



Production of Phonon Schrödinger Cat States in Benzoid Rings

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Resumen

Schrödinger cat states have been produced in trapped ions [1], cavity quantum electrodynamics, SQUIDS and more recently Bose-Einstein condensates [2]. These states are generally fragile and the observation of the process by which they lose coherence has allowed the study of the quantum-classical border. We propose a physical system in which Schrödinger cat states for phonons might be produced. We consider two identical benzoid rings coupled through a phononic mode and assume one electron molecular orbital per ring, with identical energy in absence of the phonon coupling. If one electron occupies one of the molecular states at some initial time, for example $t_0 = 0$, at which time there are no phonons, by measuring the electron at appropriate times the phononic mode is prepared in a cat state.

Palabras Clave: Schrödinger cat states, phonons, electron dynamics.

Abstract

En sistema tan diversos como iones atrapados [1], electrodinámica cuántica de cavidades, SQUIDS y más recientemente condensados de Bose-Einstein [2] se han producido estados de gato de Schrödinger. Estos estados son generalmente frágiles y la observación de los procesos por los cuales pierden coherencia ha permitido el estudio del límite clásico-cuántico. Proponemos un sistema físico en el cual podemos producir estados de gato de Schrödinger por fonones. Consideramos dos anillos benzoidales acoplados por medio de un modo fonónico y asumimos un orbital molecular electrónico por anillo, con la misma energía en ausencia del acoplamiento fonónico. Si un electrón ocupa uno de los estados moleculares en un tiempo inicial, digamos $t_0 = 0$, tiempo en el cual no hay fonones, midiendo el electrón en tiempos apropiados el modo fonónico queda preparado en un estado de gato.

Keywords: Estados de gato de Schrödinger, fonones, dinámica electrónica.

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1. Introduction

The search for electronic devices at nanometer scale has been a major goal of nanoelectronics. Molecular wires, produced assembling molecules, are expected to be the fundamental building blocks of a new generation of devices. Nature offers DNA, up to now the best nanometric molecular wire, which consists of two Watson-Crick base pair structures known as Adenine-Thymine

–coupled by two hydrogen bonds and shown in Figure 1– and Guanine-Cytosine, coupled by three hydrogen bonds. DNA possesses an important “self-assembly” property that is increasingly becoming recognized as a route to nanotechnology. Recent experimental results demonstrate the potential for using DNA to create self-assembling periodic nanostructures [3,4]. Other kinds of molecular wires that have been developed are carbon nanotubes, silicon nanotubes, boron nitride nanotubes

and others in which benzoid rings play an important role. These rings are molecules of experimental interest as molecular wires and their study involves the use of quantum mechanics to explain their electronic, optic, dynamic or thermal behavior.

On the other hand, Schrödinger's paper on *the current situation of quantum mechanics*, published in 1935[5], proposes a Gedankenexperiment to prepare superpositions of dead and alive cats, which highlights that the vast majority of states allowed by quantum mechanics are not observed in our macroscopic world. Years later coherent states were proposed as experimental feasible counterparts of the dead and alive states. In 1996 a team demonstrated the experimental realization of a quantum superposition of coherent states and its decoherence process [6], and in 2007 the Wigner function of a Schrödinger cat state was measured [7]. These states are very sensitive to decoherence, and as a result their preparation is challenging. We will demonstrate that in an experimental setup consisting of two benzoid rings in a coaxial arrangement, coupled through a phononic mode, and isolated from other sources of interaction, phonon Schrödinger cat states can be produced under certain conditions.

2. Mathematical Model

We consider a single electronic state per ring and the interaction with the torsional mode phonons. The overlap between these localized electronic states is assumed to be negligible. The Hamiltonian that describes this system is as follows:

$$\hat{H} = \varepsilon(\hat{c}_1^\dagger \hat{c}_1 + \hat{c}_2^\dagger \hat{c}_2) + \hbar\lambda(\hat{a}^\dagger + \hat{a})(\hat{c}_1^\dagger \hat{c}_2 + \hat{c}_2^\dagger \hat{c}_1) + \hbar\omega\hat{a}^\dagger \hat{a} \quad (1)$$

Here ε is the electron energy for the two states, assumed to be independent the same due to symmetry arguments. The values of λ , the electron-phonon coupling constant, are of the order of a tenth of meV lower than the phonon frequency ω , which is of the order of a hundred of meV. The symbols \hat{c}_i^\dagger and \hat{c}_i , ($i = 1, 2$) represent the creation and annihilation operators of electrons in the two states which satisfy the usual fermion anticommutation relations. The symbols \hat{a}^\dagger and \hat{a} , which stand for the creation and annihilation operators of phonons, satisfy the usual boson commutation relations.

Using a standard basis, the electronic identity operator is given by

$$\hat{I}_{1e} = |00\rangle\langle 00| + |01\rangle\langle 01| + |10\rangle\langle 10| + |11\rangle\langle 11|.$$

Taking into account that we are working in the independent electron approximation and we always have one electron, we rewrite the electronic identity operator as $\hat{I}_{1e} = |01\rangle\langle 01| + |10\rangle\langle 10|$. The Hamiltonian of our system in this subspace is given by

$$\begin{aligned} \hat{H}' &= (\varepsilon\hat{I}_{1e} + \hbar\omega\hat{a}^\dagger \hat{a}) + (\hbar\lambda(\hat{a}^\dagger + \hat{a})\sigma_x) \\ &= \hat{H}_0 + \hat{H}_1 \end{aligned} \quad (2)$$

where $\sigma_x = |10\rangle\langle 01| + |01\rangle\langle 10|$, \hat{H}_0 is the unperturbed hamiltonian and \hat{H}_1 is the interaction hamiltonian between phonons and electrons. In order to study the dynamics, we solve the Schrödinger equation for the time evolution operator

$$i\hbar \frac{\partial \hat{U}}{\partial t} = (\hat{H}_0 + \hat{H}_1)\hat{U}. \quad (3)$$

Using the Ansatz $\hat{U} = XY$, we obtain the following differential equations for X and Y

$$\frac{\partial X}{\partial t} = \frac{1}{i\hbar} \hat{H}_0 X \quad (4)$$

$$\frac{\partial Y}{\partial t} = \frac{1}{i\hbar} [e^{\frac{i\hat{H}_0 t}{\hbar}} (\hbar\lambda(\hat{a}^\dagger + \hat{a})\sigma_x) e^{-\frac{i\hat{H}_0 t}{\hbar}}] Y. \quad (5)$$

Solving (4) and (5) it is possible to obtain the time evolution operator that describes the dynamics of the electron-phonon system as follows

$$\hat{U}(t) = e^{-\frac{i\varepsilon\hat{I}_{1e}t}{\hbar}} e^{-i\omega t \hat{a}^\dagger \hat{a}} \hat{D}(\alpha) e^{-i\frac{\lambda^2}{\omega} \hat{I}_{1e}t} e^{-i\frac{\lambda^2}{\omega^2} \sigma_x^2 \sin(\omega t)} \quad (6)$$

where

$$\hat{D}(\alpha) = e^{-\frac{\lambda}{\omega} \sigma_x (e^{i\omega t} - 1) \hat{a}^\dagger + \frac{\lambda}{\omega} \sigma_x (e^{-i\omega t} - 1) \hat{a}}. \quad (7)$$

is a straightforward generalization of the displacement operator. If $|\psi(t_0 = 0)\rangle = |10\rangle \otimes |0\rangle$ describes the state of our system at the initial time $t = 0$, which corresponds to the electron in one of the two electronic states and zero phonons, $|\psi(t)\rangle = U(t, 0)|\psi(0)\rangle$ is the state at a later time.

Since the generalized displacement operator $\hat{D}(\alpha)$ contains the σ_x operator it is convenient to express the initial state in terms of its eigenvectors $|\pm x\rangle$. When the generalized displacement operator acts over a product state of an eigenvector of σ_x and the phonon vacuum state, it produces phonon coherent states

$$\begin{aligned} \hat{U}(t)|\pm x, 0\rangle &= \\ e^{-\frac{i\varepsilon\hat{I}_{1e}t}{\hbar}} e^{-i\omega t \hat{a}^\dagger \hat{a}} \hat{D}(\alpha) e^{-i\frac{\lambda^2}{\omega} \hat{I}_{1e}t} e^{-i\frac{\lambda^2}{\omega^2} \sigma_x^2 \sin(\omega t)} |\pm x, 0\rangle &= \\ = e^{if} |\pm x, \pm \frac{\lambda}{\omega} (e^{-i\omega t} - 1)\rangle, \end{aligned} \quad (8)$$

whose average values of position and momentum depend on the electron state. We can return to the original basis by

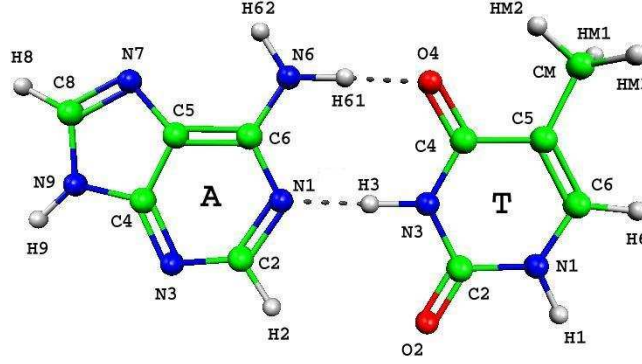


Figura 1. Base pairs Adenine-Thymine (AT) in the structure they acquire in B-DNA, the so-called Watson-Crick base pair structure.

$$\begin{pmatrix} | + x \rangle \\ | - x \rangle \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} |10 \rangle \\ |01 \rangle \end{pmatrix}. \quad (9)$$

We obtain for state of the system the expression

$$\begin{aligned} |\psi(t)\rangle &= \frac{e^{if}}{\sqrt{2}} [|10, \alpha\rangle + |10, -\alpha\rangle] \\ &+ \frac{e^{if}}{\sqrt{2}} [|01, \alpha\rangle - |01, -\alpha\rangle] \end{aligned} \quad (10)$$

where $f = -\frac{\epsilon t}{\hbar} - \frac{\lambda^2}{\omega} t + \frac{\lambda^2}{\omega^2} \sin \omega t$ and $\alpha = -\frac{\lambda}{\omega}(e^{-i\omega t} - 1)$ is a parameter that depends on the system dynamics. This is a highly entangled state involving superposition of two coherent states and the ring electronic states.

If one measures the electron on the basis of the localized electronic states, and finds it for example in the state $|10\rangle$ the phononic mode is prepared in a cat state as can be seen from the expression of the state of the total system

$$\begin{aligned} |\psi(t)\rangle &= N(t) \frac{e^{if}}{\sqrt{2}} |10\rangle \otimes \\ &\left(\left| \frac{\lambda}{\omega}(e^{-i\omega t} - 1) \right\rangle + \left| -\frac{\lambda}{\omega}(e^{-i\omega t} - 1) \right\rangle \right), \end{aligned} \quad (11)$$

where $N(t)$ is a normalization constant.

3. Conclusions

We have shown that, if the system is initially in a factorized state, where the electron happens to be in one of

the localized states and no phonons are present, the dynamics produces cat states if, at a later time a measurement of the state of the electron is made. The maximum value of the distance, in phase space, between the coherent states composing the cat state is $4\lambda/\omega$ and occurs at $t = (2n + 1)\pi/\omega$. In a more realistic experimental setup, it is necessary to include a model for the contacts, which, unavoidably, introduces decoherence effects.

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