Theoretical Concepts and Simulations for Materials Scientists
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Exercises 3

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1. Hellmann-Feynman theorem
   Consider a Hamiltonian, which depends on a parameter λ. Of course, all eigenfunctions and eigenvalues will then also depend on this parameter and the eigenvalues are given by

$$\varepsilon_n(\lambda) = \frac{\langle\psi_n(\lambda)|H(\lambda)|\psi_n(\lambda)\rangle}{\langle\psi_n(\lambda)|\psi_n(\lambda)\rangle} \quad .$$

   Here n labels different eigenstates. According to the theorem by Hellmann and Feynman any eigenstate then fulfils the relation

$$\frac{\partial\varepsilon_n(\lambda)}{\partial\lambda} = \frac{\langle\psi_n(\lambda)|\frac{\partial H(\lambda)}{\partial\lambda}|\psi_n(\lambda)\rangle}{\langle\psi_n(\lambda)|\psi_n(\lambda)\rangle} \quad .$$

   Prove the Hellmann-Feynman theorem.

2. Ritz variational method
   According to the variational principle the solutions of Schrödingers equation are characterized by a vanishing variation of the expextation value of the Hamiltonian

$$\langle H\rangle_\psi = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$$

   with respect to variations of the wave function, i.e.

$$\delta\langle H\rangle_\psi \overset{!}{=} 0 \quad .$$

   Consider the situation, where the wave function $|\psi\rangle$ can be represented as a linear combination of a set of fixed trial functions,

$$|\psi\rangle = \sum_{i=1}^{m} \alpha_i|\chi_i\rangle \quad ,$$

   and express the variational principle in terms of the Hamiltonian matrix $\langle\chi_k|H|\chi_i\rangle$ and the overlap matrix $\langle\chi_k|\chi_i\rangle$.

3. Calculate the maximum of the function

$$f(x, y) = 2x + y$$

for all pairs (x, y) falling on the ellipse with semiaxes a and b, respectively, i.e. for all pairs (x, y) fulfilling the condition

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1$$

using the method of Lagrange multipliers.

4. Yukawa potential
Calculate the Fourier transform $v_\alpha(\mathbf{q})$ of the screened Coulomb potential

$$v_\alpha(\mathbf{r}) = \frac{e^{-\alpha|\mathbf{r}|}}{|\mathbf{r}|} \quad .$$