^2}{2\,m} + \frac{1}{2}\,F\,X^2 + \frac{1}{2}\,f\,(X - r)^2\;.$$

a) Calculate the frequencies of the normal modes of the classical system.

b) Specify the Hamilton operator and calculate the eigenvalues of the corresponding quantum mechanical systems.

c) Suppose that the mass m is much smaller than M. Calculate the eigenvalues of $\hat{H}$ along the lines of the "Born-Oppenheimer approximation": in a first step neglect the motion of the heavy mass M and calculate the eigenvalues of the corresponding Hamiltonian. Thereafter solve the problem of the motion of the heavy mass M in the "effective potential", calculated in the previous step.

d) Compare your results from b) and c). It is advantageous to use the abbreviations

$$\omega = \sqrt{\frac{f}{m}}\,, \qquad \Omega = \sqrt{\frac{F}{M}} \qquad \text{and} \qquad \kappa = \sqrt[4]{\frac{m}{M}}\;.$$

Problem 2: Fourier transformation of Coulomb potential (2 points)

a) Calculate the Fourier transform

$$\tilde{v}\,(\vec{q}\,) = \frac{1}{\Omega}\int\limits_{\Omega} v\,(\vec{r}\,)\,\mathrm{e}^{-i\,\vec{q}\cdot\vec{r}}\,d^3\,r \qquad \text{of the Yukawa potential} \qquad v\,(\vec{r}\,) = \frac{\mathrm{e}^2}{4\,\pi\,\varepsilon_0}\,\frac{1}{r}\,\mathrm{e}^{-\gamma\,r}$$

in a Born-von Kármán cell with volume Ω. γ is a real constant. Replace the integral $\int\limits_{\Omega} d^3\,r$ by an integration over a sphere with radius $R \to \infty$.

b) The Coulomb potential is the $\gamma \to 0$ limit of the Yukawa potential. Determine the Fourier transform of the Coulomb potential.

Problem 3: Ewald-Method (4 points)

The calculation of the electrostatic interaction energy U_{NN} between the nuclei in a solid requires the evaluation of a sum over all lattice vectors $\vec{R}_j$. A direct summation is numerically very demanding due to the long-range Coulomb potential. In the method of Ewald, the Coulomb potential is represented by error functions $\mathrm{erf}\,(x)$ and $\mathrm{erfc}\,(x)$. One part of the sum is evaluated in Fourier space while the other part is carried out in real space.

a) Show that the sum $S = \sum_j{}' \frac{1}{|\vec{a} - \vec{R}_j|}$ can be written as $S = S_1 + S_2$ with

$$S_1 = \sum_j{}' \frac{2}{\sqrt{\pi}} \int_0^\eta \mathrm{e}^{-|\vec{a} - \vec{R}_j|^2 x^2} \, d\,x \,, \qquad S_2 = \sum_j{}' \frac{2}{\sqrt{\pi}} \int_\eta^\infty \mathrm{e}^{-|\vec{a} - \vec{R}_j|^2 x^2} \, d\,x \,.$$

Thereby is $\vec{a}$ the difference of two basis vectors $\vec{\tau}_\nu - \vec{\tau}_{\nu'}$, $\vec{R}_j$ is a lattice vector and η is a real number between 0 and ∞ which is chosen in an appropriate way for the numerical evaluation. The prime at the sum indicates that the term $\vec{R}_j = \vec{a}$ is excluded from the summation.

b) The case $\vec{R}_j = \vec{a}$ can only occur for $\vec{a} = 0$. Show that S_1 can be written as a sum without restriction in the form

$$S_1 = \sum_j \left(\frac{2}{\sqrt{\pi}} \int_0^\eta \mathrm{e}^{-|\vec{a} - \vec{R}_j|^2 x^2} \, d\,x \right) - \delta_{\vec{a},\vec{0}} \cdot \frac{2\,\eta}{\sqrt{\pi}} \,.$$

c) Represent in S_1 the Gaussian function by its Fourier transform, evaluate the sum over j and integrate with respect to the variable x.

d) Write the sum S_2 in terms of $\mathrm{erfc}\,(x)$.

e) Why is the evaluation of S_1 and S_2 as outlined above more efficient than a direct summation in S?

Remark: The divergent term in S_1 with $|\vec{G}| = 0$ is compensated by analogue terms in the electron-electron and electron-nucleus interaction.

Useful relations:

i) $$\int_0^\infty \mathrm{e}^{-b^2 x^2} \, d\,x = \frac{\sqrt{\pi}}{2\,b}$$

ii) $$\mathrm{erf}\,(y) = \frac{2}{\sqrt{\pi}} \int_0^y \mathrm{e}^{-t^2} \, d\,t$$

iii) $$\mathrm{erfc}\,(y) = 1 - \mathrm{erf}\,(y)$$

iv) $$\sum_j \mathrm{e}^{-|\vec{a} - \vec{R}_j|^2 x^2} = \sum_j \frac{1}{\Omega} \frac{\pi^{\frac{3}{2}}}{x^3} \sum_{\vec{G}} \mathrm{e}^{i\,\vec{G}\cdot(\vec{a} - \vec{R}_j)} \cdot \mathrm{e}^{-\frac{G^2}{4\,x^2}} \,.$$

Ω is the volume of the Born-von Kármán cell. There are N_{cell} lattice vectors. $\Omega_0 = \Omega / N_{\mathrm{cell}}$ is the volume of the unit cell.