Universität of Göttingen
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Methods of Computational Physics
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Sheet 3: Matrix techniques

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- **Numerical libraries for matrix diagonalization**

  Let $\mathbb{A} \in \mathbb{R}^{n\times n}$ denote a real, symmetric matrix. Initialize $\mathbb{A}$ by random values uniformly distributed in the interval $[-1:1]$ Use your favorite numerical library, e.g., LAPACK or numerical recipes, to do the following:

  a) Reduce the real, symmetric matrix $\mathbb{A}$ to the form $A = \mathbb{Q}\mathbb{T}\mathbb{Q}^\dagger$, where $\mathbb{Q}$ is an orthonormal matrix and $\mathbb{T}$ is a symmetric tridiagonal matrix. Verify your program code by explicitly checking $A = \mathbb{Q}\mathbb{T}\mathbb{Q}^\dagger$ for each matrix element. Do $\mathbb{A}$ and $\mathbb{T}$ share the same eigenvalues?

  b) Use the result of the previous task to compute all eigenvalues of $\mathbb{T}$.

  c) Calculate all eigenvalues and all eigenvectors of the real, symmetric matrix $\mathbb{A}$. Let $\mathbb{U}$ denote the orthogonal matrix formed by the normalized eigenvectors of A and Λ the diagonal matrix with the eigenvalues on the diagonal. Verify your program by explicitly checking $A = \mathbb{U}\Lambda\mathbb{U}^\dagger$ for each matrix element.

  For each task compute the CPU time as a function of the size n of the matrix $\mathbb{A}$.

- **Lanczos method**

  a) Use the Lanczos algorithm to find the smallest eigenvalue of a real, symmetric matrix $\mathbb{A}$. Initialize $\mathbb{A}$ by random values uniformly distributed in the interval $[-1:1]$. Describe the Lanczos algorithm and verify your program code by comparing the lowest eigenvalue with the result of the previous task.

  b) How does the estimate for the smallest eigenvalue change with iteration? How good are the estimates for the larger eigenvalues?

  c) How does the CPU time scale with the size n of the matrix $\mathbb{A}$.

  d) What is the largest size n that you can study?

- **[Bonus] Spinodal instability of a crystal**

  Consider a one-dimensional system with a density distribution $\rho(x) = \bar{\rho} + m(x)$ where $\bar{\rho}$ denotes the average density and $m(x)$ the deviation of the density from its average, i.e., the order parameter. $\int_0^L \mathrm{d}x\, m = 0$. The system is confined to $0 \le x \le L$, and periodic boundary conditions are applied. Associate with each density profile a free energy, $\mathcal{F}$, according to the Swift-Hohenberg functional

$$\mathcal{F}[m] = \int_0^L \mathrm{d}x\, \left\{ -\frac{m^2}{2} + \frac{m^4}{4} + \frac{1}{2} m \left[1 + \triangle\right]^2 m \right\} \tag{1}$$

  The equilibrium density distribution is characterized by the vanishing of the chemical potential

$$\mu(x|m) \equiv \frac{\delta\mathcal{F}}{\delta m(x)} = -m + m^3 + \left[1 + \triangle\right]^2 m \tag{2}$$

at each point, x, in space. $\mu(x|m)$ is a function of x that depends on the entire density profile $m(x)$. We discretize the spatial dependence

$$\begin{aligned} x_i &= i\delta_x \qquad \text{with} \quad i = 0, \cdots, N-1 \quad \text{and} \quad \delta_x = \frac{L}{N} && (3)\\ m_i &= m(x_i) && (4)\\ \mu_i &\equiv \mu(x_i|m) = \frac{1}{\delta_x}\frac{\partial \mathcal{F}(m_0, m_1, \cdots, m_{N-1})}{\partial m_i} && (5)\\ &= m_i^3 + \frac{2}{\delta_x^2}\left[m_{i+1} + m_{i-1-2m_i}\right] + \frac{1}{\delta_x^4}\left[m_{i+2} - 4m_{i+1} + 6m_i - 4m_{i-1} + m_{i-2}\right] \end{aligned}$$

and define the Hessian matrix $\mathbb{H}$ with elements

$$\mathbb{H}_{ij} \equiv \frac{\partial \mu_i}{\partial m_j} \tag{6}$$

In the following use the parameters $8.8 < L \leq 4\pi$ and $N = 128$.

a) Obviously, the homogeneous density distribution, $m_0(x) = 0$, for all x fulfills the condition $\mu(x|m_0) = 0$ for all x. This solution corresponds to a uniform liquid. For $L \approx 4\pi$ is another spatially modulated solution that is approximately

$$m_{\text{lam}}(x) \approx m_{\text{try}}(x) = \sqrt{\frac{3}{4}}\sin\left(\frac{4\pi}{L}x\right) \tag{7}$$

This solution corresponds to a crystal with lattice spacing $L/2$. Find the solution $m_{\text{lam}}(x)$ that satisfies the condition $\mu(x|m_{\text{lam}}) = 0$ for all x by a Newton-like method, i.e., starting from m_{try}, iterate

$$m(x) \to m(x) = m(x) - \int_0^L \mathrm{d}y\; H^{-1}(x,y)\mu(y|m) \tag{8}$$

or in discretized form

$$m_i \to m_i = m_i - \sum_j \left(\mathbb{H}^{-1}\right)_{ij}\mu_j \tag{9}$$

until $\frac{1}{L}\int_0^L \mathrm{d}x\; |\mu(x|m_{\text{lam}})| \approx \frac{1}{N}\sum_{i=0}^{N-1}|\mu_i| < \epsilon$ with $\epsilon = 10^{-9}$.

Plot the solution for various L starting at $L = 4\pi$ and decreasing values. At some value, $L_{\text{spin}} < 4\pi$ "suddenly" no spatially modulated solution (of that form) can be found. This marks the limit of metastability of the solution.

b) In order to consider the stability of the solution, we study small fluctuations, $\epsilon\delta m_i$, around the spatially modulated solution, $m_{\text{lam}}(x)$, where ϵ is a small parameter.

$$\begin{aligned} \mathcal{F}(m_0, \cdots) &= \mathcal{F}(m_{\text{lam},0} + \epsilon\delta m_0, \cdots) && (10)\\ &= \mathcal{F}(m_{\text{lam},0}, \cdots) + \epsilon\sum_i \underbrace{\mu_i}_{=0}\delta m_i + \frac{\epsilon^2}{2}\sum_{i,j}\delta m_i \mathbb{H}_{ij}\delta m_j + \cdot && (11) \end{aligned}$$

By diagonalizing the symmetric Hessian, we obtain the collective excitations (analog of phonons) of $m_{\mathrm{lam}}(x)$, i.e., the nth eigenmode is determined by

$$\sum_k \mathbb{H}_{ik}\delta m_k^{(n)} = \lambda^{(n)}\delta m_i^{(n)} \tag{12}$$

$\lambda^{(n)}$ are the real eigenvalues and the eigenvectors, $\delta m_i^{(n)}$, form an orthonormal basis.

$$\frac{1}{N}\sum_i \delta m_i^{(n)}\delta m_i^{(m)} = \delta_{n,m} \tag{13}$$

For these collective excitations the change of free energy is particular simple

$$\mathcal{F}(m_0,\cdots) = \mathcal{F}(m_{\mathrm{lam},0} + \delta m_0^{(n)},\cdots) = \mathcal{F}(m_{\mathrm{lam},0},\cdots) + N\frac{\epsilon^2}{2}\lambda^{(n)} + \cdots \tag{14}$$

Determine the 5 lowest lying eigenvalues, $\lambda^{(n)}$, and corresponding eigenvectors, $\delta m_i^{(m)}$, (with $n = 0, 1, 2, 3, 4$) using the QR-algorithm.

c) Numerically observe that the lowest eigenvalue, $\lambda^{(0)}$, is always 0 – this mode corresponds to a **Goldstone** mode. This Goldstone mode is related to the spontaneous breaking of translational symmetry by the crystal, i.e., if $m_{\mathrm{lam}}(x)$ is a (local) minimum of the free-energy functional $\mathcal{F}[m]$, so is also the spatially shifted density profile, $m_{\mathrm{lam},\epsilon}(x) = m_{\mathrm{lam}}(x+\epsilon)$ for all $\epsilon \in \mathbb{R}$ and $\mathcal{F}[m_{\mathrm{lam}}] = \mathcal{F}[m_{\mathrm{lam},\epsilon}]$.

   Use this symmetry to (i) show that there exists a collective excitation with vanishing eigenvalue (free-energy increase) and (ii) provide an analytical relation between $m_{\mathrm{lam}}(x)$ and $m^{(0)}(x)$. Verify your result by comparison to the numerical result. [1]

d) Upon approaching the spinodal by compressing the system (reducing L), the second (and third) largest eigenvalue(s) decrease and vanish at the spinodal, L_{spin}. Show that $\lambda^{(1)}$ approximately varies linearly with L in the vicinity of the spinodal, $L \gtrsim L_{\mathrm{spin}}$, and use this linear dependence to accurately determine L_{spin}. In the vicinity of the spinodal the corresponding eigenvector, $\delta m_i^{(1)}$, describes a low lying excitation. Illustrate the change of the density profile associated with $\delta m_i^{(1)}$ and provide a physical description.

[1] This result also implies that $\mathbb{H}$ in Equation 8 becomes singular for very fine discretization. It should not be a problem for the parameters chosen but you could avoid the difficulty by imposing $m(-x) = -m(x)$ to explicitly break translational invariance when calculating $m_{\mathrm{lam}}(x)$.