This is a testfile for vscode

Ali-loner

2020.08.02

摘要

Nam dui ligula, fringilla a, euismod sodales, sollicitudin vel, wisi. Morbi auctor lorem non justo. Nam lacus libero, pretium at, lobortis vitae, ultricies et, tellus. Donec aliquet, tortor sed accumsan bibendum, erat ligula aliquet magna, vitae ornare odio metus a mi. Morbi ac orci et nisl hendrerit mollis. Suspendisse ut massa. Cras nec ante. Pellentesque a nulla. Cum sociis natoque penatibus et magnis dis parturient montes, nascetur ridiculus mus. Aliquam tincidunt urna. Nulla ullamcorper vestibulum turpis. Pellentesque cursus luctus mauris.

Contents

1 This is a section **1**

2 Molecular Dynamics **2**

3 Probability Theory: **2**

3.1 Probability Distribution . . . 2

3.1.1 Normalization for continous variable . . . 2

3.1.2 Expected Value (aka Mean value, first moment of the distribution) . . . 2

3.1.3 Statistical Property . . . 2

3.2 Lattice Model . . . 3

4 Computer Version **3**

4.1 Rotation Matrix . . . 3

5 Homework Part **3**

5.1 Problem 5 . . . 3

5.1.1 (a) . . . 4

5.1.2 b . . . 4

5.1.3 c . . . 4

5.2 Problem 8 . . . 4

5.2.1 a . . . 4

5.2.2 b . . . 4

1 This is a section

Hello world! Hello Ali! As shown in figure 1

图 1: this is Sihan Cao

2 Molecular Dynamics

Classical mechanics can not be the whole story. Statistical Mechanics, (some system that not seem to go to the lowest energy) Today I watch 46:43

3 Probability Theory:

3.1 Probability Distribution

All Probability Distribution must be normalized: sum over all possible outcomes must be "1"! flip coin is a discrete variable (The outcome only has finite value), but in molecular dynamics we mainly think of continous variable.

3.1.1 Normalization for continous variable

: $\int_{-\infty}^{+\infty} p(x)dx = 1$

3.1.2 Expected Value (aka Mean value, first moment of the distribution)

$$\langle X \rangle = \int_{-\infty}^{+\infty} xp(x)dx \tag{1}$$

The n_{th} order moment can be calculated through:

$$\langle X^n \rangle = \int_{-\infty}^{+\infty} x^n p(x)dx \tag{2}$$

3.1.3 Statistical Property

Variance: "cumulant"

$$Var(X) = \langle X^2 \rangle - \langle X \rangle^2 \tag{3}$$

Standard Deviation: Not cumulant, but has same unit as X

$$std(x) = \sqrt{Var(X)} \tag{4}$$

3.2 Lattice Model

Space is discretizied, and each discrete cell can hold 0 or 1 particle. Microstate <—> Combinations

For the probablistic mechanics, the multi-cimponents system go to the (macro) state with the highest multiplicity (combos) 这句话是测试能否进行引用及支持中文[1]。

4 Computer Version

4.1 Rotation Matrix

$$\begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

For the linear transformation we only need to care about

$$\begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

which is the x-axis unit vector of the original coordinate and

$$\begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

which is the y-axis unit vector of the original coordinate. To use the rotation Matrixm it's just like:

$$\begin{bmatrix} x^1 \\ y^1 \end{bmatrix} = A \begin{bmatrix} x \\ y \end{bmatrix}$$

5 Homework Part

Stirling's approximation

$$N! = (\frac{N}{e})^N \ln N! \approx N \ln N - N \tag{5}$$

5.1 Problem 5

Lennard Jones law: $4\epsilon[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^6]$ For a FCC material $U(d) = \frac{1}{2}4\epsilon$

The r^{12} term is the short term repulsive term (describe Pauli Repulsion), and the r^6 is the long term attractive term (describe van der Waals force or dispersion force).

5.1.1 (a)

The sum of the energy of the material could be written as:

$$U = 4\epsilon[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^6] = \frac{1}{2}N4\epsilon(\frac{(\sigma)^{12}}{(d)^{12}}A - \frac{(\sigma)^6}{(d)^6}B) \tag{6}$$

To calculate A and B:

$$A = 2*(\frac{\sigma^{12}}{d^{12}}) + 2*(\frac{\sigma^{12}}{(2d)^{12}}) + 2*(\frac{\sigma^{12}}{(3d)^{12}}) + ... = 2.0005(\frac{\sigma^{12}}{d^{12}}) \tag{7}$$

$$B = 2*(\frac{\sigma^6}{d^6}) + 2*(\frac{\sigma^6}{(2d)^6}) + 2*(\frac{\sigma^6}{(3d)^6}) + 2*(\frac{\sigma^6}{(4d)^6}) + ... = 1.0173(\frac{\sigma^6}{d^6}) \tag{8}$$

Then,

$$U = \frac{1}{2}N4\epsilon[2.0005\frac{\sigma^12}{d^12} - 1.0173\frac{\sigma^6}{d^6}] \tag{9}$$

To calculate the equilibrium space d,

$$\frac{\mathrm{d}U}{\mathrm{d}r} = 0 \tag{10}$$

So the d is $\sqrt[6]{\frac{2\times 2.0005}{1.0173}}\sigma = 1.2564\sigma$

The d just depend on length scale σ, but has no relationship with energy scale ϵ

5.1.2 b

If there is no energy dissipation, the total system will vibrate like a wave.

5.1.3 c

The total energy of the system is $U = 2N\epsilon[A\frac{\sigma^{12}}{r^{12}} - B\frac{\sigma^6}{r^6}]$, so $\frac{\mathrm{d}^2u}{\mathrm{d}r^2} = 2N\epsilon[A\sigma^{12}(12\times 13r^{-14}) - B\sigma^6(42r^{-8})] = 2N\epsilon[2.0005\sigma^{12}\times 156\times(1.2564\sigma)^{-14} - 1.0173\sigma^6\times 42\times(1.2564\sigma)^{-8}]$ So the effective spring constant equals:$11.7938N\epsilon\sigma^{-2}$

5.2 Problem 8

5.2.1 a

For one lattice, the combination is C_N^n. Because the system has two lattices, so the total number of combinations is $C_N^n \cdot C_N^n = (C_N^n)^2$

5.2.2 b

The total number of combinations is C_{2N}^{2n}

参考文献

[1] G. J. Pottie and W. J. Kaiser. Embedding the internet: Wireless integrated network sensors. *Communications of the Acm*, 43, 2000.