«Introduction to Wolfram Mathematica»

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1 Assignment on «Patterns & Replacements»

Problem 1.1. Create a function with the same functionality as `Coefficient` using replacements.

$$\texttt{myCoefficient}[\mathit{expr\_}, \mathit{form\_}] := \ldots$$

Problem 1.2. Construct a `ComplexityFunction` that prefers $\sin^n(x)$ and $\cos^n(x)$ instead of $\sin(nx)$ and $\cos(nx)$. `Simplify` $\cos(4x)$ using it.

$$\texttt{Simplify}\left[\texttt{Cos}[4z], \texttt{ComplexityFunction} \to f[\#]\&)\right]$$

2 Assignment on «Numerical computations»

Problem 2.1. Solve Korteweg de–Vries equation

$$u_t + u_{xxx} + 6uu_x = 0$$

with two–soliton initial condition

$$u|_{t=0} = \mathrm{ch}^{-2}\left(\frac{x-5}{\sqrt{2}}\right) + \frac{3}{2}\,\mathrm{ch}^{-2}\left(\frac{x+5}{2/\sqrt{3}}\right)$$

and periodic boundary conditions (for u, u_x and u_{xx}). `Animate` the solution. Do solitons interact or pass through each other without a change?

Problem 2.2. Consider the following integral as a function of parameter a.

$$J(a) = \int_0^{10} \frac{dx}{\mathrm{ch}[(x-a)^2]}.$$

From analytical reasons it is obvious that $J(a)$ has maximum at $a = 5$. Try to obtain such result using `NMaximize` with 10–digits precision. Notice that due to very small derivate near the maximum, precision of maximum point $a_{\max}$ is much smaller than precision of maximum value $J(a_{\max})$. Construct a function that finds point of maximum with given n–digits precision.

3 Assignment on «Visualization»

Problem 3.1. Consider some non-trivial function, e.g. a sum of a Bessel and Airy functions $f(x) = J_1(x) + \mathrm{Ai}(-x)$. Find (numerically) its zeros and extrema and plot them combined with the function.

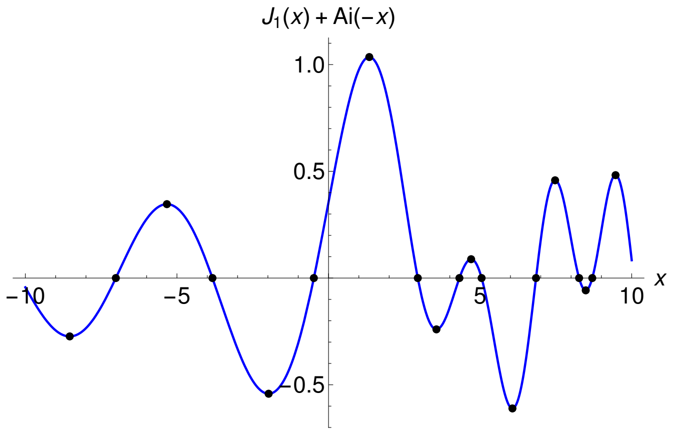

Figure 3.1: Illustration to the problem 3.1

Problem 3.2. Consider some analytic function of complex variable, e.g.

$$f(z) = \frac{z^4}{4} + \frac{z^2}{2} + e^{i\pi/3} z, \quad z \in \mathbb{C}.$$

Its real part $\mathrm{Re}\, f(z)$ as a function of $z = x + iy$ has saddle points at $f'(z_0) = 0$ and the lines of steepest descent and ascent from this points may be found from condition $\mathrm{Im}\, f(z) = \mathrm{Im}\, f(z_0)$. Find all such points and corresponding curves and plot them combined as pictured below.

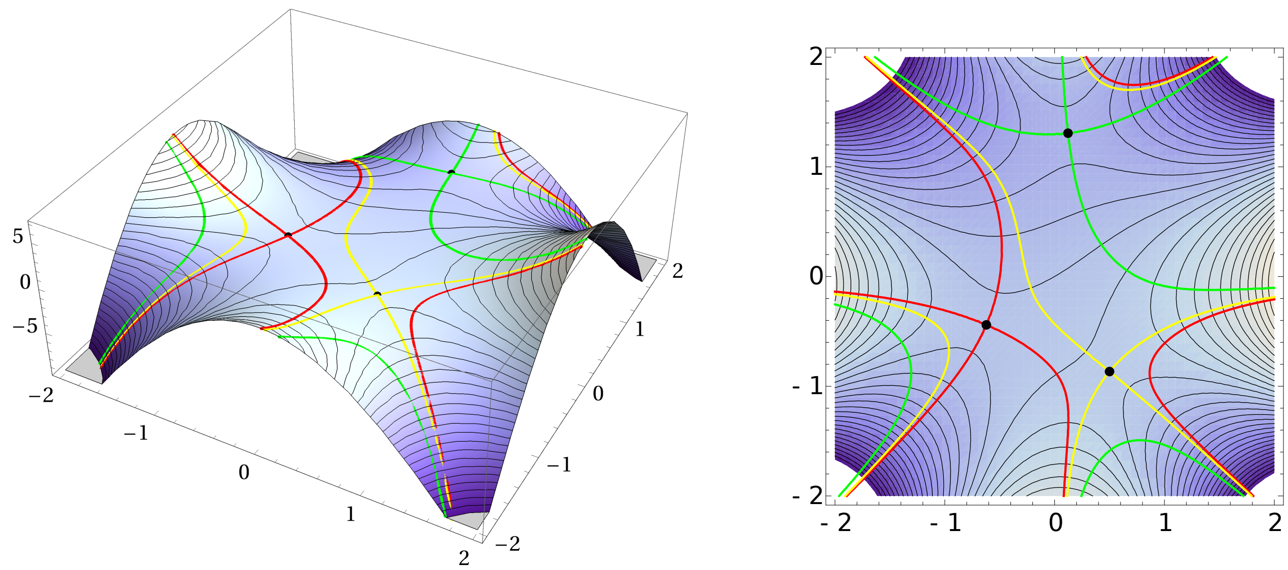

Figure 3.2: Illustration to the problem 3.2

4 Assignment on «Eigenproblems»

Problem 4.1. Consider a Pöschl–Teller potential.

$$-\psi''(x) + \psi(x) - \frac{3}{2}\frac{\psi(x)}{\operatorname{ch}^2 x} = \lambda\psi(x), \quad \psi(\pm\infty) = 0;$$

It is easy to see that it has two bounded states

$$\psi_0(x) = \sqrt{\frac{3}{8}}\frac{1}{\operatorname{ch}^2\frac{x}{2}}, \quad \psi_1(x) = \sqrt{\frac{3}{4}}\frac{\operatorname{sh}\frac{x}{2}}{\operatorname{ch}^2\frac{x}{2}}$$

with energies $\lambda_0 = 0$, $\lambda_1 = \frac{3}{4}$. Let's practice numerical methods of finding its eigensystem.

1. Can `DEigensystem` find these solutions?
2. Solve eigenproblem using `NDEigensystem`.
3. Solve eigenproblem using `ParametricNDSolve`.
4. Solve eigenproblem in finite matrix representation (using Hermite basis).

Compare results with each other and with an exact ones.

X Assigment on «Applications in Theoretical Physics»

Problem X.1 (Wick's theorem). Consider a function of order parameters φ_1, φ_2,…, all of which are normally distributed with zero mean and known variance $\langle\varphi^2\rangle$, so that

$$\langle \exp\varphi\rangle = \int d\varphi \exp\left(-\frac{\varphi^2}{2\langle\varphi^2\rangle}\right)\exp\varphi = \exp\left[\frac{1}{2}\langle\varphi^2\rangle\right].$$

Your task is to deal with expression containing exponential and trigonometric functions of order parameters, such as

$$\langle\cos\varphi_1\cos\varphi_2\rangle = \exp\left[-\langle\varphi^2\rangle\right].$$

Problem X.2 (Heisenberg antiferromagnet). Consider Heisenberg antiferromagnetic Hamiltonian with periodic boundary conditions

$$\hat{H} = \sum_{k=1}^{N}\hat{\mathbf{s}}_k\cdot\hat{\mathbf{s}}_{k+1}, \qquad N+1=1.$$

Find the spectrum of $\hat{H}$ for $s=\frac{1}{2}$ and $N=2,\,3,\,\ldots$, as well as for $s=1$ and $N=2,\,3,\,\ldots$ How large N can you achieve?

Extrapolate the ground state energy divided by number of spins E_0/N and the value of the gap

$$\Delta \eqqcolon \min_{E\neq E_0} E - E_0$$

to large $N\to\infty$ for $s=\frac{1}{2}$ as well as $s=1$. Answer the following questions:

1) Is it correct that for $s=\frac{1}{2}$ $\lim\limits_{N\to\infty} E_0/N = \frac{1}{4}-\ln 2$?
2) What is the value of $\lim\limits_{N\to\infty} E_0/N$ for $s=1$?
3) Does the gap closes with $N\to\infty$ for $s=\frac{1}{2}$? for $s=1$?

Problem X.3 (Landau levels in graphene). In the tight binding approximation effective Hamiltonian of graphene can be written as

$$H = \begin{pmatrix} 0 & \sum\limits_{n=1}^{3} e^{i\mathbf{k}\boldsymbol{\delta}_n} \\ \sum\limits_{n=1}^{3} e^{-i\mathbf{k}\boldsymbol{\delta}_n} & 0\end{pmatrix} \qquad \boldsymbol{\delta}_1 = \frac{1}{2}\begin{pmatrix}\sqrt{3}\\-1\end{pmatrix} \quad \boldsymbol{\delta}_2 = \begin{pmatrix}0\\1\end{pmatrix} \quad \boldsymbol{\delta}_3 = \frac{-1}{2}\begin{pmatrix}\sqrt{3}\\1\end{pmatrix}$$

Presence of magnetic field can be accounted for via Peierls substitution $\mathbf{k}\mapsto\mathbf{k}-\frac{e}{c}\mathbf{A}$, where $\mathbf{A}$ is a vector potential. Find energy levels in graphene in magnetic field as a function of $\mathbf{k}$ for different orientations of the field $\mathbf{B}\parallel Oz$, Ox, Oy.

Problem X.4 (Hubbard model). One of the rich model describing different phenomena in solid state physics is Hubbard model

$$\hat{H} = -t\sum_{\langle ij\rangle}\sum_{\sigma} c^+_\sigma(i)c_\sigma(j) + u\sum_i c^+_\uparrow(i)c_\uparrow(i)c^+_\downarrow(i)c_\downarrow(i).$$

Fermions live on $N\times N$ lattice with periodic boundary condition (try $N=2,\,3$). Here, I simply ask you to find quantum–statistically averaged number of fermions on the site

$$\left\langle c^+_\uparrow(i)c_\uparrow(i)\right\rangle \propto \operatorname{tr}\left[e^{-\beta\hat{H}}c^+_\uparrow(i)c_\uparrow(i)\right]$$

as a function of temperature $T=\frac{1}{\beta}$.

Problem X.5 (Over–barrier reflection)**.** Find the transmission coefficient for the over–barrier reflection in the potential $V(x) = -x^4$. In other words, you need to obtain solution of

$$\left[\frac{d^2}{dx^2} + x^4 + \varepsilon\right]\psi(x) = 0$$

that asymptotically behaves as

$$\psi(x) \sim t \cdot \frac{\exp\int_0^x \sqrt{\varepsilon - x^4}}{x}, \quad x \to \infty.$$

and then connect it with the behavior at the left end.

$$\psi(x) \sim \frac{\exp\int_0^x \sqrt{\varepsilon - x^4}}{x} + r \cdot \frac{\exp - \int_0^x \sqrt{\varepsilon - x^4}}{x}, \quad x \to -\infty.$$

Problem X.6 (Anderson model)**.** Simplest model describing impurities in conductors uses Hamiltonian

$$H = \sum_i \varepsilon_i c_i^+ c_i - t \sum_{\langle ij \rangle} c_i^+ c_j,$$

where fermion operators c_i are located on a line of size N with periodic boundary conditions. Disorder is presented via local «energies», which are uniformly distributed in $[-W, W]$ interval. Find (averaged) density of states in such model.