

# STOCHASTIC MODEL OF MOLECULAR DIFFUSION IN OPTICAL LATTICES

## MODELO ESTOCÁSTICO DE LA DIFUSIÓN DE MOLÉCULAS EN REDES ÓPTICAS

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The present study focuses in the investigation of the diffusion of polar molecules on the structures known as optical lattices (a periodic generalization of optical traps); and in the assessment of the influence of a time dependent electromagnetic field on the motion of molecule. To study this phenomenon, the particle is considered to move under the influence of a one-dimensional potential which reproduces the main characteristics of the optical lattice. Starting from the canonical representation of the electromagnetic field, it has been introduced an equivalence between this field and an ensemble of harmonic oscillators. This allows to derive an effective Langevin equation to describe the motion of the particle interacting with the bath oscillators. We analyze the influence, on the diffusion dynamics, of the parameters which determine the shape of the electromagnetic pulses, which constitutes a key ingredient for the design of optimal fields that enable an efficient control of molecular dynamics.

El presente estudio se centra en la investigación de la difusión de moléculas polares en las estructuras conocidas como redes ópticas, (una generalización periódica de las trampas ópticas), así, como la evaluación de la influencia de un campo electromagnético externo dependiente del tiempo sobre el movimiento de la molécula. Para el estudio de este fenómeno la molécula se considera sometida a un potencial unidimensional que reproduce las características esenciales de la red óptica. A partir de la forma canónica de las ecuaciones del campo electromagnético, se introduce una equivalencia entre el campo externo y un conjunto de osciladores armónicos. Esta equivalencia permitió derivar una ecuación de Langevin efectiva para describir el movimiento de la molécula en interacción con el baño de osciladores. Se analiza la influencia, sobre la dinámica de difusión, de la variación los parámetros que determinan la forma de los pulsos electromagnéticos, lo que constituye un ingrediente importante para el diseño de campos óptimos que permitan controlar de forma eficiente la dinámica molecular.

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### I. INTRODUCTION

Optical lattices are formed as a result of the interference of two laser beams that propagate in opposite directions, creating a steady pattern that repeats periodically in space. The spatial modulation of the electromagnetic field allows to trap atoms and neutral molecules within the region occupied by the optical lattice. The particles are concentrated in the vicinity of the potential minima, therefore the lattice can be considered as a periodic arrangement of micro traps. In this sense, these networks constitute the natural generalization of optical traps, which played a major role in the observation in 1995, for the first time, of the state of matter known as Bose-Einstein condensate [1].

Analogous to optical traps, lattices allow the study of atoms and molecules isolated from the environment at ultra low temperatures (of the order of micro- or nano-Kelvin) [2]. On the other hand, optical lattices provide the additional possibility to investigate the behavior of condensed-phase correlated systems [3], with potential applications in the development of quantum information, atomic transistors, analysis of dissipation mechanisms, etc. The problems that appear in the study of atoms and molecules in optical lattices

present a formal analogy with the dynamics of electrons in the periodic potential of a crystal, even though the values of the characteristic magnitudes are not the same (the spatial period of the network is of the same order as the wavelength of the laser from which it originates, about 1000 or 10000 times larger than in crystalline solids).

The most important parameters that characterize an optical lattice are the depth of the potential wells and the spatial periodicity. The well depth of an optical lattice can be adjusted in real time by changing the power of the laser. The periodicity can also be modified by varying the wavelength of the laser or by changing the relative angle between the two rays. This flexibility is one of more attractive properties of this type of systems, since atoms and molecules confined in an optical lattice can be used to study many-body effects that are difficult to observe directly in real crystals.

One of the key strategies to study the motion of the trapped particles is to act on them an additional time-dependent electromagnetic field whose intensity is much lower than that of the beams building up the network. The detailed knowledge of the characteristics of the diffusion of atomic and molecular species through is for the design of the experiments to be carried out in optical lattice, since these

displacements can facilitate or hinder the occurrence of certain phenomenon.

The purpose of this paper is to present an alternative treatment for the theoretical description of the motion of a particle in a one-dimensional potential resembling an optical lattice and under the influence of a weak, additional electromagnetic field. The methodology is based on the equivalence between the external field and a set of uncoupled one-dimensional harmonic oscillators, described in Section II. In Section III, we present the derivation of the Langevin equation and numerical examples that illustrate the validity of neglecting memory effects in the calculation of dissipative forces. In section IV the main conclusions of this work are presented.

## II. HAMILTONIAN OF THE SYSTEM

### II.1. System

The system consists in a neutral particle of mass  $m$  and dipole moment  $\vec{d}$ , which moves along the X axis under the influence of a periodic potential  $V(x) = V(x + L)$ , where  $L$  is the period of the lattice.

### II.2. Equivalence between the electromagnetic field and a set of harmonic oscillators

Using the Landau gauge [4] for the vector and the scalar potentials, the set of Maxwell equations in the vacuum (i.e., in a region free of charges and currents) can be written as follows

$$\nabla^2 \vec{A} - \frac{1}{c^2} \frac{\partial^2 \vec{A}}{\partial t^2} = 0. \quad (1)$$

The decomposition of space in a three dimensional array of cubes of lengths  $L_x, L_y, L_z$  leads to the following condition for the vector potential:  $\vec{A}$

$$\vec{A}(x, y, z) = \vec{A}(x + L_x, y + L_y, z + L_z). \quad (2)$$

Hence the solution of the wave equation (2) can be represented as:

$$\vec{A}(\vec{r}, t) = \sum_j \vec{q}_j(t) \exp(ik_j \cdot \vec{r}). \quad (3)$$

The following equation

$$\ddot{\vec{q}}_j(\vec{k}, t) + \omega_j^2 \vec{q}_j(\vec{k}, t) = 0. \quad (4)$$

To determine the vector potential at a given point in space and at a given time it is necessary to know the set of amplitudes  $\vec{q}_j(t)$ . Therefore, the state of the field is characterized by the infinite set of solutions  $\vec{q}_j(t)$  of the ordinary differential equation (4), which coincides with the equation of motion of a linear harmonic oscillator. In this way, the electromagnetic field can be formally replaced by a mechanical system comprising a set of infinite uncoupled oscillators.

### II.3. Molecule-field interaction

The original problem of a particle moving under the influence of a periodic potential and an external time-dependent electromagnetic field has been mapped (through the correspondence described above) into the equivalent problem of a particle subjected to periodic potential and interacting, at the same time, with an infinite numberable set of harmonic oscillators. The coupling between the molecule and the time-dependent field is termed  $H_{sb}$ , in analogy to the system bath interaction within the dipole approximation, it reads.

$$H_{sb} = -\vec{d} \cdot \vec{E}(t). \quad (5)$$

Assuming the electric field is linearly polarized, it can be rewritten as

$$H_{sb} = 2d \sum_j \left[ \omega_j \text{Im} \left\{ A_j \exp(ik_j x) \right\} \right], \quad (6)$$

where  $d = \vec{d} \cdot \hat{e}$  and  $\hat{e}$  is the polarization vector. Hereafter, we make use of the one-dimensional character of the problem and we employ scalar quantities only. Expressing eq. (6) in terms of the generalized coordinates  $q_j$  and momenta  $\pi_j$  of the field oscillators. The following expression for the interaction term

$$H_{sb} = d \sum_j \left[ \left( \omega_j \sqrt{\varepsilon_0 L} \sin(k_j x) \right) q_j + \left( \sqrt{\frac{1}{\varepsilon_0 L}} \cos(k_j x) \right) \pi_j \right]. \quad (7)$$

It can be casted in the form

$$H_{sb} = \sum_j (\alpha_j q_j + \beta_j \pi_j), \quad (8)$$

Which obvious definitions for the function  $\alpha(x)$  and  $\beta(x)$ . Eq (8) represent a special type of (non-linear) system-bath interaction, where the particle coordinate is coupled to both position and momenta of the bath modes.

## III. DERIVATION OF THE LANGEVIN EQUATION

The total Hamiltonian of the system [5] is

$$H = \frac{p^2}{2m} + V(x) + \frac{1}{2} \sum_j (\pi_j^2 + \omega_j^2 q_j^2) + H_{sb} + \frac{1}{2} \sum_j \left( \beta_j^2 + \frac{\alpha_j^2}{\omega_j^2} \right). \quad (9)$$

It consists of the standard contributions: the energy of the system and the bath, the system-bath coupling and the counter-term ensuring  $V(x)$  remains the bare potential Hamilton's canonical equations can be combined to yield the following equations of motion for the bath oscillators and for the position of the particle

$$\ddot{q}_j + \omega_j^2 q_j = \beta_j' \dot{x} - \alpha_j, \quad m\ddot{x} + \frac{dV}{dx} = - \sum_j (\alpha_j' q_j + \beta_j' \pi_j). \quad (10)$$

The integration of the equations of motion corresponding to the coordinates  $q_j$  can be carried out analytically using Green's method [6]. Substituting the functions  $q_j(t)$  in

Newton's second law for variable  $x$  yields Langevin equation that describes the motion of the particle

$$m\ddot{x} + \frac{dV}{dx} + \int K(t-t')\dot{x}(t')dt' = f(t). \quad (11)$$

The dissipation kernel  $K(t-t')$  is calculated using the expression

$$K(t-t') = \sum_j \left( \frac{\beta'_j}{\omega_j} \sin[\omega_j(t-t')] - \frac{\alpha'_j}{\omega_j^2} \cos[\omega_j(t-t')] \right). \quad (12)$$

Although eq. (11) is deterministic second order differential equation, if the spectrum of the electric field  $\vec{E}(t)$  is centered at high frequencies, the force

$$f(t) = \sum \cos(\omega_j t) \left[ \frac{\alpha_j \alpha'_j}{\omega_j^2} + \alpha'_j q_{j0} + \pi_{j0} \beta'_j \right] + \sum \sin(\omega_j t) \left[ \frac{\alpha'_j \pi_{jp}}{\omega_j} - \omega_j q_{j0} \beta'_j - \frac{\alpha_j \beta'_j}{\omega_j} \right] - \sum \left( \frac{\alpha'_j \alpha_j}{\omega_j^2} + \beta_j \beta'_j \right). \quad (13)$$

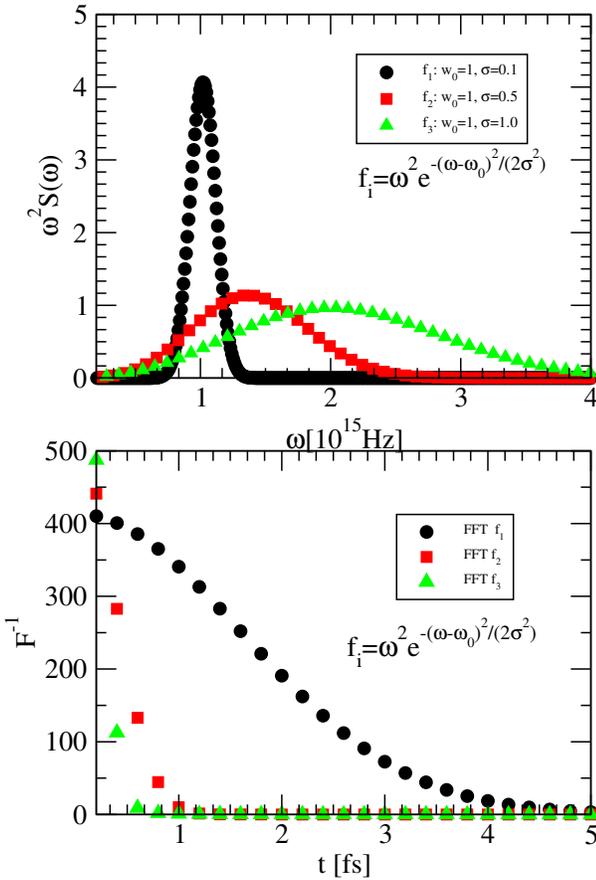


Figure 1. Top panel: Weights  $f_i(\omega)$  of bath oscillators for different widths of a Gaussian laser pulse. Bottom panel: Inverse Fast Fourier transform  $F^{-1}$  of the functions  $f_i(\omega)$ .

Can be regarded as a stochastic fluctuation after some algebra, and introducing the change of variable  $t-t' = \tau$ ,

the generalized Langevin equation can be finally written as

$$m\ddot{x} + \frac{dV}{dx} + f(t) + \pi \frac{d^2}{c^2 \epsilon_0 L} \int_0^t K(\tau) \dot{x}(t-\tau) d\tau = 0. \quad (14)$$

If we introduce the spectral density  $S(\omega) = \sum_j \delta(\omega - \omega_j)$ , it can be shown that the dissipation kernel  $K(\tau)$  can be computed as the inverse Fourier transform of the even prolongation of the function  $\omega^2 S(\omega)$ . In Figs. 1 and 2, we plot the functions  $\omega^2 S(\omega)$  and the behavior of the corresponding kernels  $K(\tau)$  for a Gaussian wavepackets  $S(\omega) = e^{-(\omega-\omega_0)^2/2\sigma^2}$  widths  $\sigma$  (Fig. 1) and centered at different frequencies  $\omega_0$  (Fig. 2).

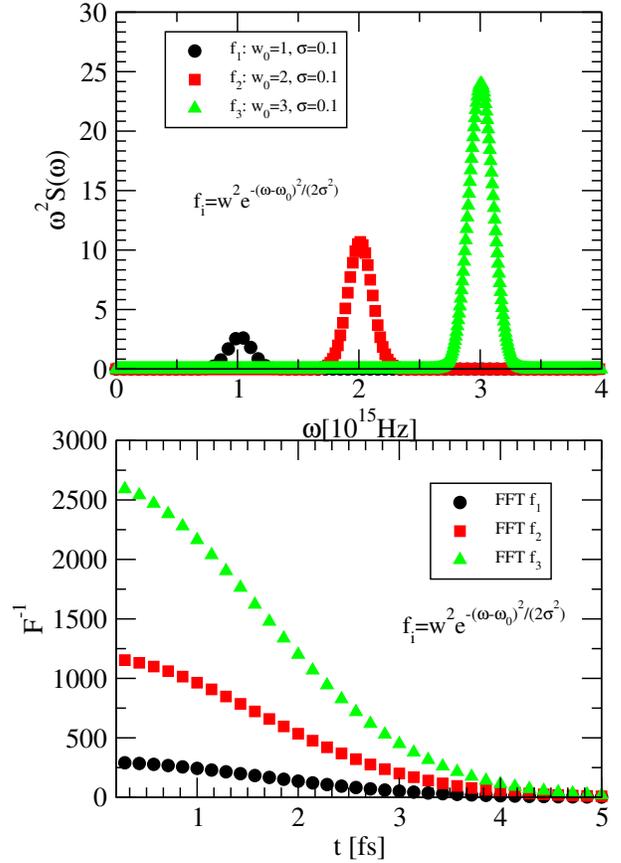


Figure 2. Top panel: Weights  $f_i(\omega)$  of bath oscillators for different central frequencies of a Gaussian laser pulse. Bottom panel: Inverse Fast Fourier transform  $F^{-1}$  of the functions  $f_i(\omega)$ .

All the cases considered correspond to rapidly decaying kernels, so the particle velocity can be regarded as constant during the typical oscillation period of the field modes. Therefore the standard (Markovian) Langevin equation [7].

$$m\ddot{x} + \frac{dV}{dx} + f(t) + \dot{x}(t) \pi \frac{d^2}{c^2 \epsilon_0 L} \int_0^t K(\tau) d\tau = 0, \quad (15)$$

represents a suitable approximation for the investigation of the diffusion of polar molecules on optical lattices under the conditions considered in this work.

#### IV. CONCLUSIONS

We present an effective Langevin equation to be used to study the motion of a polar molecule under the influence of a periodic potential and a time-dependent electromagnetic field. The equation was derived using the equivalence between the transient electromagnetic field and a set of harmonic oscillators.

Although the effective Langevin equation resembles the standard treatment of system-bath dynamics, it presents some distinct features. The molecule couple, both the coordinates and the moment of the bath oscillators. Likewise the spectral density  $S(\omega)$  contains information about the the normal modes of the distribution of field whereas the intensity of the coupling is given by the product  $\omega^2 S(\omega)$ .

From the molecular displacements, the exponent was determined that characterizes the speed of the diffusion process, being that this corresponds to the superdiffusive regime. It has been investigate the temporal evolution of the distribution of molecules on the surface. Calculations on the time evolution of the density distribution of different molecular species on the lattice, the characterization of the diffusion regime and its dependence on the characteristics of the external electromagnetic field are currently underway.

Taking into account the relative simplicity of the modeling of the effects of the interaction between a system and a thermal bath (composed of a very large number of harmonic oscillators), with respect to the theoretical treatment of the field molecule coupling subsystems. The methodology introduced in this work paves the way for a quantum study of the diffusion of neutral molecules in optical lattices using the theory of open quantum systems.

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