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Computational Physics I

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5.1. Spectra of nucleons

The lowest lying states in a nucleus can be approximated by the eigenstates of a particle inside a sphere. The radial eigenfunctions to angular momentum quantum number l are spherical Bessel functions,

$$j_l(\rho) = (-\rho)^l \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l \frac{\sin\rho}{\rho}\,, \tag{1}$$

and the eigenvalues for a sphere of radius R are determined by $j_l(k_{nl}R) = 0$ and $E_{nl} = (\hbar^2/2m)k_{nl}^2$. The indices nl label the angular momentum quantum numbers l and the order n of the zero within the sequence.

Determine the lowest wavenumbers $k_{nl}R$ and label them spectroscopically (i.e. with n running from 1 upwards and $l = 0, 1, 2, \ldots$ replaced by S, P, D, F, G,…).

How far in n and l do you have to go to get the first 10 states?

Hint: You can find Bessel functions in the module `scipy.special`.

5.2. Van der Pauw's method for the determination of resistivities

A convenient measurement technique to determine the resistivity of a 2d material uses a setup first described and analyzed by van der Pauw (see the wikipedia entry, for example). With 1 to 4 the clockwise labels of four contacts around the sample, and U_{ij} and I_{ij} the voltage differences and currents between points i and j, one can determine the pairwise resistances $R_a = U_(13)/I_{13}$ and $R_b = U_(24)/I_{24}$. van der Pauw then showed that the resistance of the sample R_s can be determined from

$$e^{-\pi R_a/R_s} + e^{-\pi R_b/R_s} = 1\,. \tag{2}$$

Show that in the dimensionless version with $x = \pi R_a/R_s$ and $\rho = R_b/R_a$, the relation between x and ρ is given by the solution to

$$e^{-x} + e^{-\rho x} = 1 \tag{3}$$

Show numerically and analytically that the solutions for $x(\rho)$ and and $x(1/\rho)$ are related by $x(\rho) = x(1/\rho)/\rho$

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5.3 Particles on a line

Program a gradient and a Newton method for the determination of equilibrium points for N particles on a line, repelling each other with a potential $V(r) = 1/r$, and held together by an external harmonic potential. That is, with x_i the positions of the particles, the potential becomes

$$V(x_1, \dots, x_N) = \frac{1}{2}\sum_i x_i^2 + \frac{1}{2}\sum_{i \neq j} V(|x_i - x_j|) \tag{4}$$

Determine the equilibria and the normal modes for $N = 1$, 2, 3, and 4.

What happens if the stepsize in the gradient method becomes too large?
Instead of computing the derivatives analytically, you may also compute them numerically: do you notice any differences?

5.4. Symmetric many particle equilibria

Consider a system of N charged particles in the plane, trapped by a harmonic potential $V_h = \mathbf{x^2}/2$ and repelling each other by Coulomb forces, $V_{12}(\mathbf{x}_1, \mathbf{x}_2) = 1/|\mathbf{x}_1 - \mathbf{x}_2|$.

For a few particles, on can guess simple configurations, like N particles on a line or at the vertices of a regular polygon, with or without a particle in the middle. One benefit of such configurations is that they depend on a single parameter only so that the corresponding configurations can be found by a one-dimensional search.

Reduce to one-dimensional searches and determine the equilibrium positions for the cases of (a) two particles on a line, (b) three particles on a line with one in the middle, (c) N particles on the vertices of a regular polygon and (d) $N + 1$ particles where one is in the middle and N particles are arranged as in (c).