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Operating mode of Fourier series and transforms in molecular dynamics

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Summary: This article explores the use of Fourier series and transforms in the context of molecular dynamics. The Fourier transform is a powerful tool for analyzing random phenomena such as molecular motions and incoherent radiation. Starting from Schrödinger's formulation and concepts from quantum mechanics, the article highlights how Fourier series allow molecular motions to be decomposed into oscillations of different frequencies. Experimental results, often obtained from macroscopic samples, are compared with theoretical predictions, illustrating the challenges inherent in the study of dynamical systems. Practical applications, such as vibration analysis, X-ray diffraction, and second harmonic generation, are also discussed, highlighting the importance of these analytical methods. Finally, the article suggests perspectives for future research, particularly on the impact of molecular characteristics on random phenomena, thus strengthening the link between theory and experiment in chemistry and physics.

Keywords: Fourier Transform, Molecular Dynamics, Quantum Mechanics, Vibration Analysis, X-ray Diffraction, Second Harmonic Generation, Random Phenomena.

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Introduction

Schrödinger's formulation of quantum mechanics reveals the time independence of the system's Hamiltonian. The evolution equation can then be reduced to a stationary form, forgetting the time dimension. The precise resolution of this relationship is far from being an easy task; it remains one of the major challenges of quantum chemistry. The many-body problem, dear to mechanics teachers, sees its paroxysm in the determination of the electronic structure of molecular structures.

However, simple models can be used to understand and predict molecular geometries, such as Lewis theory or the VSEPR approach. Concepts such as symmetry, electronegativity, and overlap allow chemical phenomena to be simply rationalized. Frontier orbital theory and the fragment approach, crowned by the Nobel Prize awarded to Roald Hoffmann and Kenichi Fukui in 1981, have made it possible to qualitatively understand a large number of experimental results based on relatively simple analyses in a language accessible to all chemists.

However, the vast majority of experimental observations, with which theoretical predictions are confronted, are observed from samples of macroscopic dimension, involving a large number of molecules, under certain experimental conditions, of temperature, pressure, concentration, etc. In addition, the natural times of spectroscopic methods are variable; some techniques are slow compared to the characteristic molecular vibrational times, others are of the same order of magnitude, or even faster. Finally, some reaction mechanisms are essentially governed by an entropic effect, which is difficult to reproduce by a static theoretical study. It must be kept in mind that a chemical process is above all a dynamic process involving the displacement of molecules and within them the movement of nuclei.

How can we take some of these effects into account from a theoretical point of view?

To solve one of these problems, this article aims to make a contribution on the principle of using Fourier series and transforms in molecular dynamics.

Let the random distance be , for different time intervals T, this distance can be decomposed into an infinite series of oscillations of frequency (or pulsation: and amplitudes, expressed by the Fourier series$f(t)nv_0 n\omega_0 = n2\pi v_0 = \frac{2\pi n}{T}\{a_n, et\ b_n\}$

$$f(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty}\{a_n \cos(n\omega_0 t) + b_n \sin(n\omega_0 t)\} \quad (1)$$

$$= \frac{a_0}{2} + \sum_{n=1}^{\infty}\left\{a_n \cos\left(\frac{2\pi n}{T}t\right) + b_n \sin\left(\frac{2\pi n}{T}t\right)\right\}$$

Demonstration of the Fourier series

The function can be written as a Fourier series:$f(t)$

$$f(t) = a_O + \sum_{n=1}^{\infty}\left\{a_n \cos\left(\frac{2\pi n}{T}t\right) + b_n \sin\left(\frac{2\pi n}{T}t\right)\right\}$$

Demonstration:To show that any periodic function can be expressed in this form, we begin by defining the Fourier coefficients:$f(t)$

$$a_O = \frac{1}{T}\int_0^T f(t)dt$$

$$a_n = \frac{2}{T}\int_0^T f(t)\cos\left(\frac{2\pi n}{T}t\right)dt$$

$$b_n = \frac{2}{T}\int_0^T f(t)\sin\left(\frac{2\pi n}{T}t\right)dt$$

These formulas allow us to determine the Fourier coefficients for any continuous and integrable function over a period interval $.f(t)T$

By the convergence of the Fourier series, we can affirm that:

$$\lim_{N\to\infty}\left(a_0 + \sum_{n=1}^{N}\left(a_n \cos\left(\frac{2\pi n}{T}t\right) + b_n \sin\left(\frac{2\pi n}{T}t\right)\right)\right) = f(t) \qquad (2)$$

In the case of random motions, the amplitude of the random signal varies over time and from one molecule to another. The result of the experimental measurement is therefore an average of the motion of individual particles, averaged over time, on the one hand, and over all particles, on the other hand. We see from the Fourier relation that the value averaged over the observation time T that we will call is equal to zero since:$f(t) < f(t) >$

$$\int_0^T \cos\left(\frac{2\pi n}{T}t\right)dt = \int_0^T \sin\left(\frac{2\pi n}{T}t\right)dt = 0 \qquad (3)$$

$$< f(t) > = 0$$

The time average of a function is zero if is periodic.$f(t)f(t)$

Demonstration:Let's calculate the time average over a period interval:T

$$< f(t) > = \frac{1}{T}\left(\int_0^T a_0 + \sum_{n=1}^{\infty}\left(a_n \int_0^T \cos\left(\frac{2\pi n}{T}t\right)dt + b_n \int_0^T \sin\left(\frac{2\pi n}{T}t\right)dt\right)\right)$$

The integrals of the cosine and sine functions over a full period interval are zero:

$$\int_0^T \cos\left(\frac{2\pi n}{T}t\right)dt = 0, \int_0^T \sin\left(\frac{2\pi n}{T}t\right)dt = 0 \qquad (4)$$

Thus, the time average becomes:

$$< f(t) > = \frac{1}{T}\,.\,a_0.T = a_0$$

If the values of the coefficients and are non-zero at a given time and for a particular molecule, they become zero when averaged over time; we can therefore derive no information about the instantaneous value of and from observations of the average behavior of a set of particles.$a_n b_n a_n b_n$

However, if we do an experiment that measures the square of , that is, an experiment that measures the intensity rather than the amplitude of a movement, remembering that:$f(t)$

$$\frac{1}{T}\int_0^T \cos^2\left(\frac{2\pi n}{T}t\right)dt = \frac{1}{T}\int_0^T \sin^2\left(\frac{2\pi n}{T}t\right)dt = \frac{1}{2}$$

we obtain for the time average (denoted by) of a particle that:<>

$$< f^2(t) > = \sum_{n=1}^{\infty}\frac{a_n^2 + b_n^2}{2} \qquad (5)$$

Then performing the average over all the particles (noted by the upper bar):

$$P(n\omega_n) = \frac{\overline{a_n^2 + b_n^2}}{2}$$

$$\text{And}: \overline{< f^2(t) >} = \sum_{n=1}^{\infty} P(n\omega_n)$$

For a given particle, we can a priori say nothing about the function at a given time.$f(t)$

However, if we have information about the motion being studied, for example, if we know the value of the diffusion coefficient, we can assume that the value of the function at time will differ only slightly from the value of the function at time if is small. We will say that, for small values of , the values of the functions and are "correlated". On the other hand, if time becomes significant, we will no longer be able to specify the behavior of the function. The functions and are at that point said to be "uncorrelated". Since the time required for the functions and to become uncorrelated depends on the characteristics of the motion, for example, the molecular diffusion coefficient, we can hope to obtain information about the random phenomenon by studying the correlation function:$t + \tau t\tau\tau f\,(t)f(t + \tau)\,\tau f(t + \tau).f(t)f(t + r)f(t + \tau)f(t)$

$$G(\tau) = G(0)e^{-\tau/\tau c} \qquad (6)$$

Demonstration:The correlation function is defined as:

$$G(\tau) =< f(t)f(t+\tau) >$$

Substituting , we obtain:$f(t) = \sum_{n=1}^{N}(a_n \cos(\omega_n t) + b_n \sin(\omega_n t))$

$$G(\tau) = \sum_{n=1}^{\infty}(a_n^2 \cos(\omega_n \tau) + b_n^2 \sin(\omega_n t))$$

For diffusic motions, with a constant diffusion coefficient, it can be shown that the correlation decreases exponentially, which is typical of disordered systems.

From the elements described during the study of Fourier transforms, we are able to obtain without difficulty the Lorentzian function, transform of the exponential decay:

$$P(\omega) = s\,\frac{2}{\pi}G(0)\int_0^{\infty} e^{-\tau/\tau c}\cos(\omega\tau)d\tau \qquad (7)$$

$$= \frac{2}{\pi}G(0).\left(\frac{\tau_c}{1+\omega^2\tau_{c^2}}\right)$$

Some applications

Atomic diffusion factor

X-ray diffraction of liquid structures

Second harmonic generation in linear optics

Nonlinear optics relies on molecular polarization in the presence of an external electric field. If the field is weak, it is commonly assumed that the polarization is proportional to the intensity of the external electric field:

$$P = \varepsilon_0 \chi E$$

Where is the linear electric susceptibility. The answer here is directly proportional to the field.χ

In the presence of intense electric fields such as those produced by lasers, non-linear terms appear:

$$P = \varepsilon_0 \chi E + \varepsilon_0 \chi_2 E^2 + \varepsilon_0 \chi_3 E^3 + .. (8)$$

Where are the first and second (nonlinear) hyperpolarizabilities? The introduction of an oscillating electric field causes the polarization which, by trigonometric expansion or by Fourier series expansion, gives us a total polarization which is no longer proportional to the incident field and which is, therefore, a non-symmetrical response:$\chi_2\ et \chi_3\ E\ =\ E_0\ sin(\ \omega t)$

$$P = \varepsilon_0 \chi E + \varepsilon_0 \chi_2 E^2 + \varepsilon_0 \chi_3 E^3 + ..$$

$$= \varepsilon_0(\chi E_0 sin\omega t + \chi_2 (E_0 sin\omega t)^2 + \chi_3 (E_0 sin\omega t)^3 + \cdots)$$

$$= \varepsilon_0 \left[\chi E_0 \sin(\omega t) + \frac{1}{2}\chi_2 E^2(1 - \cos(2\omega t) + ..\right]$$

$$= \varepsilon_0 \tfrac{1}{2}\chi_2 E^2 \qquad \Longrightarrow Composante\ fixe$$

$$+\varepsilon_0 \chi E_0 sin\omega t \qquad \Longrightarrow Composante\ fondamentale$$

$$-\varepsilon_0 \frac{1}{2}\chi_2 E^2 \cos(2\omega t) + .. \Longrightarrow \sec onde\ harmonique$$

We can therefore see that a frequency field generates a double frequency response. This is the phenomenon of second harmonic generation (SHG). For example, laser radiation in the red range passes through an ammonium dihydrogen phosphate crystal and emerges with a double frequency in the blue. If we had carried the Fourier expansion up to the terms coming from , we would have obtained the mathematical form of third harmonic generation (THG). Note that in French, we should logically use the term "first and second harmonics" instead of "second and third" harmonics. This is a franglicism where the "first floor" corresponds to the ground floor, the "second floor" to the first floor, and so on.$\omega\ =\ 2\pi v 2\omega\ =\ 4\pi v \sin^3(\omega t)$

1. Fourier Transform in Signal Processing

The Fourier transform of a signal is given by:$f(t)$

$$F(\omega) = \int_{-\infty}^{\infty} f(t)e^{-i\omega t}dt$$

Or$F(\omega)$represents the frequency spectrum of the signal.

Example 1.1: In audio signal processing, the Fourier transform is used to decompose a complex sound into its constituent frequencies. For example, an audio file containing multiple musical instruments can be analyzed to determine which frequencies are present and their intensity. This is essential for applications such as audio mixing.

2. Vibration Analysis

For a mass system with an excitation force , the equation of motion can be written:$F(t)$

$$m\frac{d^2x}{dt^2} + c\frac{dx}{dt} + kx = F\ (t) \qquad (9)$$

By applying the Fourier transform, we obtain:

$$m\omega^2 X(\omega) - i\omega X(\omega) + kX(\omega) = F(\omega)$$

Example 2.1: In engineering, vibration analysis of a structure (such as a bridge) can be performed using Fourier series. By measuring the vibrations and applying the Fourier transform, engineers can identify the structure's natural frequencies and predict its behavior under dynamic loads.

3. Pattern recognition

The discrete Fourier transform (DFT) of an image is given by:$I(x,y)$

$$F(u,v) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} I(x,y)e^{-i(ux+vy)}\,dxdy$$

Or $F(u,v)$represents the frequency components of the image

Example 3.1: In image recognition, Fourier transform-based techniques can be used to identify patterns or shapes in images. For example, an algorithm can analyze an image to detect edges or contours by transforming the image into the frequency domain.

4. Modeling of dynamic systems

The differential equation of a harmonic oscillator is:

$$m\frac{d^2x}{dt^2} + kx = 0 \qquad (10)$$

By applying the Fourier transform, we obtain:

$$x(t) = A\cos(\omega t + \phi)\, o\grave{u}\ \omega = \sqrt{\frac{k}{m}}$$

Example 4.1: In the modeling of dynamic systems, differential equations can be solved using the Fourier transform. For example, a system of springs and masses can be analyzed to determine its oscillatory behavior by decomposing the applied forces into their frequency components.

5. Representations of molecular interactions

- **Force Matrices**: In molecular dynamics, the forces between atoms can be represented by a force matrix. Each element of this matrix describes the interaction between two atoms, making it easy to calculate the net forces on each atom.
- **Example 5.1**: For a system of three atoms, the force matrix can be defined as:F

$$F = \begin{pmatrix} F_{11} & F_{12} & F_{13} \\ F_{21} & F_{22} & F_{23} \\ F_{31} & F_{32} & F_{33} \end{pmatrix}$$

6. Modeling of potential energies

- **Hessian Matrices**: The Hessian matrix, which contains the second derivatives of potential energies with respect to atomic coordinates, is used to analyze the stability of molecular configurations. This matrix allows the determination of vibration modes and critical energy points.

  . Example 6.1: For a system with atoms, the Hessian matrix is:nH

$$H = \begin{pmatrix} \frac{\partial^2 E}{\eth x_1^2} & \frac{\partial^2 E}{\partial x_1 \partial x_2} & \cdots \\ \frac{\partial^2 E}{\partial x_2 \partial x_1} & \frac{\partial^2 E}{\eth x_1^2} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

7. Coupling Systems

- **Coupling of Vibrational Modes**: The vibrational modes of a molecule can be modeled by matrices that describe the coupling between the different modes. These matrices make it possible to study the complex interactions between vibrations.

  . Example7.1: The coupling matrix can be used to relate the amplitudes of the vibrational modes:C

$$C = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix}$$

8. Linear transformations in configuration space

- **Coordinate transformations**: Transformation matrices are used to perform rotations and translations of molecules in space. This is essential for simulating the movements of molecules during chemical reactions.

  -Example 8.1: A rotation in space can be represented by a rotation matrix:$3DR$

$$\boldsymbol{R} = \begin{pmatrix} \boldsymbol{\cos\theta} & \boldsymbol{-\sin\theta} & \boldsymbol{0} \\ \boldsymbol{\sin\theta} & \boldsymbol{\cos\theta} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{1} \end{pmatrix}$$

9. Solving systems of linear equations

- **Equations of motion**: The equations of motion for a system of molecules can be formulated as systems of linear equations, which can be solved using algebraic techniques. Matrices make it easier to manage these systems.

  - Example9.1: For a dynamical system, the equations can be written in matrix form:

$$M\ddot{x} = F$$

  where is the mass matrix, is the vector of accelerations, and is the vector of applied forces.$M\ \ddot{x}, F$

Matrices are powerful tools for modeling complex molecular systems, facilitating the analysis of interactions, dynamics, and properties of molecules. The use of matrices simplifies calculations and yields meaningful results in molecular dynamics studies.

Conclusion

The use of Fourier series and transforms in molecular dynamics offers fascinating and essential perspectives for understanding random phenomena at the molecular level. This article has highlighted how these mathematical tools allow the analysis of molecular motions and the interpretation of complex experimental data.

We have demonstrated that Fourier series can decompose random signals into their frequency components, thus facilitating the identification of dynamic behaviors of molecules. The ability of

these methods to address diverse phenomena, such as diffusion, system vibrations, and nonlinear response of materials, underlines their importance in diverse research fields, ranging from quantum chemistry to materials science.

In the future, it would be beneficial to further explore the implications of these techniques in practical applications, such as the design of new materials or the modeling of complex biological systems. Moreover, the increasing integration of artificial intelligence in data analysis could open new avenues to improve the accuracy and efficiency of methods based on Fourier series and transforms.

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