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Effect of phonons on optical properties of RbCl quantum pseudodot qubits

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Abstract In this work, an electron which is strongly coupled to the strong electron-longitudinal optical (LO) phonon in RbCl quantum pseudodot qubits is considered. First, we employ the Pekar variational method and obtain the eigenenergies and eigenfunctions of the ground and the first-excited states of the system. Then, we have studied optical properties of the system under strong electron-LO phonon coupling. In this regard, the refractive index changes and absorption coefficient of the system are obtained using compact-density-matrix approach and iterative method. It is found that the absorption coefficients show saturation in the presence of phonon effect. This behavior occurs at small quantum size and for different potential height. Our results show that both the structure parameters and phonon effect have a great effect on the total absorption and refractive index changes.

Keywords Quantum pseudodot · Optical properties · Phonon

1 Introduction

With recent rapid advances of modern nanotechnology field, many researchers have been investigating various new quantum nanostructures like quantum dots, quantum wells, quantum wires and quantum pseudodots (Khordad 2016; Li et al. 2012; Feng and Xiao 2016). These quantum nanostructures have been central points of experimental and theoretical researches.

During recent years, quantum computation and quantum information processing have been interesting subjects for quantum computers. Knowledge about the behaviors or the

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physical properties of a quantum computer is essential to its processing. It is demonstrated that quantum computer with a large number of qubits would be more realizable in solids (Togan et al. 2010), especially by invoking semiconductor quantum dot (QD) (Roloff et al. 2010). In quantum theory, the two-level system is usually employed as the elementary unit for storing information which is usually called as the quantum bit (qubit). Recently, there has been a large amount of theoretical (Nielsen and Chang 2000; Mosca 2012; Passante et al. 2011) and experimental (Weedbrook et al. 2012; Feng et al. 2013; Schindler et al. 2011) works on quantum computers.

The physical properties of quantum dot qubits and quantum pseudodot qubits have been studied during past years (Hansom et al. 2014; Xiao 2014; Xiao 2014). For example, (Sun et al. 2016) have investigated effect of phonons in quantum pseudodot qubits. Ezaki et al. (1998) have investigated the electronic structures in a triangular bound potential quantum dot. Ikhdair and Hamzavi (2012) calculated the electronic properties of an electron confined in a two-dimensional quantum pseudodot. Xiao (Xiao 2013) has studied the electric field on an asymmetric quantum dot qubit. Wang and Xiao (2007), Wang et al. (2008) studied the properties of a two-level parabolic quantum dot qubit. Chen and Xiao (2008) recently examined the temperature effects on the parabolic linear bound potential QD qubit.

The study of optical properties of quantum dot qubits is an interesting subject. So far, optical properties of quantum dot with and without external factors have been extensively investigated. Among optical properties of nanostructures, the refractive index changes and absorption coefficients are important. Although the optical properties of quantum dots have been studied in the past few years, no attempt has been made to study the phonons dependent optical properties of quantum pseudodot qubits. For this reason, we intend to investigate the phonons effect on optical properties of pseudodot qubits using Pekar variational method and compact-density-matrix approach.

2 Theory and model

Consider an electron is moving in a polar crystal quantum pseudodot with pseudoharmonic potential. It is interacting with bulk LO phonons. The Hamiltonian of the system can be written as

$$H = \frac{P^2}{2m^*} + V(r) + \sum_q \hbar\omega_{LO} a_q a_q^+ + \sum_q \left[V_q a_q e^{iq\cdot r} + h\cdot c\right] \tag{1}$$

where $\boldsymbol{p} = \left(p_x, p_y, p_z\right)$ and $\boldsymbol{r} = (r, \theta)$ are the momentum and position vectors of the electron, $a_q^+\left(a_q\right)$ is the creation (annihilation) operator of the bulk LO phonon with wave vector $\boldsymbol{q}$ and frequency ω_{LO}. $V_{\boldsymbol{q}}$ in Eq. (1) is expressed as

$$V_q = i\left(\frac{\hbar\omega_{LO}}{q}\right)\left(\frac{\hbar}{2m\omega_{LO}}\right)^{\frac{1}{4}}\left(\frac{4\pi\alpha}{V}\right)^{\frac{1}{2}} \tag{2}$$

where α is the electron-LO phonon coupling strength and is given by

$$\alpha = \left(\frac{e^2}{2\hbar\omega_{LO}}\right)\left(\frac{2m\omega_{LO}}{\hbar}\right)^{\frac{1}{2}}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right) \tag{3}$$

The second term in Eq. (1) denotes the pseudoharmonic potential as (Xiao 2015)

$$V(r) = V_0\left(\frac{r}{R_0} - \frac{R_0}{r}\right)^2 \tag{4}$$

where V_0 is the chemical potential of the two-dimensional electron gas and R_0 is the zero point of the pseudoharmonic potential.

Employing the Pekar variational method (Pekar 1954; Pekar and Deigen 1948; Landau and Pekar 1948), the trial wave function $|\psi>$ of the strong-coupling polaron can be separated into two parts, the electron and the phonon parts, as

$$|\psi\rangle = |\phi\rangle U|0_{ph}\rangle \tag{5}$$

where $|\phi>$ relates to the electron coordinate, $|0_{ph}>$ denotes the zero phonon state which satisfies $a_q|0_{ph}> = 0$ and $U|0_{ph}>$ is the coherent state of the phonon. In above relation, we have

$$U = \exp\left[\sum_q \left(f_q a_q^+ - f_q^* a_q\right)\right] \tag{6}$$

where $f_q\left(f_q^*\right)$ is the variational function. By employing this unitary transformation to Eq. (1), the transformed Hamiltonian can be written as

$$H' = U^{-1}HU \tag{7}$$

The trial ground and the first-excited state wave functions of the electron to be

$$|\psi_0\rangle = |\phi_0\rangle|0_{ph}\rangle = \pi^{-3/4}\eta_0^{3/2}\exp\left[-\eta_0^2 r^2/2\right]|0_{ph}\rangle \tag{8}$$

$$|\psi_1\rangle = |\phi_1\rangle|0_{ph}\rangle = \left(\frac{\pi^3}{4}\right)^{-1/4}\eta_1^{5/2} r\cos\theta\exp\left[-\eta_1^2 r^2/2\right]|0_{ph}\rangle \tag{9}$$

By minimizing the expectation value of the Hamiltonian, we obtain the ground state energy $E_0 = <\phi_0|H'|\phi_0$ and the first excited state energy $E_1 = <\phi_1|H'|\phi_1$ as follows

$$E_0 = \frac{3\hbar^2\eta_0^2}{4m^*} + \frac{3V_0}{2\eta_0^2 R_0^2} + 2V_0\eta_0^2 R_0^2 - 2V_0 - \sqrt{\frac{2}{\pi}}\alpha\hbar\omega_{LO}\eta_0 R_0 \tag{10}$$

and

$$E_1 = \frac{5\hbar^2\eta_1^2}{4m^*} + \frac{5V_0}{2\eta_1^2 R_0^2} + \frac{2}{3}V_0\eta_1^2 R_0^2 - 2V_0 - \frac{3}{4}\sqrt{\frac{2}{\pi}}\alpha\hbar\omega_{LO}\eta_1 R_0 \tag{11}$$

where η_0 and η_1 are the variational parameters and $R_0 = \sqrt{\hbar/2m^*\omega_{LO}}$ is the polaronic radius.

3 Optical absorption coefficients and refractive index changes

In order to calculate the optical properties of our system, we consider the interaction of a polarized monochromatic electromagnetic field with the system. Then, we employ the density matrix formalism for computing the absorption coefficients and refractive index changes related to an optical transition. The electromagnetic field vector with the frequency ω can be expressed by

$$E(t) = Ee^{i\omega t} + E^* e^{-i\omega t}. \tag{12}$$

With respect to the time-dependent interaction of electromagnetic field with the system, the time evolution of the matrix elements of one-electron density operator, ρ, is given by the von-Neumann equation (Boyd 2003; Ahn and Chuang 1987; Aspnes 1976)

$$\frac{\partial \rho_{ij}}{\partial t} = \frac{1}{i\hbar}[H_0 - erE(t), \rho]_{ij} - \Gamma_{ij}\left(\rho - \rho^{(0)}\right)_{ij}, \tag{13}$$

where $\rho^{(0)}$ is the unperturbed density matrix, H_0 is the Hamiltonian of this system without the electromagnetic field $E(t)$, and q is the electronic charge. The symbol [,] is the quantum mechanical commutator, Γ is the phenomenological operator responsible for the damping due to collisions among electrons, and etc. We can solve Eq. (13) with applying the standard iterative method (Aspnes 1976). After obtaining the density matrix, we can determine the electronic polarization $P(t)$ and $\chi(t)$ susceptibility as

$$P(t) = \varepsilon_0 \chi_\omega^{(1)} \widetilde{E} e^{i\omega t} + \varepsilon_0 \chi_{2\omega}^{(2)} \widetilde{E}^2 e^{2i\omega t} + \varepsilon_0 \chi_0^{(2)} \widetilde{E}^2 + \varepsilon_0 \chi_{3\omega}^{(3)} \widetilde{E}^3 e^{3i\omega t} + c.c, \tag{14}$$

where $\chi_\omega^{(1)}$, $\chi_{2\omega}^{(2)}$, $\chi_0^{(2)}$, and $\chi_{3\omega}^{(3)}$ are the linear susceptibility, second-harmonic generation, optical rectification and third-harmonic generation, respectively. The electronic polarization of the n th order electronic polarization follows,

$$P^{(n)}(t) = \frac{1}{V} Tr\left(\rho^{(n)} qr\right), \tag{15}$$

where V and ρ are the volume of system and the one-electron density matrix. Also ε_0 is the permittivity of free space, and the symbol Tr (trace) denotes the summation over the diagonal elements of the matrix.

In this work, we have considered the linear and the third-order nonlinear refractive index changes which are expressed as (Kuhn et al. 1991):

$$\frac{\Delta n^{(1)}(\omega)}{n_r} = \frac{\sigma_v^2 e^2 |M_{21}|^2}{2n_r^2 \varepsilon_0} \left[\frac{E_{21} - \hbar\omega}{(E_{21} - \hbar\omega)^2 + (\hbar\Gamma_{12})^2}\right], \tag{16}$$

$$\begin{aligned} \frac{\Delta n^{(3)}(\omega)}{n_r} = & -\frac{\sigma_v e^4 |M_{21}|^2}{4n_r^3 \varepsilon_0} \frac{\mu c I}{\left[(E_{21} - \hbar\omega)^2 + (\hbar\Gamma_{12})^2\right]^2} \\ & \times \left[4(E_{21} - \hbar\omega)|M_{21}|^2 - \frac{(M_{22} - M_{11})^2}{(E_{21})^2 + (\hbar\Gamma_{12})^2}\right. \\ & \left. \times \left\{(E_{21} - \hbar\omega)\left[E_{21}(E_{21} - \hbar\omega) - (\hbar\Gamma_{12})^2\right] - (\hbar\Gamma_{12})^2(2E_{21} - \hbar\omega)\right\}\right], \end{aligned} \tag{17}$$

where σ_v is the carrier density, μ is the permeability, $E_{ij} = E_i - E_j$ is the energy difference, and $M_{ij} = |\langle i|x|j\rangle|$ is the electric dipole moment matrix element. Using Eqs. (16) and (17), one can write the total refractive index change as

$$\frac{\Delta n(\omega)}{n_r} = \frac{\Delta n^{(1)}(\omega)}{n_r} + \frac{\Delta n^{(3)}(\omega)}{n_r}. \tag{18}$$

The absorption coefficient $\alpha(\omega)$ is also calculated from the imaginary part of the susceptibility $\chi(\omega)$ as

$$\alpha(\omega) = \omega\sqrt{\frac{\mu}{\varepsilon_R}}\mathrm{Im}[\varepsilon_0\chi(\omega)]. \tag{19}$$

The linear and third-order nonlinear absorption coefficients can be written as (Adachi 1985; Unlu et al. 2006):

$$\alpha^{(1)}(\omega) = \omega\sqrt{\frac{\mu}{\varepsilon_R}}\left[\frac{\sigma_v e^2\hbar\Gamma_{12}|M_{21}|^2}{(E_{21}-\hbar\omega)^2 + (\hbar\Gamma_{12})^2}\right], \tag{20}$$

$$\begin{aligned}\alpha^{(3)}(\omega, I) = -\omega\sqrt{\frac{\mu}{\varepsilon_R}}\left(\frac{Ie^4}{2n_r\varepsilon_0 c}\right)\frac{\sigma_v\hbar\Gamma_{12}|M_{21}|^2}{\left[(E_{21}-\hbar\omega)^2 + (\hbar\Gamma_{12})^2\right]^2} \\ \times\left\{4|M_{21}|^2 - \frac{(M_{22}-M_{11})^2\left[3E_{21}^2 - 4E_{21}\hbar\omega + \hbar^2(\omega^2 - \Gamma_{12}^2)\right]}{(E_{21})^2 + (\hbar\Gamma_{12})^2}\right\},\end{aligned} \tag{21}$$

where c is the speed of light in free space and I is the optical intensity of the incident wave, and it is given by

$$I = 2\sqrt{\frac{\varepsilon_R}{\mu}}|E(\omega)|^2. \tag{22}$$

Using Eqs. (20) and (21), one can express the total absorption coefficient as

$$\alpha(\omega, I) = \alpha^{(1)}(\omega) + \alpha^{(3)}(\omega, I) \tag{23}$$

4 Results and discussion

In this section, we have performed the numerical results for RbCl quantum pseudodot qubits. The parameters used in the calculation are (Adachi 1985) $\hbar\omega_{LO} = 21.45$ meV, $n_r = 1.49$, $\sigma_v = 2.9 \times 10^{20}$ cm^{-3}, $m = 0.432m_0$, $\theta = \pi/3$.

Figure 1 shows linear, nonlinear and total refractive index changes of RbCl quantum pseudodot qubits as a function of photon energy under phonon effect with $I = 0.2$ MW/cm^2, $\alpha = 3.81$, $V_0 = 10$ meV and $R_0 = 10$ nm. The linear term generated by the $\Delta n^{(1)}$ term is the opposite in sign of the nonlinear change generated by the $\Delta n^{(3)}$ term. Thus, the total refractive index change will be reduced. Thus, the calculation of the refraction index change applying with only the linear term, may not be correct for systems, operating especially with a high optical intensity, because of the strong dependence of $\Delta n^{(3)}$ on the incident optical intensity.

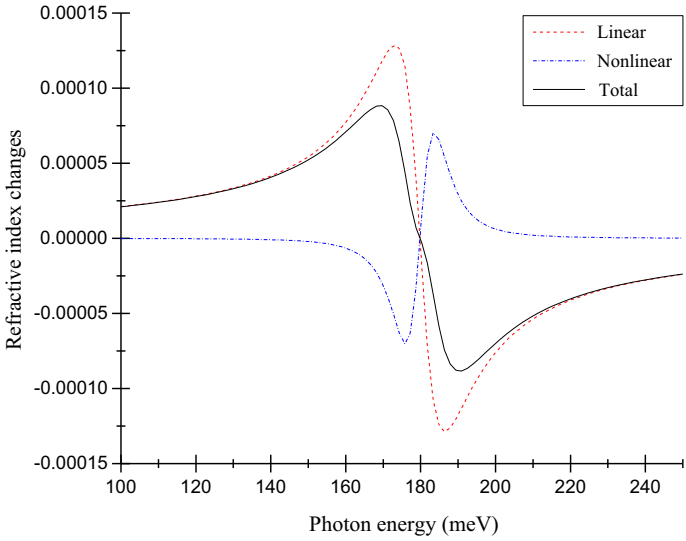

Fig. 1 The variation of linear, third-order and total refractive index changes with the photon energy

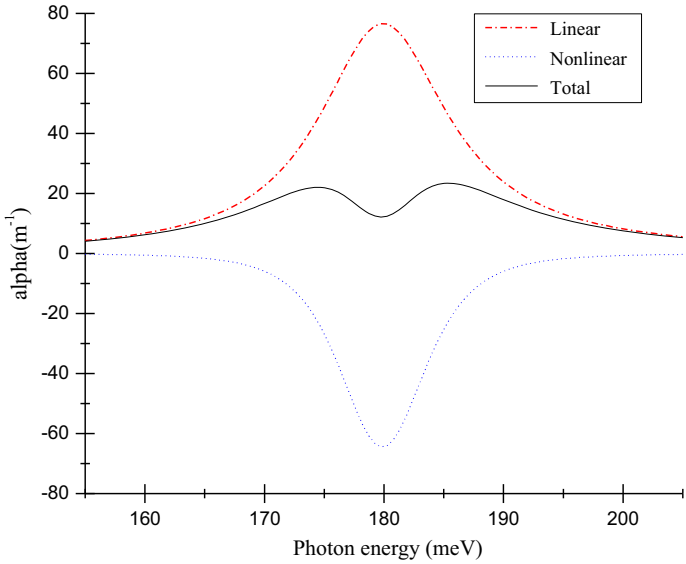

Fig. 2 The variation of linear, third-order and total absorption coefficients with the photon energy

In Fig. 2, the variations of linear, third-order nonlinear and total absorption coefficients of RbCl pseudodot quantum qubits are plotted as a function of the photon energy with $I = 0.2$ MW/cm^2, $\alpha = 3.81$, $V_0 = 10$ meV and $R_0 = 10$ nm. There is a resonance peak at a photon energy value of 180 meV as expected, which corresponds to the energy difference between the levels considered with phonon effect.

Figure 3 shows the total changes in the absorption coefficient as a function of the photon energy for four different V_0 as 10, 12, 14, and 16 meV with $R_0 = 10$ nm. We

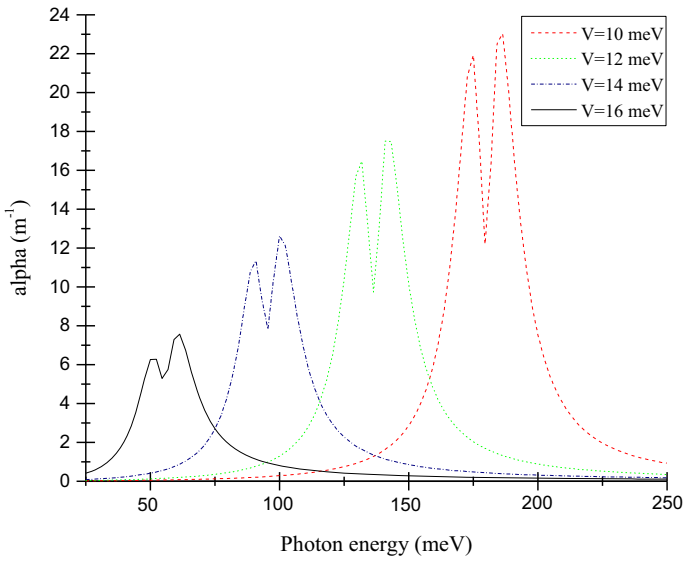

Fig. 3 The variation of total absorption coefficients with the photon energy for different V_0

observe from the figure that the total changes in the absorption coefficient will be significantly reduced as V_0 increases and shifts toward lower energies due to the presence of phonons. There is an interesting point in the figure. Due to the presence of phonon effect, the total absorption coefficients show the saturation.

In Fig. 4, the variations of total absorption coefficient are plotted as a function of the photon energy of RbCl pseudodot quantum qubits for four different quantum sizes as 1,

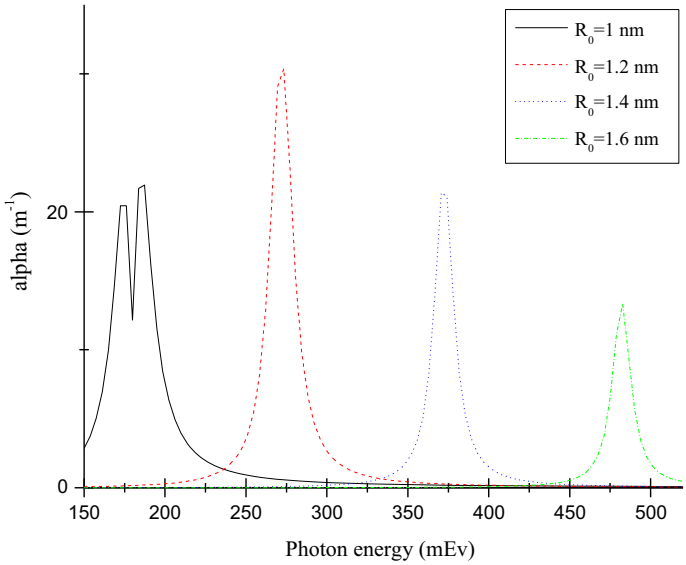

Fig. 4 The variation of total absorption coefficients with the photon energy for different quantum sizes

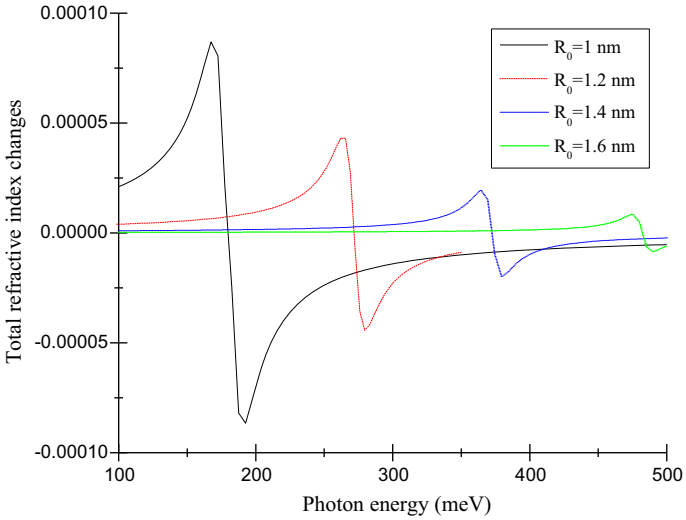

Fig. 5 The variation of total refractive index changes with the photon energy for different quantum sizes

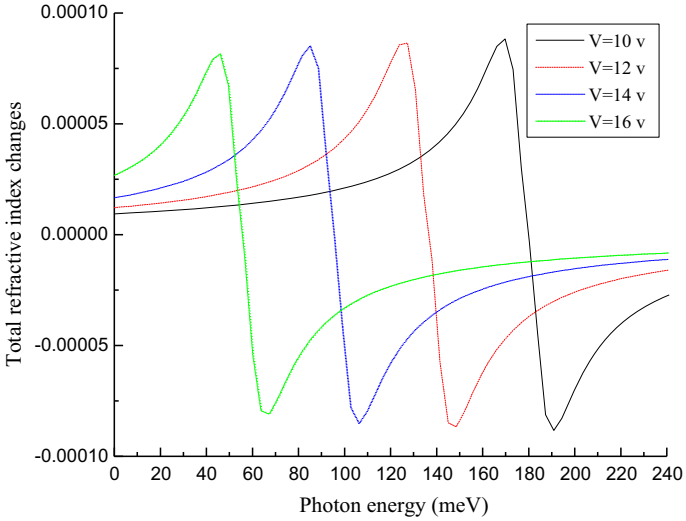

Fig. 6 The variation of total refractive index changes with the photon energy for different V_0

1.2, 1.4, and 1.6 nm with $V_0 = 12$ meV. It is seen that from the figures the total absorption coefficients increase with enhancing quantum size. It is observed from the figure that saturation occurs at quantum size 1 nm.

Figures 5 and 6 display the refractive index changes as a function of photon energy of RbCl pseudodot quantum qubits for different quantum sizes and V_0. It is clear that the refractive index changes reduce and shift toward higher energies with increasing quantum sizes. But, the parameter reduces and shift towards lower energies with increasing V_0.

This physical behavior in the figures is due to the fact that the states, ground and first excited states, coherently exchange energies under electron–phonon interaction.

5 Conclusions

In the present work, we have employed Pekar variational method to obtain the ground and first excited state energy of polaron in RbCl pseudodot quantum qubits under phonon effect. By using the compact-density matrix approach, the expressions for the linear and third-order nonlinear optical properties in pseudodot quantum qubits have been theoretically deduced and some numerical computations have been performed for selected material parameters. Acording to the results, it is found that the linear changes in the absorption coefficient and refractive index is not related to the incident optical intensity, whereas the incident optical intensity has a great influence on the third-order nonlinear change, as it is expected from theoretical expressions. We hope that this study can make a significant contribution both to the experimental works and also the other theoretical analysis on this subject.

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