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Letter

On the dynamics of confined particles: a laser test

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Abstract
Reduced dimensionality systems (RDS) are materials extending along one or two dimensions much more than the other(s). The degrees of freedom of the small dimension are not explored by the electrons since their energy is very large. The time dependent wave function of a particle in a short nanotube, taken as a paradigm of the RDS family, is calculated by solving the Klein–Gordon equation; the confining condition produces a small change in the mass of the particles and of the energy levels. These changes are of relativistic origin and therefore small, but can be measured by use of a weak resonant laser field which produces cumulative effects in the time development of the wave function. The shift of the energy of the levels are within today's spectroscopy capacity.

Keywords: reduced dimensionality systems, strong fields

(Some figures may appear in colour only in the online journal)

1. Introduction

Modern techniques permit the fabrication of new materials endowed of properties that, as yet, are not fully explored. Here we like to mention quantum rings and those carbon allotropes such as fullerene, graphene, nanotubes, which display astounding geometry and symmetry.

Quantum rings are slender, annular structures that can be fabricated with predetermined radius and thickness [1]. Fullerene or, more properly, C_{60}, is formed by 60 carbon atoms located at the corner of hexagons and pentagons and closely resembles a soccer ball. Graphene is a monoatomic layer of carbon atoms arranged in a honeycomb-like pattern and paving a large surface; it is the thinnest known material and, probably, will retain such a record for it does not appear at the horizon the possibility of making material layers thinner than the atom; graphene's C_6 symmetry gives to electrons the dispersion relation of massless Dirac particles, feature that can be used to test relativistic behaviour without use of huge accelerators [2–4]; the unit hexagonal cell may be seen as a small ring-like structure. Nanotubes are strips of graphene rolled in single or double walled cylindrical tubes of radius and length predetermined almost at will; the ratio between length and radius spans several orders of magnitude [5]; here again a short tube is basically a quantum ring.

The list of applications of these molecules is everyday growing; thus fullerene's cage can be used for in situ drug delivery and graphene fragments provide the plates for measuring Casimir forces [6–8]. Very recently, laser driven carbon allotropes have been shown to be good emitters of harmonics of the fundamental laser frequency [9–21]. Moreover rings appear to provide the base for designing and implementing fast operating logic circuits [22–24]. Today the possibility of controlling the yield and the polarization of the electromagnetic radiation is required; several schemes have been proposed to achieve this goal by using the possibilities offered by high order harmonic generation in atoms and molecules [25, 26]; rings can be designed almost at will and may open a road toward the control of the polarization of the emission [27].

The above quoted structures, having an extension along one or two dimensions much larger than the other(s), can be treated as reduced dimensionality systems (RDS). In fact the degree of freedom pertaining to the dynamics along the small dimensions are characterized by large energy separation between their eigenstates and are essentially frozen unless large temperature is reached or large energy is provided to the system. When dealing with RDS, to disregard from the treatment the frozen degree of freedom is often a safe procedure. In this way, by judicious exploitation of the symmetries of the systems, to simplify the analysis and to obtain appealing analytical expressions is possible [28]. One of the motivations of this letter is the exam of the consequences of the reduced dimensionality condition.

By applying a weakly relativistic analysis to RDS and in particular to a short quantum tube, in this letter we show that the mere existence of the small – and frozen – degree of freedom affects the electron (*rest*) mass and the energy of the quantum levels for a very tiny but measurable amount. We propose to probe such small effects by use of a weak and resonant laser field. If the duration of the driving pulse is long, cumulative effects in the evolution of the wave function of the electron result in modifications of the dynamics which are, at least in principle, measurable.

2. Theory

To carry out the analysis, we consider one electron bound on a cylindrical surface with axis along z; the radius and the length of the cylinder are respectively R and s and we suppose that $s \ll R$, therefore the longitudinal eigenstates pertaining to the z degree of freedom are very separated in energy. To start the discussion, to consider one bound electron with weakly relativistic energy is convenient.

From the dispersion relation $E^2 = \boldsymbol{p}^2 c^2 + m^2 c^4$, with the usual substitutions $E \to \mathrm{i}\hbar\partial_t$ and $\boldsymbol{p} \to -\mathrm{i}\hbar\boldsymbol{\nabla}$, the Klein–Gordon equation is arrived at:

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2\right)\Psi(\boldsymbol{r}, t) = -\mu^2\Psi(\boldsymbol{r}, t) \tag{1}$$

with

$$\mu^2 = \frac{m^2c^2}{\hbar^2}, \tag{2}$$

m the mass and $\Psi(\boldsymbol{r}, t)$ the wave function of the electron. In cylindrical coordinates and with $r = R$ the Klein–Gordon equation becomes

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{1}{R^2}\frac{\partial^2}{\partial\varphi^2} - \frac{\partial^2}{\partial z^2}\right)\Psi(\varphi, t) = -\mu^2\Psi(\varphi, t) \tag{3}$$

which can be solved by separating the variables: $\Psi(\boldsymbol{r}, t) = Y(\varphi, t)Z(z)$. The boundary condition $Z(0) = Z(s) = 0$ gives

$$Z_N(z) = A\sin\left(\frac{N\pi}{s}z\right), \quad N = 1, 2\ldots \tag{4}$$

with A the irrelevant normalization constant; the integer N counts the excitation quanta pertaining to the z degree of freedom. By substituting (4) into (3), the Klein–Gordon equation is reduced to

$$\left(\frac{1}{c^2}\frac{\mathrm{d}^2}{\mathrm{d}t^2} - \frac{1}{R^2}\frac{\mathrm{d}^2}{\mathrm{d}\varphi^2}\right)Y_N(\varphi, t) = -\mu_N^2 Y_N, \quad \mu_N^2 = \mu^2 + \left(\frac{N\pi}{s}\right)^2. \tag{5}$$

This expression tells us that the longitudinal degree of freedom can be disregarded from the dynamics provided the substitution $\mu \to \mu_N$. The particle in the ring appears now to have a new mass

$$m_N = m\sqrt{1 + \frac{\pi^2\hbar^2}{m^2c^2}\frac{N^2}{s^2}} \tag{6}$$

and N becomes a hidden variable from the point of view of the transverse space. If we want to read this formula by going much beyond the restricted scope of this letter, we may assert that in a reduced dimensionality world no particle can be massless. At the moment only photons are known to be surely massless elementary particles while gluons and gravitons are still in the foggy realm of hypothesis. The existence of massive photons has been discussed since many years [29] and it would invalidate the expression of Coulomb law; maybe the r^{-2} Coulomb force is a hint that the world is 4 dimensional.

If, as it should be, the correction to the mass is small, we can deduce a first order approximation to the electron mass for a quick estimation:

$$m_N \cong m\left(1 + \frac{\pi^2\hbar^2}{2m^2c^2}\frac{N^2}{s^2}\right). \tag{7}$$

The motion of the electron over a cylindrical surface is now reduced to a rotation along the circle. The standard energy levels of one electron in a ring

$$\hbar\omega_n = \frac{\hbar^2 n^2}{2mR^2}, \quad n = 0, \pm 1, \pm 2\ldots \tag{8}$$

now appear shifted to the new values (with two subscripts separated by a semicolon)

$$\hbar\omega_{N;n} = \frac{\hbar^2 n^2}{2m_N R^2} = \frac{\hbar\omega_n}{\sqrt{1 + \frac{\pi^2\hbar^2}{m^2c^2}\frac{N^2}{s^2}}} \tag{9}$$

or, at first order of approximation:

$$\hbar\omega_{N;n} \cong \hbar\omega_n\left(1 - \frac{\pi^2\hbar^2}{2m^2c^2}\frac{N^2}{s^2}\right) = \hbar\omega_n\left(1 - 2.6\cdot 10^{-4}\frac{N^2}{(s/a_0)^2}\right) \tag{10}$$

with a_0 the Bohr radius and $\hbar n$ the orbital angular momentum. The energy of the eigenstates is modified by a quantity which is independent from the radius of the ring and depends only upon the length of the tube s and the excitation number N of the longitudinal modes, or more precisely, from their ratio.

Unfortunately the physical parameters enter the expression in parenthesis of equation (10) in such a way to make the assembly of a device for the experimental determination of the corrections difficult; in fact, a large energy shift of the levels would require a high degree of longitudinal excitation and/or a very thin cylinder so that $Na_0/s \gg 1$; nevertheless ratios $\Delta\omega/\omega \approx 10^{-6}$ are within the possibility of modern spectroscopy and leave margin for experiments. Thus, if we set $R = 5a_0$ for the radius of the quantum ring, the energy

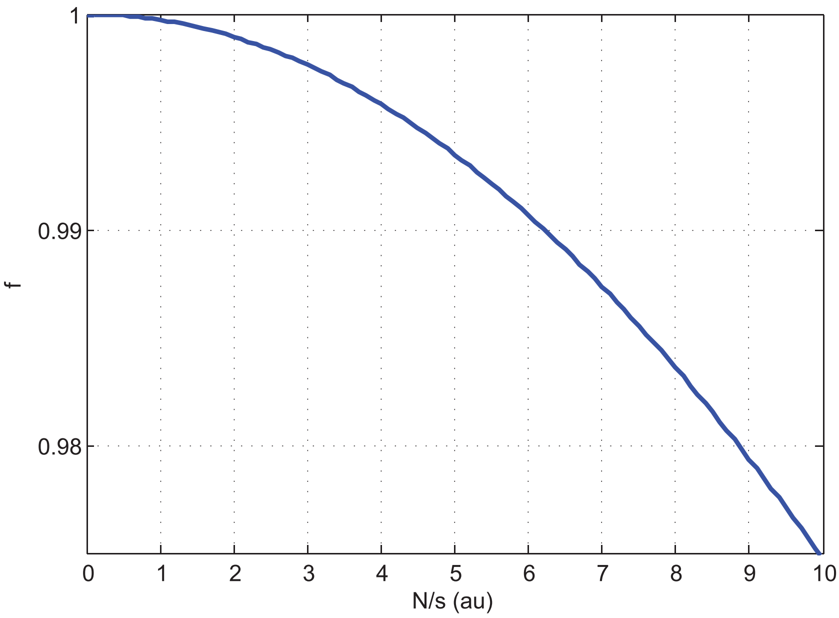

Figure 1. Plot of the factor $f = \left(\sqrt{1+\frac{\pi^2\hbar^2}{m^2c^2}\frac{N^2}{s^2}}\right)^{-1}$ versus N/s in au.

difference between the two lowest levels is in the infrared range ($\Delta\omega = 0.54$ eV). The Raman radiation emitted by the ring at different longitudinal excitation states, i.e. with different value of N, can be used to measure $\omega_{N;n}$ versus N. In this case the strong quadratic dependence of the energy upon N is a favourable condition. A microcromator with a 1 m of focal length, a 1000 lines per mm grating and a long optical path should have the required precision. In figure 1 the factor $f = \left(\sqrt{1+\frac{\pi^2\hbar^2}{m^2c^2}\frac{N^2}{s^2}}\right)^{-1}$ is plotted versus N/s.

We must add that our theoretical method of confining the longitudinal modes with a wall is used only for mathematical simplicity. Of course any efficient confining potential for the electron would work and a discussion can be found in [30]. We think that the short tube might be sandwiched between two strata of an opportune material which allows the excitation of longitudinal modes by irradiation with electromagnetic fields. As a final comment, small relativistic corrections to the hydrogen energy spectrum were discussed Sommerfeld as far as 1916 and experimentally detected [31, 32].

3. The laser

Large modifications on the wave function of electrons in atoms and molecules are effectively induced by the presence of a laser field of frequency ω_L resonant with a molecular transition. The effect that we propose to observe with a laser is small and can be better seen by producing a slow and cumulative change in the time evolution of the electron wave function. At resonance, even a weak field is efficient and ensures stability to the operation of the lasing device for many optical cycles, favourable condition for observing the wanted cumulative effects.

Let $\boldsymbol{\mathcal{E}} = \epsilon_x \mathcal{E}_0 f(t)\sin\omega_L t$ be the electric field of the laser taken in dipole approximation and linearly polarized along the x axis; $f(t)$ describes the pulse envelope. Hereafter we take $\omega_L = \omega_1$, that it to say, we consider always a nominal exact one-photon resonance between the ground and first excited state of the ring. Accordingly to our theory, the energy of the eigenstates is slightly shifted, and therefore a very small detuning is present.

Now, the electron is a bound over a circle of radius R, and the Hamiltonian of the laser-ring interaction is

$$\hat{H} = \frac{\hbar^2}{2m_N R^2}\hat{\ell}_z^2 + \hbar\,\Omega f(t)\cos\varphi\sin(\omega_L t). \tag{11}$$

with $\hbar\,\Omega \equiv e\mathcal{E}_0 R$. Here $\hbar\hat{\ell}_z$ is the z component of the angular momentum operator whose eigenstates $\hat{\ell}_z|n\rangle = n|n\rangle$ are:

$$|n\rangle \to \frac{\mathrm{e}^{\mathrm{i}n\varphi}}{\sqrt{2\pi}} \tag{12}$$

and can be used to expand the time dependent solution of the Schroedinger equation (TDSE): $\mathrm{i}\hbar\partial_t|\psi\rangle = \hat{H}|\psi\rangle$:

$$|\psi\rangle = \sum_{k,-\infty}^{\infty} a_{N;k}(t)|k\rangle. \tag{13}$$

Substitution of (13) into the TDSE and projection into the generic state $\langle n|$ gives

$$i\dot{a}_{N;n} = \omega_{N;n}a_{N;n} + \Omega f(t)\sum_{m,-\infty}^{\infty}\langle n|\cos\phi|m\rangle\sin(\omega_L t)a_{N;m}; \tag{14}$$

by using the relation $\langle n|\cos\phi|m\rangle = (\delta_{m,n-1}+\delta_{m,n+1})/2$ the ladder of coupled differential equations:

$$\begin{cases} i\dot{a}_{N;n} = \omega_{N;n}a_{N;n} + \dfrac{\Omega}{2}f(t)\sin(\omega_L t)[a_{N;n-1}+a_{N;n+1}] \\ \dot{a}_{N;|n|>M} = 0 \\ a_{N;n}(t=0) = \delta_{n0} \end{cases} \tag{15}$$

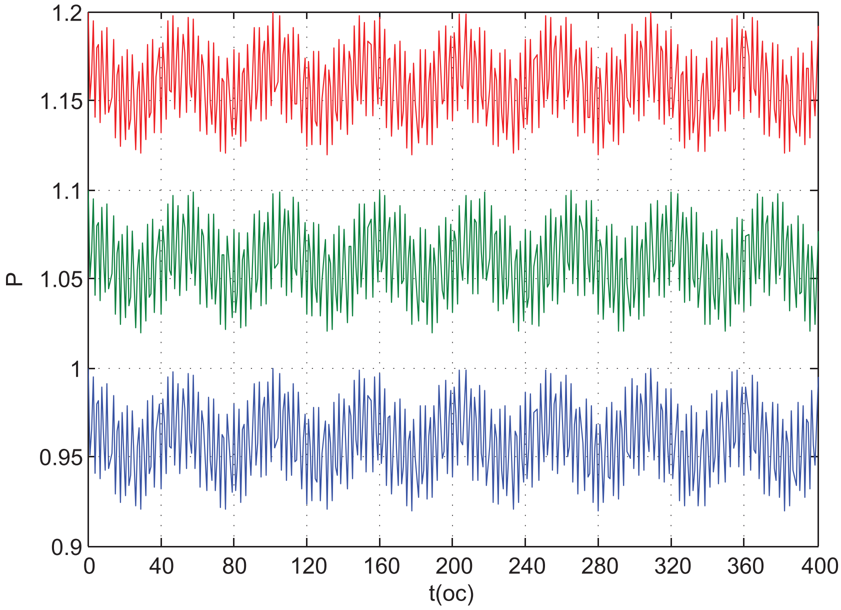

Figure 2. Population of the ground state of the laser driven quantum tube for different lengths of the tube as a function of time (in oc). The lower plot (blue) corresponds to the case with uncorrected mass. Central plot (green) has $N = 1$ and $s = 1$. The upper plot has: $N = 1$ and $s = 3$.

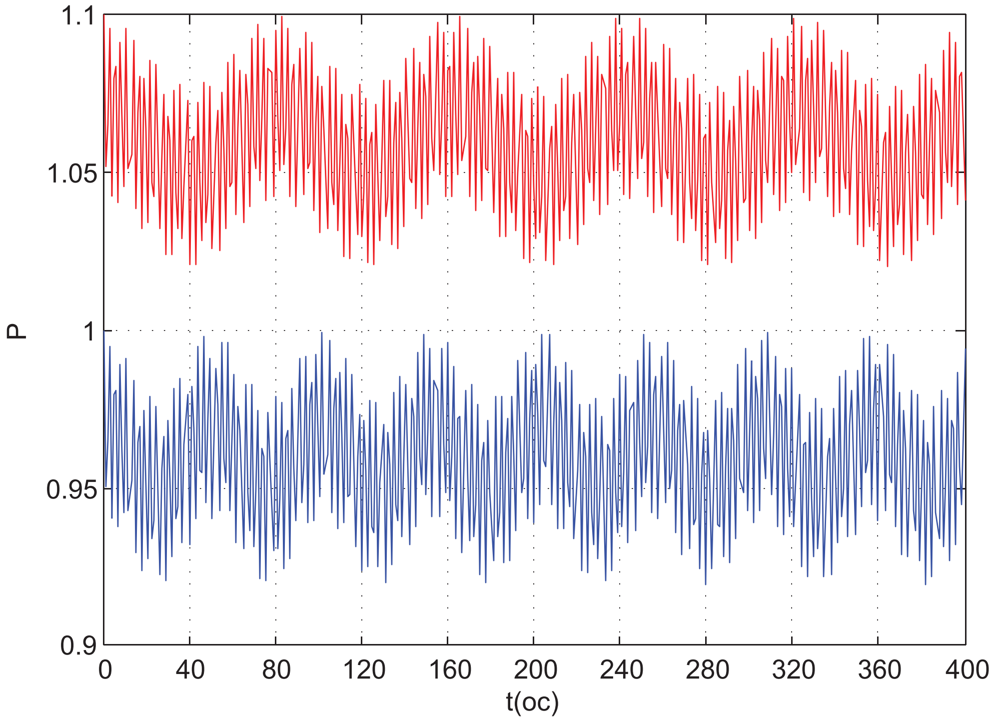

Figure 3. Population of the ground state of the laser driven quantum tube as a function of time (in oc). The lower plot (blue) corresponds to the case with uncorrected mass; upper plot (red) has $N = 3$ and $s = 1$.

is readily obtained; for further details and generalizations the reader is referred to [15, 18, 20]. M labels the highest angular momentum eigenstate that has a non vanishing probability to be populated during the laser operation. Moreover, to avoid features induced by a particular pulse shape, throughout the letter we set $f(t) = 1$; this should not be a severe assumption in pulses as long as those here used.

We have numerically solved the system in (15) by using $\mathcal{E}_0 = 10^{-2}e/a_0^2$ and $R = 5a_0$. In figure 2 we display the plot of the population of the ground state for three different cases as a function of time. In all the following figures, the plot with uncorrected mass is shown at the bottom (in blue). Adopting a small vertical offset to help visualisation, we show the cases with $N = 1$ and $s = 1$ (central plot) and $s = 3$ (top plot). The points are stroboscopically taken at any optical cycle (oc). We observe oscillations of the population of the ground state with period of about 40 oc. But although small, there is a detectable difference between the period of oscillations with uncorrected and with corrected mass. At the beginning of the time evolution, the plots are almost the same; but after a while it is evident that the oscillations with corrected masses have a different period; actually, after a while the oscillations of the population of the central plot are in opposite phase with respect to the bottom one. By increasing *s* the effect is less pronounced since this parameter appears in the denominator of equation (10). In figure 3 we show the rather favourable case of $N = 3$ and $s = 1$, but it requires three excitation quanta of the longitudinal degree of freedom.

The calculations here presented are carried out in the assumption that the system is not severely ionised by the applied electric field requiring that $\mathcal{E}_0 \ll e/a_0^2$. Of course no real system behaves as two-dimensional object and radial degrees of freedom exist and can be excited. However if the ring is slender enough, also these degrees of freedom can be disregarded from the calculations leaving only a small contribution to the mass of the electron.

4. Conclusion

The accessible space of the charges in a RDS is restricted by physical constraints; in some materials such constraints can be so effective to realize a good approximation of 1D or 2D systems. We have seen that the effect of the confinement can be treated in the orthogonal space as a small modification of the mass of the charges. Essentially what happens is that under convenient symmetries, the charge dynamics along a physical dimension can be disentangled from the dynamics along the others. The excitation state or energy content of the separated dimension introduces a tiny modifications of the mass of the charges. A resonant laser coupling induces fast oscillations of the wave function of the electrons pertaining to the large dimension and of course the period of oscillation depends upon the inertia of the charges. We checked our conjecture with a short quantum tube driven by a weak and long laser field. By an opportune choice of the ring size (radius and length) it is possible to regulate the type of laser to use, so that this is not a problem in the planning of the experiments. The modifications on the transition Bohr frequency of the angular levels for short and long tube can be measured since lie in a difficult but non impenetrable range. Moreover we predict that a difference between the population of the ground states for long or short tube of order of 10% are to be expected. In conclusion a weak laser field opens the possibility to penetrate weak relativistic effects.

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