DISCRETE FREE PATHS IN THERMODYNAMICAL SYSTEMS

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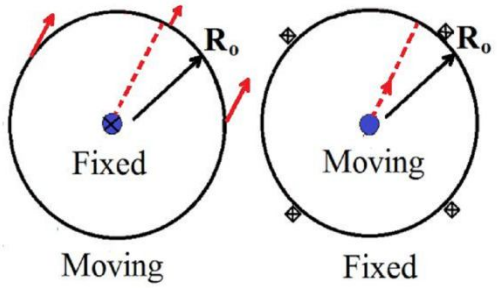
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Abstract- thediscrete path problem has been the subject of extended literature. Physically, the free path concept starts from thermodynamics and then merges into other fields of study. This article describes the free path as a spatial correlation functions. Finally, the most important free path equations are summarized.

Keywords- Chord Length, Discrete Free Path, Line Of Sight, Accessible Radius, Spatial Correlation Functions.

I. INTRODUCTION

In 1858, Clausius published a paper, in which, he first introduced the idea of the mean free path. His paper owed its origin to an objection raised by the Dutch metrologist Christoph Buys-Ballot (1817-1890), who had argued that if it were true, as Joule and Clausius claimed, that if the molecules of gas moves at speeds of several hundred meters a second, gases should mix much more rapidly than they do.



The mean free path λ in thermodynamics is the average distance travelled by a moving particle (such as an atom, a molecule, a photon) between successive impacts (collisions). Impacts modify the particle's direction or energy. Equivalently, the mean free path λ is defined as the average speed of a particle, c divided by the average number of collisions experienced, n[1]-[3]).

$$\lambda = \frac{\text{speed}}{\text{number of collisions}} = \frac{c}{n} \qquad (1)$$

The classical free path equation is written as:

$$\lambda = \alpha \frac{1}{(\pi\rho\sigma^2)} \qquad (2)$$

Where ρ is the density,σ is the collision radius. α is a speed correction factor to count for the effect of speed distribution,(e.g. Maxwell calculates α to equal $1/\sqrt{2}$).

In order to transfer heat and mass from a point to another in thermodynamic systems, the concept of free path is essential. Any conduction or transfer of thermodynamic phenomena to other points in the system requires accurate definition of the path between the two points.

III. THREE TYPES OF DISCRETE LINES IN NATURE

In this section, we will overview and classify different types of path and their mathematical definitions.fig.1 is a graphical representation of the three types of lines;

The free path is usually known as the two points patial correlation function. Moreover, it can be defined mathematically; Start by defining Q to be a suitable geometry. For any two distinct points a and b in Q, we define interval notation analogous to that on the real line. (This type of classification is well-known, see for example [4])

$$[a,b] := \{\delta a + (1-\delta)b | 0 \le \delta \le 1\}$$
$$[a,b[\ = \ ]a,b] := \{\delta a + (1-\delta)b | 0 < \delta \le 1\} \qquad (3)$$
$$]a,b[:= \{\delta a + (1-\delta)b | 0 < \delta < 1\}$$

Point – point path $]\boldsymbol{a},\boldsymbol{b}[$

A path that starts at the surface of one object and ends at another surface. This path is a surface-surface path, symbolically $[a,b]$, notice the square bracket in both sides, it means that the starting surface and ending surface are included in the path. Example of this path is the path of the particles created in atomic reactions. A particle is created at point A, and then it moves to point B where it vanishes. Another example is taken from stereology; it is the line of sight in which a line segment of length z is wholly in one phase of the material. Both linesdo not need the concept of surface to be defined

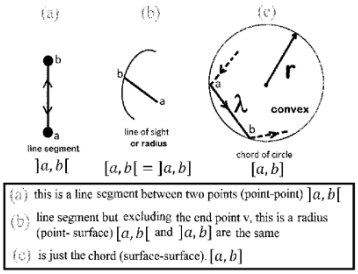


Fig .1:The three types of free path correlation functions

A. Surface-point path $[\boldsymbol{a}, \boldsymbol{b}[$

Similarly, a path that starts at the surface and ends at any internal points inside the geometry is a surface-point path, symbolically $[a, b[$. Notice the reversed square bracket in one side of the interval, it means that either the start or end point is excluded from the path. Example of this type of path is a point source that emits a particle at point A. Then the particle diffuses until it collides with a surface at point B. In bounded geometries, the integration of this measure is equivalent to the average radius. It is a generalization of the geometry radius. The radius of unbounded geometries is undefined. Radius is calculated for disconnected geometrical systems. For example, deep inside a forest, despite the trees being disconnected, it is impossible to look out of the forest. In every direction you look there is a tree blocking your line of sight. The "accessible radius" concept describes the path of an OC diffuses from a specific central point until it collides with the surface.

The mean free path $\lambda_\circ$ for a radially diffusing OC equals the "accessible radius" of the geometry:

$$\lambda_\circ = r_\circ \qquad (4)$$

B. Surface – surface path $[\boldsymbol{a}, \boldsymbol{b}]$

Finally, a path that starts at any point and ends at any other internal points inside the geometry, this path is a point-point path, symbolically $]a, b[$. The reversed square bracket in both sides of the interval means that the start and end points of the path are not surfaces. An example of surface-surface path is the path of a particle in a circle. The mean free path in a circle is equivalent to the mean chord length. Cauchy formula i.e.

$$path\ of\ the\ type\ [\mathbf{a}, \mathbf{b}] = 4V/A \qquad (5)$$

It is used to calculate the mean chord length. Where Aand V are the area and volume of the geometry or body. The free chord concept, describes the path of an OC collides, successively and only, with the surface. The free chord follow similar laws used to calculate the chord in connected geometries like circles, triangles and closed polygons. The Cauchy formula is widely accepted as a measure of free chord. Mathematically, at any point a on the boundary surface ∂Q of the geometry Q. Let $\mathfrak{L}(\theta,\varphi)$ be the length of the line $[a, b]$ connecting a with an opposite boundary point b at an angles (θ, φ) to the inward normal at a. The averaging over different chord lengths $\mathfrak{L}(\theta, \varphi)$ starting from a will involve an integration over the solid angle of 2π-steradians above the tangent plane at the point a, with a measure $d(\theta, \varphi)$, in hard sphere systems, the reflection and incidence angles are equal. The invariant measure in the spherical coordinates is

$$d(\theta, \varphi)_{[\,]} = c_{[\,]}(\mathrm{v}\cdot\mathrm{n})\sin\theta\, d\theta d\varphi = c_{[\,]}\cos\theta\sin\theta\, d\theta d\varphi \qquad (6)$$

$$l_{[\,]} = \int \mathfrak{L}(\theta,\varphi)d\mu(\theta,\varphi) \qquad (7)$$

The [ ] in $l_{[\,]}$ denote the surface-surface mean chord length. The resulting mean chord length is then defined by

$$\lambda_\circ = \frac{\int_{\partial Q} l_{[\,]}\, dS}{|\partial Q|} \qquad (8)$$

IV. AVERAGING THE DYNAMIC STAR SHAPE KERNELS

In 2D and 3D bounded geometries this equation reduces to [5]

$$\lambda_\circ = \mathfrak{L}_\circ = \int_0^\infty l.f(l)dl = \begin{cases} \frac{\pi \cdot A}{U}\ ;\ in\ 2D \\ \frac{4 \cdot V}{A}\ ;\ in\ 3D \end{cases} \qquad (9)$$

Where $\lambda_\circ$ the mean free chord for OC. V is the volume and A is the surface area of the kernel and U is the circumference length of the area, and $f(l)$ is the chord's probability distribution function. The following relation is correct 3D sphere

$$\mathfrak{L}_\circ = \beta_m r_\circ \qquad (10)$$

$\lambda_\circ$ is the free path in dynamic systems like gases, $\mathfrak{L}_\circ$ is the geometric chord length in the equivalent static or stationary system and $r_\circ$ is the equivalent radius of the geometry. In 3D it reduced to

$$\lambda_\circ = \mathfrak{L}_\circ = \frac{4}{3} r_\circ \qquad (11)$$

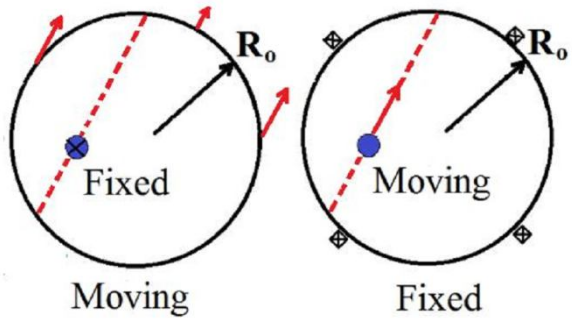


Fig.3 : In the left circle, the OC is fixed whereas the VC is moving, every surface-surface line describe a chord. In the right VC, the OC is moving whereas the VC is fixed, every surface-surface line describe a chord. The two chords are equivalent.

In this paper, we focus on the last two classes of free path correlations; point-surface and surface-surface correlation because they have the minimum geometric requirements to define a dynamic system. The point-point correlation function, like line of sight is used for secondary purposes only. Later, the line of sight will be used to define the concept of visibility.

C. Relation between the three types:

The three types of paths are interconnected, in the case of anyconvex X, with volume V and surface area S by

$$lf_{[\,]}(x) = \frac{4V}{A} f_{[[}(x) = \frac{12V^2}{\pi A}\frac{1}{l^3} f_{]][}(x) \qquad (12)$$

Where$f_{[\,]}$,$f_{[[}(l)$and$f_{]][}(l)$ are the probability distribution functions for the three lines And the relations between the radii and the moments of the chords for smooth connected geometries are:

$$r_\circ = \langle [a,b[\rangle = \frac{\langle \Omega^2 \rangle}{2\Omega_\circ} = \frac{\langle [a,b]^2 \rangle}{2\langle [a,b] \rangle} \qquad (13)$$

Among the three types of lines it is possible to define two types of "paths" only. An essential condition to define the free path distribution inside any surface is thepresence of a surface that bounds the OC at every point and instance in the system. Hence, the free path is definable in bounded (systems) geometries. Collisions between the OC happen at the system's boundaries or within the system volume with other identities, which in turn, is considered by the particle as a part of a bounding surface.

V. THE MEAN FREE PATH

Statistical mechanics had been used extensively to study the mean free path in gases; the literature is rich of papers about the effect of speed on free path calculation, see section D. Starting from Maxwell's free path which is obtained by dividing $\bar{c}$, the average speed, by n, the average free number of collisions per second averaged over all the molecules. On the other hand, Tait takes the value of the free path c/n appropriate to each speed and averages this over all the molecules. Obviously, still another free path would be obtained, if the average value of the speed $\bar{c}$ were to be multiplied by the value of $1/\lambda$ averaged over all themolecules, and still others could be obtained by averaging in different ways.

Later Jeans [6] showed that the distribution of free path depends on the average velocity, and the fluctuations due to the distributions of velocity is negligible. the frequency of collisions is proportional to the density of scatterers, whereas, the mean-free path λ is inversely proportional to the density.[7]

"different particles are moving at different speeds" (20)

D. Clausius calculation of number of collisions and free path

In Clausius paper, the question of the collisions of spherical particles of radius r_p with other particles or with the walls, is replaced by the equivalent problem of the collision of a point with a surface1[8]. Clausius determined the free path by considering the condition

"all the particles are static " (14)

Since all particles are static then there is no need for relative speed correction. The correction factor $\alpha_\circ$ in equation () is unity

$$\alpha_\circ = 1 \qquad (15)$$

The free path value when all the surrounding particles are static equals

$$\lambda_\circ = \frac{1}{(\pi\sigma^2\rho)} \qquad (16)$$

Then Clausius supposed that

"all the particles are moving at constant average speed" (17)

The relative speed correction α_C for this condition equals to

$$The mean relative speed correction = \alpha_C = 0.75 \qquad (18)$$

Hence, Clausius free path is

$$\lambda_C = 0.75\frac{1}{(\pi\sigma^2\rho)} \qquad (19)$$

It is generally conceived that Clausius free path independency of the speed distribution, was because he wasn't aware of the importance of Maxwell's speed distribution function.

E. Maxwell's calculation of number of collisions and free path

Maxwell's free path is obtained by dividing$\bar{c}$, the mean speed by $\boldsymbol{n}$, the mean number of collisions per second $\langle \bar{c}/n \rangle$ averaged over all the molecules. Maxwell determined the free path by considering the condition that

He proposed a relative speed correction α_M equals to the integral

$$\alpha_M = \frac{1}{\bar{c}}\frac{4}{\alpha^3\sqrt{\pi}}\left[\int_0^{\bar{c}} \frac{3\bar{c}^2 + v^2}{3\bar{c}} v^2 e^{-\frac{v^2}{\alpha^2}} dv + \int_{\bar{c}}^{\infty}\int_0^{\bar{c}} \frac{3v^2 + \bar{c}^2}{3v} v^2 e^{-\frac{v^2}{\alpha^2}} dv\right] \qquad (21)$$

Where $\bar{c}$ the average is speed and v is the speed of the other particle and α is a constant. Given that every free path terminates two collisions2. This is a hard integral. And can be solved only numerically. Notice that the integral is a function in speed only. The value of α_M is

$$\alpha_M = 0.7071 \qquad (22)$$

The Maxwell's free path is

$$\lambda_M = 0.7071\frac{1}{(\pi\sigma^2\rho)} \qquad (23)$$

"Although Clausius was obviously uncomfortable with Maxwell's use of the mean free path, he did not attack Maxwell's method on physical grounds; he only remarked on his misgivings about the use of statistics … Clausius did not use the statistical

[2]The free path results from two successive collision with a surface.

distribution even after Maxwell derived it independently of the mean free path. He only used the distribution function once, to find the mechanical expression for the heat added to a gas" [9]

F. Tait's calculation of number of collisions and free-path

Tait takes the value of the free path $c/\boldsymbol{n}$ appropriate to each speed and averages this over all the molecules $\langle c/n \rangle$. Tait's determined the free path by considering the condition

"different speeds give different number of collisions" (24)

He proposed a relative speed correction α_T equals to the integral

$$\alpha_T = \int_0^{\infty} \frac{4x^4 \exp -x^2 \, dx}{\Psi(x)} \qquad (25)$$

The function $\Psi(x)$ is given by

$$\Psi(x) = x \exp -x^2 + (2x^2 + 1) \int_0^{\infty} \exp -y^2 \, dy \qquad (26)$$

$x = \frac{c}{\beta}$ and $y = \frac{c'}{\beta}$ where c and c' are the speed of the two particles. β is constant. This integration can be solved numerically. Notice that the integral is function in speed only. The calculated value of α_T by this integral is

$$\alpha_T = 0.667 \qquad (27)$$

So that the Tait free path is

$$\lambda_T = 0.667 \frac{1}{(\pi\sigma^2\rho)} \qquad (28)$$

CONCLUSION

Discrete free path arespatial correlation functions. Thermodynamically,at equilibrium, the free path depends on the constant$1/\rho\pi\sigma^2$ for their order of magnitude. Averaging the effect of speedgives a correction factor α. The value of correction factor α in (2) is as follows

$$\alpha = \begin{cases} \alpha_\circ = 1 & forcondition(14) \\ \alpha_C = 0.75 & forcondition(17) \\ \alpha_M = 0.7071 & \text{for condition Error! Reference source not found.} \\ \alpha_T = 0.667 & \text{for condition (24)} \end{cases}$$

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