

Application of Quantum Breathers in SRR based metamaterials: Femtosecond Response

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Abstract: The quantum breathers (QB) state in terms of two-phonon bound state (TPBS) via detailed quantum calculations was already shown in important ferroelectrics in a periodic boundary condition with Bloch function. In this work on metamaterials for application in split-ring resonators in antenna arrays, only the temporal variation of the number of quanta in more sites in a non-periodic boundary condition is detailed for a generalized Klein-Gordon lattice. A generalized Hamiltonian is considered which was then quantized by bosonic operators to study the temporal evolution of quanta. Moreover, the time of redistribution of quanta that is proportional to QB's lifetime shows important variation with different quanta at different permittivity, which has important implications in devices.

Keywords: Metamaterials; Quantum breathers; Two phonon bound states; SRR.

I. Introduction

In the field of condensed matter physics, a fertile ground is created by a tremendous amount of both theoretical and experimental research work on nonlinear optics, particularly on discrete breathers that depend on nonlinearity. The majority of these investigations have been carried out with the help of nonlinear Schrodinger equation (NLSE) on nonlinear optical materials, such as ferroelectrics, metamaterials, and others. In a recent work [1] on metamaterials, it has been shown that nonlinear Klein-Gordon equation can also be used in describing the modal behaviour of such engineered materials. A careful analysis of both NLSE and NLKG indicates that apart from showing both dark and bright discrete breathers, the presence of breather pulse can also be observed through NLKG, but not by NLSE. In further upgradation of this work from classical breathers to quantum breathers or two-phonon bound states (TPBS) is first explored in this work within periodic boundary condition. Moreover, our main focus remains on the temporal evolution of such quantum breathers for the first time on metamaterials on Klein-Gordon lattice and that also in a non-periodic boundary condition approach. Let us briefly introduce metamaterials.

Substances with both negative dielectric constant (ϵ) and magnetic permeability (μ) are predicted to possess a negative index (NI) of refraction, and consequently they exhibit a variety of optical properties that are not found in positive indexed materials. With negative refraction, reversing light is an interesting observation [2], and such materials have quite an interesting history in terms of fabrication and measurement techniques [3-9]. However, these NI materials called metamaterials (MM) do not occur in nature, and only recently it has been possible to artificially fabricate them. In saying that metamaterials possess a negative index is a special case nowadays, if cloaking is considered for example [10]. Also many anisotropic materials, like calcite, exhibit negative refraction, as discussed by Boardman et al [11].

The experimental realization of such materials was demonstrated by Smith, et al [12] based on the theoretical work of Pendry et al [3,13], where a type of metamaterial was made as an artificial structure. From the theoretical standpoint, the linear and nonlinear split-ring-resonators (SRR) have been described by equivalent resistor-inductor-capacitor (RLC) circuits [14] featuring a self-inductance L from the ring, a ring Ohmic resistance R to take care of dissipation, and a capacitance C from the split in the ring. MMs are then formed as a periodic array of SRRs which are coupled by mutual inductance and arrayed in a material of dielectric constant ϵ . It is to be noted that unlike natural materials, MMs also show relatively large magnetic response at femtoseconds (fs) and hence their THz applications assumes special significance.

Due to RLC configuration of the SRRs, there exists a resonant frequency for this type of circuit model. It is observed that the (capacitively loaded) magnetically induced (MI) waves propagate within a band near the resonant frequency of the SRRs. Also, the magnetic permeability does not depend on the intensity of the electromagnetic (EM) field in the linear regime of MI wave propagation in a MM. For this purpose, the nonlinearity is incorporated in the system by embedding the SRRs in a Kerr-type medium [15,16]. Kourakis et al [17] studied the self-modulation of the waves propagating in nonlinear magnetic metamaterials on the basis of nonlinear Schrodinger equation that led to spontaneous energy localization via the generation of localized envelope structures, i.e. so called envelope solitons, and the dynamics of the nonlinear RLC circuit gave rise to a governing equation for SRRs in both space and time dimensions. There are important observations made on the appearance of multisolitons by controlling various parameters by a number of authors with numerical solutions [18,19]. Lazarides and co-workers [14] also studied classical discrete breathers in MM systems. Next, let us discuss about discrete breathers (DBs).

Discrete breathers (DB) [20], also known as intrinsic localized modes, are nonlinear excitations that are produced by the nonlinearity and discreteness of the lattice. These excitations are characterized by their long time oscillations and are highly localized pulses in space that are found in the discrete nonlinear model formulation. Unlike the plane wave like modes, DBs have no counterparts in the linear system, but exist only because of the system nonlinearity in a periodic lattice [21]. They are formed as a self-consistent interaction or coupling between the mode and the system nonlinearity. Thus, DB modifies the local properties of the system that provides the environment for the DB to exist. In relevance to metamaterials, Smith and Pendry [22] showed that inclusions smaller than EM wavelength of interest could be considered only through homogenization of field in any periodic structure via field-averaging method for several basic metamaterial structures.

As the continuum limit formulation cannot be applied to their study, the present formulation is appropriate to highly localized pulses having widths that are not large compared to that of domain of interest [23]. So, the question is about the appropriate length scale, which drives us to nano-range in metamaterials consisting of SRR elements. Thus, localization also assumes more significance. As the nonlinearity arises in SRR based metamaterials due to the nonlinear Kerr medium, it could also give rise to the localization, possibly with the coupling within the SRR system that is embodied in the discrete Hamiltonian [14]. DBs are discrete solutions, periodic in time and localized in space and whose frequencies extend outside the phonon spectrum [20,21]. After discussing about classical breathers, next let us look for quantum breathers (QBs).

For the characterization of DBs or classical breathers [24], the bulk system was the right tool, but for systems that are very small, the laws of classical mechanics are not valid, which brings us to the quantum breathers (QBs) [20]. Once generated, QBs modify system properties such as lattice thermodynamics and introduce the possibility of non-dispersive energy transport [20]. These are observed in many systems viz. ladder array of Josephson junction for superconductors, BEC in optical lattices, optical waveguides, micro-mechanical arrays, DNA, SRR based metamaterials in antenna arrays, two-magnon bound states in antiferromagnets, and two-phonon bound states (TPBS), i.e. quantum breathers in ferroelectrics (see ref. [25] for all the references). As pointed out by Zheludev [9], the quantum-effect enabled systems via metamaterials route will bring a range of exciting applications in the future.

For QBs, it is important to consider detailed information on phonons and their bound state concept, which is sensitive to the degree of nonlinearity. The branching out of the QB state from the single-phonon continuum is quite noteworthy in nonlinear systems with charge defects [25]. Thus, the goal of this paper is to explore whether SRR system, through engineering of their geometry (i.e. change of coupling between different SRR elements) shows any sensitivity on coupling and permittivity by quantum calculations hitherto not done on metamaterials. This study is quite realistic to understand the quantum localization due to nonlinearity, which is essential for many nano devices. Quantum localization behavior in Klein-Gordon (K-G) lattice has been studied by many researchers in terms of four atom lattice with periodic Bloch function by Provile [26], dimer case for targeted energy transfer by Aubry et al [27], delocalization and spreading behavior of wave-packets by Flach and coworkers [20]. A generalized method is presented for any number of sites and quanta without periodic boundary condition to show the QB states in metamaterials. It is pertinent to mention that metamaterials can occur in nature as well. However, it is not the issue that we are discussing here. Our issue is: could we explain the phenomenon in its quantum-counterpart? or, could we observe some noticeable effects in quantum-regime or not? - that are not explained in the classical regime. In such a case, we were inclined to see it by dependence of permittivity, while plotting QB's lifetime against number of quanta (see later in Section 3).

Here, our main focus will be on the temporal variation of the number of quanta, as it is also convenient to characterize QBs by this method. Importantly, we also calculate critical times of redistribution of quanta in fs under various physical conditions with an eye on THz applications. It has to be noted that in an anharmonic K-G model, the levels in the potential energy are non-equidistant that could have important implications from the application viewpoint [20].

Finally, it needs to be mentioned that despite the existence of an extensive literature in the area of metamaterials, this is concentrated only in the classical domain. Very few papers have been published on its quantum point of view. Hence, we are trying to study metamaterials from its quantum perspective. In such a case, one could make the fastest switch using metamaterials by studying the temporal-evolution of the number of quanta. For this study, we have to theoretically study temporal-evolution and vary the concerned parameters to optimize the results and then it could eventually be used in the device applications, such as antenna arrays, modulation instability based gadgets, quantum metamaterials based superconductors, etc.. Hence, from the application point of view, the present study assumes special importance.

The paper is organized as follows: In Section II, the theoretical model of the one-dimensional chain of inductively coupled SRRs is described to obtain the Klein-Gordon equation for the system and then the quantization with bosonic operators is done for non-periodic boundary condition. In Section III, the results and discussion are presented for the time of redistribution of quanta against number of quanta. Section IV contains the conclusions.

II. Theoretical Model

Let us consider the following case of three adjacent split-ring resonators, as shown in Fig. 1. A one-dimensional discrete, periodic array of identical non-linear SRRs, that consists of the simplest realization of a MM in one dimension, is considered here. This array is shown here to emphasize that the concerned SRR domains are periodic array, and as pointed out by Segev and coworkers [28] that periodicity is important in creating discrete breathers. In one dimension, the SRRs form a linear array with their centers separated by distance d . Each of the SRRs has self-inductance L , and mutual inductance M . However, a device-oriented optimized model can be considered for the antenna-array application having a varying L and M values. It should be mentioned that almost everything about the above system and also about how the nearest neighbour interactions are considered for weaker coupling in ref. [14]. In ref. [1], wherein the effects of further than first neighbour couplings in the SRR system are also discussed. It is an anisotropic situation, since nonlinear medium does not tend to be isotropic.

As done by Lazarides et al [14], the Hamiltonian of such a system involving the non-dimensional charge (q) and time (t) is given by:

$$H = \sum_n \left[\left(\frac{1}{2} \dot{q}_n^2 - \lambda \dot{q}_n \dot{q}_{n+1} + V(q_n) \right) \right] \quad (1)$$

where, $\frac{dq_n}{dt} = \dot{q}_n = i_n$ (i is the current in SRR), $\lambda = M/L$ (coupling parameter); and the term $V_n = \int_0^{q_n} f(q'_n) dq'_n$ is nonlinear

$$\text{on-site potential and after truncation, this is expressed as: } f(q_n) \approx q_n - \left(\frac{\alpha}{3\epsilon_l} \right) q_n^3 \quad (2)$$

The above eq. (1) can also be tackled by our type of discrete Hamiltonian [23,29]. With a magnetic field H and magnetization σ of each SRR, the Hamiltonian is modified as:

$$H = \sum_n \left[\left(\frac{1}{2} \dot{q}_n^2 - \lambda \dot{q}_n \dot{q}_{n+1} + V(q_n) - \sigma H \right) \right] \quad (3)$$

Now, after putting the value of magnetization (σ), as done by Shadrivov et al [15], we develop the Lagrangian and by using the variational principle (Euler-Lagrange equation), the governing equation in the x -direction is derived to show the Klein-Gordon dynamical equation as [1]:

$$\frac{\partial^2 q}{\partial \tau^2} - ab \frac{\partial^2 q}{\partial x^2} + b \left[q - \frac{\alpha}{3\epsilon_l} q^3 \right] - b\Lambda\Omega \sin(\Omega\tau) + \gamma \frac{\partial q}{\partial \tau} = 0 \quad (4)$$

$a = \lambda'/(1 + 2\lambda')$ and $b = 1/(1 + 2\lambda')$; here λ that is equal to ab being an interaction constant or coupling within the SRR system in a Klein-Gordon lattice, ϵ_l is the linear part of the permittivity that appears to be an important parameter for THz application (see later), $\alpha = +1$ (-1) corresponds to a self-focusing (self-defocusing) in a nonlinear Kerr medium, Ω is a non-dimensional frequency factor and τ is the time, with non-zero external field involving a term Λ and finally a damping term (γ) [1]. The eq. (4) is useful for stability analysis, as normally done in a nonlinear system.

It should be pointed out that we have simply derived Klein-Gordon equ. by variational principle from Lazarides Hamiltonian. It should be made clear that even our discrete Hamiltonian as given in refs. [23,29] with magnetic components could be used for this purpose. It is pertinent to mention that in our recent work, both K-G equation and nonlinear Schrodinger equation (NLSE) show dark and bright solitons, and also dark and bright breathers; however, K-G equation in addition shows breather pulses, whereas NLSE does not show such pulses. This work could also be relevant for important nonlinear optical materials [1]. Next, let us describe the quantum breather state.

The generalized Hamiltonian for the Klein-Gordon system for order parameter (y_n) at nth site is written as:

$$H = \sum_n \frac{p_n^2}{2m} + \frac{A}{2} y_n^2 + \frac{B}{4} y_n^4 + k(y_n - y_{n-1})^2 \quad (5)$$

The first term is momentum at nth site (p_n), the second and third terms are nonlinear potential formulation and the last one contains a term (k) involving coupling. Here A and B are two constants having implication for breather formation. From the above equ. (5), after deducing the classical equation of motion and rescaling of time, we get the revised Hamiltonian as:

$$\tilde{H} = \sum_n \frac{1}{2} p_n^2 + \frac{1}{2} y_n^2 + \eta y_n^4 + \lambda (y_n - y_{n-1})^2 \quad (6)$$

Now, in the corresponding equation of motion, we rescale time as follows: $t = (1/\alpha)\tau$ and we take $\alpha^2 = A/m$, where m is the electronic mass. In such a case, the scale of time is 3.048 fs for an interaction constant value of 0.01, where $\eta = B/4A$ and $\lambda = k/2A$. The term η involves linear permittivity (ϵ_l) and focusing (defocusing) nonlinearity (α) with a value of +1 (-1). Now, we could quantize the Hamiltonian by using creation and annihilation Bosonic operators at the nth site as follows:

$$a_n^+ = \frac{(y_n - ip_n)}{\sqrt{2}}, \quad a_n = \frac{(y_n + ip_n)}{\sqrt{2}} \quad (7a)$$

$$H = \sum_n \frac{1}{2} + a_n^+ a_n + \frac{\eta}{4} (a_n^{+4} + 4a_n^{+3} a_n + 4a_n^+ a_n^3 + 6a_n^{+2} a_n^2 + a_n^4) + \frac{\lambda}{2} (a_n^{+2} + a_n^2 + 2a_n^+ a_n + a_{n-1}^{+2} + a_{n-1}^2 + 2a_{n-1}^+ a_{n-1} + 2) - \lambda (a_n^+ a_{n-1}^+ + a_n a_{n-1} + a_n^+ a_{n-1} + a_n a_{n-1}^+) \quad (7b)$$

After having done the second quantization as described above, to account for the above mentioned terms in a proper way, a general 'basis' with non-number conserving of particles needs to be formed. In an important work done by Proville [26] (see references therein) the periodic boundary condition approach for four sites and an arbitrary number of particles are shown. However, the method presented above gives a generalized way to solve the system for arbitrary number of particles on arbitrary number of sites. So, our method is clearly distinguished from the other investigations. For the characterization of quantum discrete breathers, we need to make the Hamiltonian time-dependent. Let us resort to temporal evolution of number of quanta $\langle n_i \rangle(t) = \langle \psi_t | \hat{n}_i | \psi_t \rangle$ at each site of the system. We take i-th eigen state of the Hamiltonian, and then we make it time dependent as follows:

$$|\Psi_i(t)\rangle = \sum_i b_i \exp(-iE_i t / \hbar) |\psi_i\rangle \quad (8)$$

where ψ_i and E_i are the i-th eigenvector and eigenvalue respectively, t is time, the Planck's constant (\hbar) taken as unity and $b_i = \langle \psi_i | \Psi(0) \rangle$ for each site i and for a given range of t, where $\Psi(0)$ stands for initial state. In our computation by 'mathematica', we need to specify the initial states at $t=0$ wherein there is localization in the initial state and then as time is varied, there is a continuous evolution of the number of quanta.

In contrast with the Discrete Non-Linear Schrodinger equation, where complete energy transfer takes place [27], in case of nonlinear K-G lattice, complete energy transfer does not take place between the anharmonic oscillators and there is a critical time of redistribution for the quanta. This is an important point to be noted. In our computation, this critical time is measured when the number of quanta meets or almost meets on the time axis. In the above approach, we have not used any periodic function, such as Bloch function. With this methodology, we can now proceed to deal with the application of non-periodic boundary condition approach in metamaterials.

III. Results and Discussion

As a preamble for the existence of quantum breather state, here we first show an eigenspectrum of two-phonon bound state (TPBS) that is a signature of the quantum breathers, by using the formalism as described in ref. [25] for a periodic boundary condition with a Bloch function. For SRR based metamaterials, for a very low value of permittivity of 0.002 with focusing nonlinearity $\alpha=+1$ and a small value of interaction constant of 0.001, it is noted from Fig. 2 that a continuum of states with single phonon and QB state can also be observed. As revealed by our numerical simulation, the SRRs are weakly coupled and when the coupling value increases beyond 0.05, the formation of QB becomes relatively more difficult. The reason of taking a smaller value of permittivity is to merely show the presence of QB in metamaterials, even these smaller values may be considered practically unrealistic. Having established the presence of quantum breather states in SRR based metamaterials, we may go to our main focus area of temporal evolution of the number of quanta.

For a non-periodic boundary condition, the temporal evolution spectra were generated from 4 quanta to 12 quanta on 3 sites. The time of redistribution of quanta that is proportional to QB's lifetime in fs was calculated from each spectra. All these data are shown in table-I for four different values of linear permittivity (ϵ_1) by changing 3 orders of magnitude from 0.002 to 2.0 and taking only one value of coupling of $\lambda=0.01$.

Typical spectra are shown in Fig. 3: for a relatively large value of linear permittivity, as taken by Lazarides et al [14] $\epsilon_1 = 2$, for a focusing nonlinearity $\alpha = +1$, and a smaller value of coupling between the SRR elements $\lambda=0.01$. This simulation was carried out for 6 particles on 3 sites with $|\psi(0)\rangle = |5,1,0\rangle$. Here, the initial localization is mainly at the first site and then there is a fast redistribution of quanta between the other two sites until they become equal or almost equal, and the critical time for redistribution (t_{re}) is 50.89. This is about 155.1 fs for this value of coupling. This value seems to be on the higher side as compared to that in ferroelectrics with 6 quanta ($t_{re}=13.45-14.27$ for a coupling between 0.1 and 0.9) despite having the same number of quanta, but with lower value of coupling within the SRR assembly. It is known that by engineering the geometry of the SRR assembly, the interaction between SRR elements can be varied. Hence, the study of QB in non-periodic boundary condition in terms of temporal evolution of the number of quanta seems to reveal a different picture for different types of materials, which both are important as nonlinear optical materials.

Finally, the time of redistribution of quanta or QB's lifetime (t_{re}) is plotted against number of quanta at four different values of linear permittivity in Fig. 4. It is seen that t_{re} is low for lower permittivity values of 0.002 and 0.02, but it increases slightly up to a value of $\epsilon_1 = 0.2$, whereas there is a significant increase afterwards towards higher value. This change is quite noticeable at lower number of quanta in that QB's lifetime at 4 quanta changes from 76.8 fs to 266.8 fs between 0.2 and 2. TPBS parameters show significant variation with coupling after a value of 0.05 making the quantum breather formation relatively more difficult. This shows that QB's lifetime is quite sensitive to a change of coupling as well as linear permittivity of the SRR based metamaterials.

It is important to mention from the physics viewpoint that smaller values of permittivity (0.002 and 0.02) were merely taken to show the variation of number operators in our simulation. These smaller values of permittivity may be considered unrealistic from the practical point of view, but Fig. 4 shows that these values have insignificant role in the overall behaviour of QB's lifetime. This could be considered as an important piece of information for application. For a highly absorbing sort of material, the linear part of the permittivity could be low enough, but it cannot be said about its lower limit. However, the variation of QB's lifetime between 0.2 and 2 (i.e. an increase of an order of magnitude) is still very significant. A study of QB's band gap against permittivity could possibly throw some light on the subject. It is pertinent to mention that for a macromolecule, Tretiak et al [26] observed that the lifetime of discrete breathers increases as the crystals become more and more defective. As the defect or disorder could create localization, it is congenial for the formation of QB giving us insight on quantum localization [20,26]. This might be an important consideration for device applications. Moreover, from a design viewpoint of SRR assembly, the behavior shown in Fig. 4 indicates that for increasing QB's lifetime, the linear permittivity which is embodied in our Hamiltonian has an important role to play in terms of changing the temporal evolution of the number of quanta. This piece of information could be useful for future directions of study.

IV. Conclusion

In a periodic boundary condition approach, the branching out of two-phonon bound state from a single phonon continuum is a signature for quantum breathers in SRR based metamaterials, which is sensitive to coupling. For a non-periodic boundary

condition approach, the temporal evolution spectra show a decrease of time of redistribution with increasing number of quanta for each value of linear permittivity except at lower value of 0.002, which does not have much significance. It is also observed that as the permittivity increases, the lifetime of QBs increases substantially from 76.8 to 266.8 fs after a value of 0.20 to 2.0 for 4 quanta and such effect is reduced on increasing the number of quanta. This piece of information is considered useful for a future study in this new field of investigation of QBs in SRR based metamaterials and other THz applications of QBs in important nonlinear optical materials. Here, an attempt has been made to study quantum localization in metamaterials that is expected to trigger new class of investigations on the subject. As per Zheludev [9], the quantum-effect enabled systems through metamaterials route will bring a range of exciting applications in the future.

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Table – I

QB's lifetime in fs at 4 different values of permittivity for 5 different quanta
(coupling, $\lambda=0.01$)

No. of Quanta	$\epsilon_1=0.002$	$\epsilon_1=0.02$	$\epsilon_1=0.2$	$\epsilon_1=2.0$
4	1.5	8.8	76.8	266.8
6	2.6	4.8	22.8	155.1
8	2.9	4.4	6.3	58.0
10	3.7	4.6	4.4	24.8
12	6.4	3.2	3.6	16.2

Note: The difference of QB's lifetime between two values of permittivity is to be noted.

Figure Captions

Fig. 1: Three adjacent split-ring-resonators having self-inductance L and mutual inductance M .

Fig. 2: Typical eigenspectrum for $\lambda=0.001$, $\epsilon_1 = 0.002$ and $\alpha=+1$. The spectra represent single phonon continua and the quantum breather band or two-phonon bound state in the upper branch of the spectrum.

Fig. 3: Temporal-evolution spectra for metamaterials with SRR assembly for 6 particles on 3 sites with $|\psi(0)\rangle = |5,1,0\rangle$, $\epsilon_1 = 2$, $\alpha = +1$, and $\lambda=0.01$ ($t_{re} = 155.1$ fs).

Fig. 4: The time of redistribution data (t_{re}) against number of quanta at four different values of linear permittivity showing a slight increase up to a value of $\epsilon_1 = 0.2$, whereas there is a significant increase afterwards towards higher value. The timescale has to be multiplied by 3.048 fs.



Fig. 1

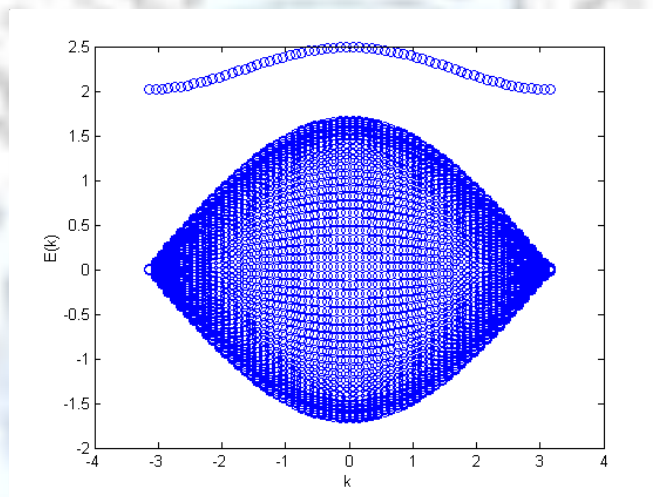


Fig. 2

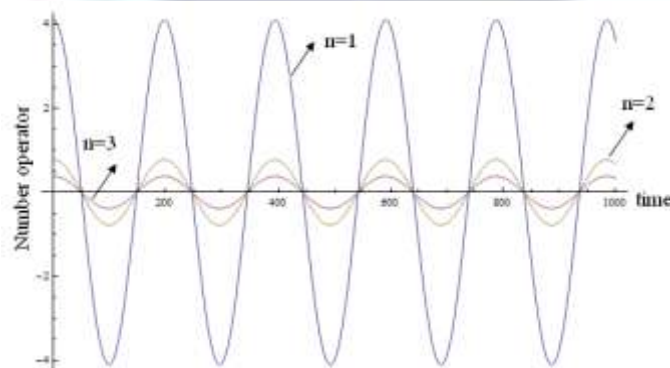


Fig. 3

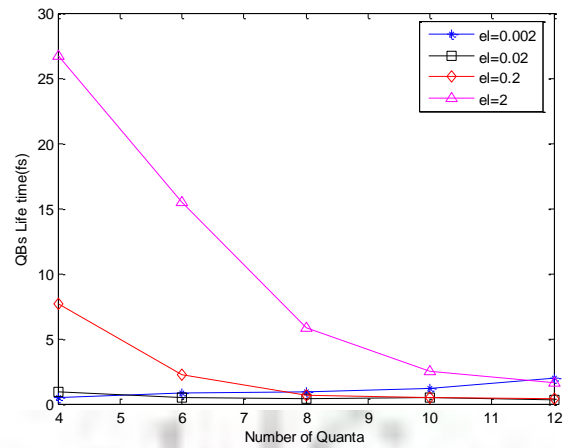


Fig. 4