Additional Notes --- brownian motion and mathematical tools

Yining He

1) Paper (A) The dynamic mean-field density functional method and its application to the mesoscopic dynamics of quenched block copolymer melts

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1) why study the quenching dynamics? (short relaxation time!)

"Yet from an industrial perspective, **even a rough description of irregular nonequilibrium states** is **much more desired than a detailed analysis of pure equilibrium structures**. Typically, the industrial processing time of a melt is orders of magnitude shorter than the thermodynamic relaxation time and thus in many cases intermediate nonperfect states must contribute substantially if not dominate the behavior of the final macroscale material."

2) Terminology

2.1 "Kronecker function"

https://en.wikipedia.org/wiki/Kronecker_delta

Kronecker delta

From Wikipedia, the free encyclopedia

Not to be confused with the Dirac delta function, nor with the Kronecker symbol.

In mathematics, the **Kronecker delta** (named after Leopold Kronecker) is a function of two variables, usually just non-negative integers. The function is 1 if the variables are equal, and 0 otherwise:

$$\delta_{ij} = \begin{cases} 0 & \text{if } i \neq j, \\ 1 & \text{if } i = j. \end{cases}$$

克罗内克δ函数 [编辑]

维基百科，自由的百科全书

提示：本条目的主题不是狄拉克δ函数，也不是克罗内克符号。

在数学中，**克罗内克函数**（又称克罗内克δ函数、克罗内克δ）δ_{ij} 是一个二元函数，得名于德国数学家利奥波德·克罗内克。克罗内克函数的自变量（输入值）一般是两个整数，如果两者相等，则其输出值为1，否则为0。

$$\delta_{ij} = \begin{cases} 1 & (i = j) \\ 0 & (i \neq j) \end{cases} 。$$

克罗内克函数的值一般简写为 δ_{ij} 。

克罗内克函数和狄拉克δ函数都使用δ作为符号，但是克罗内克δ用的时候带两个下标，而狄拉克δ函数则只有一个变量。

2.2 "Trace" or "迹" in linear algebra

https://en.wikipedia.org/wiki/Trace_(linear_algebra)

迹 [编辑]

维基百科，自由的百科全书

在线性代数中，一个$n \times n$的矩阵$\mathbf{A}$的**迹**（或**迹数**），是指$\mathbf{A}$的主对角线（从左上方至右下方的对角线）上各个元素的总和，一般记作$\operatorname{tr}(\mathbf{A})$或$\operatorname{Sp}(\mathbf{A})$：

$$\operatorname{tr}(\mathbf{A}) = \mathbf{A}_{1,1} + \mathbf{A}_{2,2} + \cdots + \mathbf{A}_{n,n}$$

其中$\mathbf{A}_{i,j}$代表矩阵的第i行j列上的元素的值[1]。一个矩阵的迹是其特征值的总和（按代数重数计算）。

迹的英文为trace，是来自德文中的Spur这个单字（与英文中的Spoor是同源词），在数学中，通常简写为“Sp”或“tr”。

In linear algebra, the **trace** (often abbreviated to tr) of a square matrix $\mathbf{A}$ is defined to be the sum of elements on the main diagonal (from the upper left to the lower right) of $\mathbf{A}$.

The trace of a matrix is the sum of its (complex) eigenvalues, and it is invariant with respect to a change of basis. This characterization can be used to define the trace of a linear operator in general. The trace is only defined for a square matrix ($n \times n$).

The trace is related to the derivative of the determinant (see Jacobi's formula).

Definition [edit]

The **trace** of an $n \times n$ square matrix $\mathbf{A}$ is defined as[1]:34

$$\operatorname{tr}(\mathbf{A}) = \sum_{i=1}^{n} a_{ii} = a_{11} + a_{22} + \cdots + a_{nn}$$

where a_{ii} denotes the entry on the ith row as well as ith column of $\mathbf{A}$.

Example [edit]

Let $\mathbf{A}$ be a matrix, with

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} = \begin{pmatrix} -1 & 0 & 3 \\ 11 & 5 & 2 \\ 6 & 12 & -5 \end{pmatrix}$$

Then

$$\operatorname{tr}(\mathbf{A}) = \sum_{i=1}^{3} a_{ii} = a_{11} + a_{22} + a_{33} = -1 + 5 + (-5) = -1$$

2.3 “Kernel (linear algebra)”

Kernel (linear algebra)

From Wikipedia, the free encyclopedia

For other uses, see Kernel (disambiguation).

In mathematics, more specifically in linear algebra and functional analysis, the **kernel** of a linear mapping, also known as the **null space** or **nullspace**, is the set of vectors in the domain of the mapping which are mapped to the zero vector.[1][2] That is, given a linear map $L : V \to W$ between two vector spaces V and W, the kernel of L is the set of all elements $\mathbf{v}$ of V for which $L(\mathbf{v}) = \mathbf{0}$, where $\mathbf{0}$ denotes the zero vector in W,[3] or more symbolically:

$$\ker(L) = \{\mathbf{v} \in V \mid L(\mathbf{v}) = \mathbf{0}\}.$$

2.4 “fluctuation-dissipation theorem”

(1) https://en.wikipedia.org/wiki/Fluctuation-dissipation_theorem

Fluctuation-dissipation theorem

From Wikipedia, the free encyclopedia

The **fluctuation–dissipation theorem** (**FDT**) or **fluctuation–dissipation relation** (**FDR**) is a powerful tool in statistical physics for predicting the behavior of systems that obey detailed balance. Given that a system obeys detailed bal~~ance, the theorem is a general proof that thermodynamic fluctuations~~ in a physical variable predict the response quantified by the admittance or impedance of the same physical variable (like voltage, temperature difference, etc.), and vice versa. The fluctuation–dissipation theorem applies both to classical and quantum mechanical systems.

The fluctuation–dissipation theorem was proven by Herbert Callen and Theodore Welton in 1951 [1] and expanded by Ryogo Kubo. There are antecedents to the general theorem, including Einstein's explanation of Brownian motion [2] during his *annus mirabilis* and Harry Nyquist's explanation in 1928 of Johnson noise in electrical resistors.[3]

Qualitative overview and examples [edit]

The fluctuation–dissipation theorem says that when there is a process that dissipates energy, turning it into heat (e.g., friction), there is a reverse process related to thermal fluctuations. This is best understood by considering some examples:

- *Drag and Brownian motion*

  If an object is moving through a fluid, it experiences drag (air resistance or fluid resistance). Drag dissipates kinetic energy, turning it into heat. The corresponding fluctuation is Brownian motion. An object in a fluid does not sit still, but rather moves around with a small and rapidly-changing velocity, as molecules in the fluid bump into it. Brownian motion converts heat energy into kinetic energy—the reverse of drag.

- *Resistance* and *Johnson noise*

  If electric current is running through a wire loop with a resistor in it, the current will rapidly go to zero because of the resistance. Resistance dissipates electrical energy, turning it into heat (Joule heating). The corresponding fluctuation is Johnson noise. A wire loop with a resistor in it does not actually have zero current, it has a small and rapidly-fluctuating current caused by the thermal fluctuations of the electrons and atoms in the resistor. Johnson noise converts heat energy into electrical energy—the reverse of resistance.

Examples in detail [edit]

The fluctuation–dissipation theorem is a general result of statistical thermodynamics that quantifies the relation between the fluctuations in a system that obeys detailed balance and the response of the system to applied perturbations.

Brownian motion [edit]

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For example, Albert Einstein noted in his 1905 paper on Brownian motion that the same random forces that cause the erratic motion of a particle in Brownian motion would also cause drag if the particle were pulled through the fluid. In other words, the fluctuation of the particle at rest has the same origin as the dissipative frictional force one must do work against, if one tries to perturb the system in a particular direction.

From this observation Einstein was able to use statistical mechanics to derive the Einstein–Smoluchowski relation

$$D = \mu\, k_B T$$

which connects the diffusion constant D and the particle mobility μ, the ratio of the particle's terminal drift velocity to an applied force. k_B is the Boltzmann constant, and T is the absolute temperature.

Notes:
Clarifications for some Physical terms.

(A) Drag (physics) (https://en.wikipedia.org/wiki/Drag_(physics))
In fluid dynamics, drag (sometimes called fluid resistance) **is a force acting opposite to the relative motion of any object moving with respect to a surrounding fluid**. This can exist between two fluid layers (or surfaces) or a fluid and a solid surface. Unlike other resistive forces, such as dry friction, which are nearly independent of velocity, drag forces depend on velocity. **Drag force is proportional to the velocity** for a laminar flow (层流) and the squared velocity for a turbulent flow (湍流).

(B) Thermal fluctuations (https://en.wikipedia.org/wiki/Thermal_fluctuations)
"In statistical mechanics, thermal fluctuations are **random deviations of a system from its average state, that occur in a system at equilibrium.** All thermal fluctuations become larger and more frequent as the temperature increases, and likewise they decrease as temperature approaches absolute zero.

Thermal fluctuations are a basic manifestation of the temperature of systems: A system at nonzero temperature does not stay in its equilibrium microscopic state, but instead randomly samples all possible states, with probabilities given by the Boltzmann distribution.

Thermal fluctuations generally affect all the degrees of freedom of a system: There can be random vibrations (phonons), random rotations (rotons), random electronic excitations, and so forth.

Thermodynamic variables, such as pressure, temperature, or entropy, likewise undergo thermal fluctuations. For example, for a system that has an equilibrium pressure, the system pressure fluctuates to some extent about the equilibrium value.

Only the 'control variables' of statistical ensembles (such as the number of particles N, the volume V and the internal energy E in the microcanonical ensemble) do not fluctuate.

Thermal fluctuations are a source of noise in many systems. The random forces that give rise to thermal fluctuations are a source of both diffusion and dissipation (including damping and viscosity). **The competing effects of random drift and resistance to drift are related by the fluctuation-dissipation theorem**. Thermal fluctuations play a major role in **phase transitions** and **chemical kinetics**.

Notes: Central limit theorem (https://en.wikipedia.org/wiki/Thermal_fluctuations)
(Gamma Function: For any positive integer n,

$$\Gamma(n) = (n-1)!$$

for complex numbers with a positive real part the gamma function is defined via a convergent improper integral:

$$\Gamma(z) = \int_0^\infty x^{z-1} e^{-x}\, dx, \qquad \Re(z) > 0$$

Central limit theorem [edit]

The volume of phase space $\mathcal{V}$, occupied by a system of $2m$ degrees of freedom is the product of the configuration volume V and the momentum space volume. Since the energy is a quadratic form of the momenta for a non-relativistic system, the radius of momentum space will be $\sqrt{E}$ so that the volume of a hypersphere will vary as $\sqrt{E}^{2m}$ giving a phase volume of

$$\mathcal{V} = \frac{(C \cdot E)^m}{\Gamma(m+1)},$$

where C is a constant depending upon the specific properties of the system and Γ is the Gamma function. In the case that this hypersphere has a very high dimensionality, $2m$, which is the usual case in thermodynamics, essentially all the volume will lie near to the surface

$$\Omega(E) = \frac{\partial \mathcal{V}}{\partial E} = \frac{C^m \cdot E^{m-1}}{\Gamma(m)},$$

where we used the recursion formula $m\Gamma(m) = \Gamma(m+1)$.

The surface area $\Omega(E)$ has its legs in two worlds: (i) the macroscopic one in which it is considered a function of the energy, and the other extensive variables, like the volume, that have been held constant in the differentiation of the phase volume, and (ii) the microscopic world where it represents the number of complexions that is compatible with a given macroscopic state. It is this quantity that Planck referred to as a 'thermodynamic' probability. It differs from a classical probability inasmuch as it cannot be normalized; that is, its integral over all energies diverges—but it diverges as a power of the energy and not faster. Since its integral over all energies is infinite, we might try to consider its Laplace transform

$$\mathcal{Z}(\beta) = \int_0^\infty e^{-\beta E}\,\Omega(E)\,dE,$$

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which can be given a physical interpretation. The exponential decreasing factor, where β is a positive parameter, will overpower the rapidly increasing surface area so that an enormously sharp peak will develop at a certain energy $E^\star$. Most of the contribution to the integral will come from an immediate neighborhood about this value of the energy. This enables the definition of a proper probability density according to

$$f(E;\beta) = \frac{e^{-\beta E}}{\mathcal{Z}(\beta)}\Omega(E),$$

d

whose integral over all energies is unity on the strength of the definition of $\mathcal{Z}(\beta)$, which is referred to as the partition function, or generating function. The latter name is due to the fact that the derivatives of its logarithm generates the central moments, namely,

$$\langle E\rangle = -\frac{\partial \ln \mathcal{Z}}{\partial\beta}, \qquad \langle (E-\langle E\rangle)^2\rangle = \langle(\Delta E)^2\rangle = \frac{\partial^2 \ln \mathcal{Z}}{\partial\beta^2},$$

and so on, where the first term is the mean energy and the second one is the dispersion in energy.

The fact that $\Omega(E)$ increases no faster than a power of the energy ensures that these moments will be finite.[2] Therefore, we can expand the factor $e^{-\beta E}\Omega(E)$ about the mean value $\langle E\rangle$, which will coincide with $E^\star$ for Gaussian fluctuations (i.e. average and most probable values coincide), and retaining lowest order terms result in

$$f(E;\beta) = \frac{e^{-\beta E}}{\mathcal{Z}(\beta)}\Omega(E) \approx \frac{\exp\{-(E-\langle E\rangle)^2/2\langle(\Delta E)^2\rangle\}}{\sqrt{2\pi\langle(\Delta E)^2\rangle}}.$$

This is the Gaussian, or normal, distribution, which is defined by its first two moments. In general, one would need all the moments to specify the probability density, $f(E;\beta)$, which is referred to as the canonical, or posterior, density in contrast to the prior density Ω, which is referred to as the 'structure' function.[2] This is the central limit theorem as it applies to thermodynamic systems.[3]

If the phase volume increases as E^m, its Laplace transform, the partition function, will vary as β^{-m}. Rearranging the normal distribution so that it becomes an expression for the structure function and evaluating it at $E = \langle E \rangle$ give

$$\Omega(\langle E \rangle) = \frac{e^{\beta(\langle E \rangle)\langle E \rangle} \mathcal{Z}(\beta(\langle E \rangle))}{\sqrt{2\pi \langle (\Delta E)^2 \rangle}}.$$

It follows from the expression of the first moment that $\beta(\langle E \rangle) = m/\langle E \rangle$, while from the second central moment, $\langle (\Delta E)^2 \rangle = \langle E \rangle^2/m$. Introducing these two expressions into the expression of the structure function evaluated at the mean value of the energy leads to

$$\Omega(\langle E \rangle) = \frac{\langle E \rangle^{m-1} m}{\sqrt{2\pi m} m^m e^{-m}}.$$

The denominator is exactly Stirling's approximation for $m! = \Gamma(m+1)$, and if the structure function retains the same functional dependency for all values of the energy, the canonical probability density,

$$f(E;\beta) = \beta \frac{(\beta E)^{m-1}}{\Gamma(m)} e^{-\beta E}$$

will belong to the family of exponential distributions known as gamma densities. Consequently, the canonical probability density falls under the jurisdiction of the local law of large numbers which asserts that a sequence of independent and identically distributed random variables tends to the normal law as the sequence increases without limit.

Central limit theorem (**in Probability Theory**)

In probability theory, the central limit theorem (CLT) establishes that, in some situations, when independent random variables are added, their **properly normalized sum** tends toward a normal distribution (informally a bell curve) even if the original variables themselves are not normally distributed. The theorem is a key concept in probability theory because it implies that probabilistic and statistical methods that work for normal distributions can be applicable to many problems involving other types of distributions.

Mathematically, if $X_1, X_2, \ldots, X_n$ is a random sample of size n taken from a population with mean μ and finite variance σ^2 and if $\bar{X}$ is the sample mean, the limiting form of the distribution of $Z = \left(\frac{\bar{X}-\mu}{\sigma/\sqrt{n}}\right)$ as $n \to \infty$, is the standard normal distribution.[1]

(b) https://web.stanford.edu/~peastman/statmech/largenumbers.html#the-central-limit-theorem

The Central Limit Theorem:

Consider the sum

$$S = \sum_{i=1}^{N} x_i$$

where the values x_i are independently drawn from a distribution with mean μ_x and standard deviation σ_x. In the limit $N \to \infty$, the sum S is distributed according to a normal distribution with mean $\mu = N\mu_x$ and standard deviation $\sigma = \sqrt{N}\sigma_x$.

(2) The Fluctuation-Dissipation Theorem
https://web.stanford.edu/~peastman/statmech/friction.html

2.5 “Ginzburg-Landau theory”
太难，以后再试一下