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Computational Physics I
WS 2017/18

Deadline: Dec 11, 2017

7.1. Eigenmodes of many-body systems
Extend the programs for the computation of force equilibria so that also the eigenfrequencies and eigenmodes are determined and displayed.

7.2. Finite difference representation for a 1-d Schrödinger equation
Approximating the second derivative with centered finite difference, develop a matrix representation of the 1-d Schrödinger equation. Calculate the eigenvalues for the potential $V(x) = V_0/\cosh(x/a)$ for $\mathcal{V}_0 = 2ma^2\, V_0/\hbar^2 = 5\,.$

7.3 Finite difference representation for the radial Schrödinger equation
Approximating the second derivative with centered finite difference, develop a matrix representation for the radial Schrödinger equation for a 3-d central potential and calculate the eigenvalues for the Lennard-Jones potential $V(r) = V_0((a/r)^{12} - 2(a/r)^6)$ for different angular momenta. Compare the results for the parameters of Argon ($V_0 = 1.65 \cdot 10^{-21}$J and $a = 3.8 \cdot 10^{-10}$m) with those for Helium ($V_0 = 0.13 \cdot 10^{-21}$J and $a = 3.8 \cdot 10^{-10}$ m).