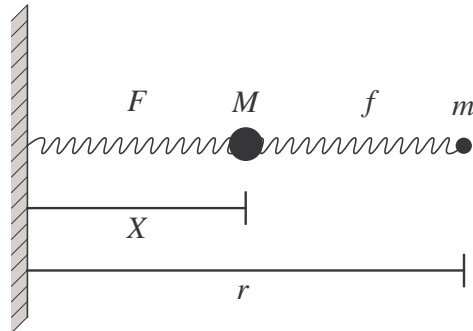


Problem 1: Dynamics of two coupled masses

[4 points]

Consider the Hamilton function of two particles in one dimension:



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

- 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

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

Problem 2: Fourier transformation of Coulomb potential

[2 points]

- a) Calculate the Fourier transform

$$\tilde{v}(\vec{q}) = \frac{1}{\Omega} \int_{\Omega} v(\vec{r}) e^{-i\vec{q}\cdot\vec{r}} d^3 r \quad \text{of the Yukawa potential} \quad v(\vec{r}) = \frac{e^2}{4\pi\epsilon_0} \frac{1}{r} e^{-\gamma r}$$

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

- b) The Coulomb potential is the $\gamma \rightarrow 0$ 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 $\text{erf}(x)$ and $\text{erfc}(x)$. 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

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

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

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

- 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 $\text{erfc}(x)$.
- 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) $\int_0^\infty e^{-b^2 x^2} dx = \frac{\sqrt{\pi}}{2b}$
- ii) $\text{erf}(y) = \frac{2}{\sqrt{\pi}} \int_0^y e^{-t^2} dt$
- iii) $\text{erfc}(y) = 1 - \text{erf}(y)$
- iv) $\sum_j e^{-|\vec{a} - \vec{R}_j|^2 x^2} = \sum_j \frac{1}{\Omega} \frac{\pi^{\frac{3}{2}}}{x^3} \sum_{\vec{G}} e^{i\vec{G} \cdot (\vec{a} - \vec{R}_j)} \cdot e^{-\frac{G^2}{4x^2}}.$

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