计算物理/研, USTC
Prof. Ming Gong (LQCC)
物质楼 C 栋 812
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Homework 1

Please submit your homework(s) use a pdf file. If you are not familiar with LATEX, a scanned pdf file is also acceptable.

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Due date and Due time: Friday, 9/30/2021, 12:00 pm. These who really have difficulties in finishing these problems can postpone their homework by, at most, one week. Homework delay by more than one week will obtain at most 50% of the total marks.

You can finish the homework using any language (c, c++, fortran, python, matlab, MATHEMATICA, $\cdots$); however, be sure to submit your code together with your homework, demonstrating that you finish this work by yourself, independently. Plagiarism is strictly not allowed.

Problem 1 (10 points)

Obtain a general feeling of numerical physics. Please summarize the major models and algorithms in any book of ”numerical methods”.

Ref. 张韵华等，数值计算方法和算法, 科学出版社。

Hint: 插值、极值、求根、迭代、本征值、随机数、FFT、积分、Runge-Kutta 等。

Problem 2 (10 points)

Summary the models in physics. Please summary as many models as possible in the books you have, which need to be calculated numerically. Models from literature are also welcome. The techniques in solving these problems are the focus of this course.

Ref. 普通物理、四大力学、非线性物理、多体物理、量子信息等.

Hint: Some of the most important problems in physics: Dynamical problems, Eigenvalues,

Homework 1

Stochastic problem and Extreme value problems (动力学问题、本征值问题、随机问题、极值问题). All of them will become extremely complicated when $N \to \infty$ (or large enough).

For these reasons, the following models are important

1. Newton equation in coupled systems; Chaos; synchronization;
2. Application of newton equation in other fields, such as network, bird flocking, molecular dynamics and medicine designing，traffic jam *etc.*
3. Maxwell equation (requiring of Gauge invariant);
4. Partial function $Z = \text{tr}(e^{-\beta H})$ in statistical physics;
5. Eigenvalues of Hamiltonian, and their eigenvalues in the many-body models;
6. Stochastic process, such as the Brown motion and Langevin equation; Dissipation in quantum qubits interacting with the bath;
7. The ground state energy E_g of a model with many-body interaction, such as that in DFT.
8. Mean-field theory and self-consistent solution of some nonlinear equations;
9. Monte Carlo simulation: from classical physics to quantum physics.
10. $\cdots$

Problem 3 (10 points)

Analytical programming language. MATHEMATICA is very important in this course because a lot of calculations need to be done based this software. So install MATHEMATICA in your own computer; and summary the major commands in MATHEMATICA from the textbooks. Try some of them in your own computer.

Ref. 张韵华、王新茂，Mathematica 7 实用教程，中国科学技术大学出版社。

Hint: The following commands are exceptional important in this course:

1. Mathematical constants: Pi, E, I, Infinity, GoldenRatio, EulerGamma.

2. D, Series, FullSimplify, Assumption, Clear, Show, N, %.

3. Solve, DSolve, NSolve, Integrate, NIntegrate.

4. Complex numbers: I, Complex, Re, Im, Abs, Arg, Sign, Conjugate, Reduce.

5. Plot, Plot3D, ContourPlot, ListPlot.

6. Matrix: Dot, Inverse, Transpose, Tr, Det, MatrixExp, Eigensystem, Eigenvectors, Eigenvalues, QRDecomposition, LUDecomposition.

7. Table, Array, Dot, Cross, Norm, MatrixForm.

8. Loops and outputs: Do, While, Write.

9. Special functions: Gamma, Beta, Erf, LegendreP, HermiteH, LaguerreL, JacobiP, EllipticK, EllipticF, Zeta, PolyLog, MathieuS, MathieuC, MathieuSPrime, MathieuCprime, BesselJ, BesselY, BesselI, BesselK, AiryAi, SphericalBesselJ, AiryAiPrime $\cdots$.

Problem 4 (20 points)

Tricks in numerical calculations: I use the following simple, but important examples, to illustrate some importance tricks in numerical and analytical calculations, which will be frequently used in this course.

1. Please generate numbers x_i and y_i, where $i = 1 - L$ (with $L = 10000$), then calculate

$$z = \prod_{i=1}^{L} x_i + \prod_{i=1}^{N} y_i.$$

2. Please plot the following function

$$P(x) = \sum_{k=1}^{\infty} \frac{x^{k/2}}{(3k)!}, \quad x = (0, 1000).$$

3. Determine the approximate polynomial of $P(x)$, with error less than 10^{-10} for $x \in (0, 1000)$.

Homework 1

4. About the Stirling's approximation for $n!$

$$n! = n^n e^{-n}\sqrt{2\pi n}F(n), \quad F(n) = 1 + \frac{1}{12n} + \frac{a_2}{n^2} + \frac{a_3}{n^3} + \frac{a_4}{n^4} + \cdots .$$

Please determine the values of $a_i \in \mathbb{Z}$ in the higher-order terms by numerical method.

5. Consider the Morse potential

$$V(r) = U(1 - \exp(-a(r - r_e)))^2 - Fr, \quad U, a, r_e > 0.$$

Assume that $F \to 0$, find analytically the minimal position of $V(r)$, to the accuracy of F^3, that is, $V'(x) = 0$, with

$$x = r_e + a_1 F + a_2 F^2 + a_3 F^3.$$

Then determine a_i analytically using perturbation theory; and verify them numerically.