Electron localization in graphene quantum dots

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We study theoretically a localized state of an electron in a graphene quantum dot with a sharp boundary. Due to Klein's tunneling, the "relativistic" electron in graphene cannot be localized by any confinement potential. In this case the electronic states in a graphene quantum dot become resonances with finite trapping time. We consider these resonances as the states with complex energy. To find the energy of these states we solve the time-independent Schrödinger equation with outgoing boundary conditions at infinity. The imaginary part of the energy determines the width of the resonances and the trapping time of an electron within quantum dot. We show that if the parameters of the confinement potential satisfy a special condition, then the electron can be strongly localized in such quantum dot, i.e., the trapping time is infinitely large. In this case the electron localization is due to interference effects. We show how the deviation from this condition affects the trapping time of an electron. We also analyze the energy spectra of an electron in a graphene quantum ring with a sharp boundary. We show that in this case the condition of constructive interference can be tuned by varying internal radius of the ring, i.e., parameters of confinement potential.

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I. INTRODUCTION

The recent discovery of elusive two-dimensional form of carbon called graphene[1] has unusual electronic properties that may be useful in the design of new electronic devices. Recently there has been great deal of interest in this high mobility conducting material.[2–4] One of the factors which makes graphene so attractive for research is that the low-energy dynamics of electrons in graphene. Those electron can be described by a two-dimensional Dirac-Weyl equation and electrons in graphene behave as massless chiral fermions,[5] i.e., "relativistic" electrons. Due to this unique property, the electrons in graphene cannot be localized by any confinement potential. This effect is called Klein's paradox[6] and is related to the fact that electrons in graphene can have both positive and negative energies. Therefore, when a propagating electron reaches the potential barrier it penetrates through it and emerges inside of the barrier in the state with the negative-energy-hole state. This tunneling, Klein's tunneling, introduces an efficient escape channel from any trapping potential.

Therefore, taking into account Klein's tunneling, we can conclude that there are no conventional quantum dots in graphene, i.e., quantum dots,[7] which can localize electrons within finite spatial regions. At the same time for future electronic applications of graphene it is quite important to realize the quantum dot trapping potential for relativistic electrons. A zero dimensionality of quantum dots and possibility of tuning the confinement potential and the electron-density externally result in very broad applications of quantum dots in conventional semiconductors, ranging from lasers[8] and photodetectors[9] to quantum information processing and quantum computers.[10] Recently the quantum dots created in carbon nanotubes[11,12] and graphitic systems[13] have also been reported.

Since the electron in graphene cannot be localized we need to discuss not the localization but the trapping of an electron. Here the trapping means that the electron should stay within finite spatial region for a very long time. The problem of trapping of electron has been studied in the case of a one-dimensional wire in zero[14–16] and in finite[17] magnetic fields and for a quantum dot with smooth[18] and sharp[19] boundaries. It was shown that the trapping potential for relativistic electron in graphene is produced by transverse momentum.[14,18,20] In the case of a quantum dot the transverse potential is related to an electron angular momentum.[18] The larger the angular momentum, the more efficient trapping potential is created. Another factor, which strongly affects the trapping time, is the sharpness of the quantum dot boundaries, i.e., the sharpness of the confinement potential. The sharpness of the boundary of a quantum dot determines the width of the trapping potential. Therefore the most efficient trapping is realized in a smooth confinement potential and for electronic states with large angular momentum. The trapping time of an electron in a quantum dot has exponential dependence on the angular momentum and the slope of the confinement potential.[18] Since the electron with large trapping time can be considered as almost localized, below we use both terms *trapping* and *localized* to describe electron states in graphene quantum dot.

Although the most efficient trapping is realized in a smooth potential, some trapping should be expected in the confinement potential with sharp boundaries.[19] In this case the trapping time has no exponential dependence but a power dependence on the parameters of the confinement potential.

In the present paper we show that even in the case of confinement potential with sharp boundaries, we can realize the trapping of the relativistic electron for a very long time. For special parameters of the confinement potential, which can be achieved by an additional tuning of the potential, the escape rate from some states of the quantum dot can be even exactly zero. Therefore, the relativistic electrons in such states are *strongly localized* with infinite trapping time. This localization is achieved not due to a large trapping potential barrier but due to interference effects within the quantum dot. It means that the trapping properties of the quantum dot with sharp boundaries depend on the distribution of the con-

finement potential within the whole region of quantum dot. This opens another possibility for tuning of the trapping properties of an electron in quantum dots. We show below that by introducing additional holes in the quantum dots, we can strongly suppress the escape rate of an electron from the quantum dot. We illustrate this effect by considering the trapping properties of quantum rings with sharp boundaries.

The quantum dot considered in this paper has the same structure as the one studied in Ref. 19. Matulis and Peeters[19] discussed the resonances of the quantum dots, which are revealed as peaks in the scattering cross section.[21] From the width of the peaks the lifetime or escape rate can be extracted. Our approach to the problem of the trapped states of the quantum dots is different from Ref. 19. Namely, we consider the resonances as the long-lived states in the decay process.[21] It means that we define the resonances of the quantum dots as the time-independent solution of the Schrödinger equation, which is characterized by the outgoing boundary conditions at infinity and a complex energy. The imaginary part of the energy determines the width of the resonances and the trapping time of the electron within quantum dot. Namely, if E is the complex energy of the localized state, then the trapping time is $\tau=\hbar/\mathrm{Im}[E]$. Here $\mathrm{Im}[E]$ is imaginary part of the electron energy and $\hbar$ is reduce Planck constant. This approach allows us to obtain in the closed form the equation for the complex energy of the trapped states of the quantum dot. From this equation we can obtain the condition of strong localization of an electron within quantum dot and derive some analytical results for the imaginary part of electron energy.

The paper is organized as follows. In Sec. II we introduce the main system of equations for graphene quantum dot and derive the energy eigenvalue equation. In Sec. III we provide the analysis of the energy spectra of the quantum dot and derive the condition that the quantum dot has a strongly localized state. In Sec. IV we introduce the main system of equations for a quantum ring system and derive the corresponding energy eigenvalue equation. In Sec. V we discuss the possible tuning of the trapping properties of the quasilocalized states of the quantum ring by varying the internal radius of the ring.

II. MAIN EQUATIONS: QUANTUM DOT

To introduce a quantum dot in graphene we consider a cylindrically symmetric confinement potential, which has the following form:

$$V(r)=\begin{cases}0 & \text{if } r<R\\ V_0 & \text{if } r>R,\end{cases} \tag{1}$$

where $V_0>0$ and R is the radius of the quantum dot. This shape of confinement potential allows us to obtain analytical expressions for the trapping time of the states of the quantum dot. The confinement potential in Eq. (1) has sharp boundaries and based on the analysis of Ref. 18 we can conclude that the trapping time of the electron within such a quantum dot is relatively small. This means that any trapping of the electron in such potential should be related to the behavior of the wave functions within the whole region of quantum dot, i.e., the trapping properties are determined by the interference effects within the quantum dot.

The Hamiltonian of a single electron in graphene with potential, determined by Eq. (1), is given by an expression[5,22]

$$\mathcal{H}=\frac{\gamma}{\hbar}(\vec{\sigma}\cdot\vec{p})+V(r), \tag{2}$$

where $\vec{\sigma}$ are the Pauli matrices, $\vec{p}=-i\partial/\partial\vec{r}$, and $\gamma=\sqrt{3}a_0\gamma_0/2$ is the band parameter. Here $a_0=0.246$ nm is the lattice constant and $\gamma_0\approx 3.03$ eV is the transfer integral between the nearest-neighbor carbon atoms.[23] In expression (2) for the Hamiltonian of the system we consider a single valley only, taking into account the double valley degeneracy of the energy levels. The potential in Eq. (1) does not introduce any mixture between the different valleys and does not lift the valley degeneracy. In addition to the valley degeneracy each level has double spin degeneracy. Therefore, each energy level, we discuss below, has a fourfold degeneracy.

The wave function, $\psi(\vec{r})$, corresponding to Hamiltonian (2), is a two-component function. Here the two components correspond to two different sublattices of graphene honeycomb lattice. For cylindrically symmetric confinement potential the two-component wave function has the following form:

$$\psi(r,\theta)=e^{i(m-1/2)\theta}\begin{pmatrix}\chi_1(r)\\ \chi_2(r)e^{i\theta}\end{pmatrix}, \tag{3}$$

where r and θ are cylindrical coordinates and $m=\pm 1/2,\pm 3/2,\cdots$ is orbital angular momentum. With this form of the wave function the Schrödinger equation corresponding to the Hamiltonian in Eq. (2) becomes

$$V(r)\chi_1-i\gamma\frac{d\chi_2}{dr}-i\gamma\frac{m+1/2}{r}\chi_2=E\chi_1, \tag{4}$$

$$V(r)\chi_2-i\gamma\frac{d\chi_1}{dr}+i\gamma\frac{m-1/2}{r}\chi_1=E\chi_2. \tag{5}$$

To find the energy, E, of the level we need to solve the system of Eqs. (4) and (5) with the following boundary conditions: (i) at $r=0$ both χ_1 and χ_2 should be finite and (ii) at infinity we have outgoing boundary conditions, i.e., $\chi_1,\chi_2\propto\exp(ikr)$.

By eliminating χ_1 or χ_2 in the system [Eqs. (4) and (5)] we can easily obtain that χ_1 and χ_2 satisfy Bessel's differential equations of the order $|m-1/2|$ for functions χ_1 and of the order $|m+1/2|$ for function χ_2. Then the general solution of the system of Eqs. (4) and (5) inside the quantum dot, where $V=0$, has the form

$$\begin{pmatrix}\chi_1(r)\\ \chi_2(r)\end{pmatrix}=A\begin{pmatrix}J_{|m-1/2|}(\varepsilon r/R)\\ iJ_{|m+1/2|}(\varepsilon r/R)\end{pmatrix}, \tag{6}$$

where J_n is the Bessel function of the nth order and we introduced the dimensionless energy $\varepsilon=RE/\gamma$. The energy and correspondingly the dimensionless energy are complex in our approach.

Outside the quantum dot, i.e., at $r>R$, the solutions of the corresponding Bessel differential equations should describe the outgoing waves, $\propto\exp(ikr)$. Therefore at $r>R$, the solutions of Eqs. (4) and (5) are Hankel functions of the first kind. Then the general solution of the system of Eqs. (4) and (5) at $r>R$, where $V=V_0$, is

$$\begin{bmatrix} \chi_1(r) \\ \chi_2(r) \end{bmatrix} = B \begin{Bmatrix} H^{(1)}_{|m-1/2|}[(\varepsilon-\nu_0)r/R] \\ iH^{(1)}_{|m+1/2|}[(\varepsilon-\nu_0)r/R] \end{Bmatrix}, \tag{7}$$

where $H^{(1)}_n$ is the Hankel function of the first kind and of the nth order and we introduced the dimensionless confinement potential $\nu_0=RV_0/\gamma$.

At the boundary of the quantum dot, i.e., at $r=R$, the two-component wave function should be continuous. From this condition we can find the energy eigenvalue equation, which takes the form

$$\frac{H^{(1)}_{|m-1/2|}(\varepsilon-\nu_0)}{H^{(1)}_{|m+1/2|}(\varepsilon-\nu_0)} = \frac{J_{|m-1/2|}(\varepsilon)}{J_{|m+1/2|}(\varepsilon)}. \tag{8}$$

The solution of the eigenvalue equation [Eq. (8)] determines the complex energy spectrum of the quantum dot. The imaginary part of the energy characterizes the electron trapping time at the corresponding state of the dot.

We can see that Eq. (8) is symmetric with respect to the change of the sign of the angular momentum, $m\to -m$. It means that the energy spectra of an electron with positive and negative angular momenta are identical. Therefore below we consider only positive values of m, $m=1/2,3/2,\cdots$.

III. STRONGLY LOCALIZED STATES IN QUANTUM DOTS

For a given angular momentum, m, we solve the eigenvalue equation [Eq. (8)] numerically. We show the results of calculations in Fig. 1 for a few lowest values of m. The results are shown in the complex energy plane. As we can see from these data the typical imaginary part of the energy is of the order of 1 (in dimensionless units). This is valid for all values of m. These results are consistent with the main conclusion of Ref. 18, where it was shown that the strong trapping can be achieved only in smooth confinement potential, in which the trapping time is exponentially large.

Based on the data shown in Fig. 1 we can estimate the typical trapping time of the electron within quantum dot. In the real units the imaginary part of the energy is of the order of γ/R. Then the trapping time $\tau\sim\hbar R/\gamma$. For a quantum dot of size $R=50$ nm we obtain $\tau\sim 10^{-13}$ s. This is a relatively small time and we should consider the electron in such a quantum dot as weakly trapped.

Although an electron in the confinement potential as in Eq. (1) is only weakly localized (the typical imaginary part of the energy is large) we can see in Fig. 1 that there is a region of energies, where the imaginary part of the energy becomes small. Within this region the real part of the energy is close to the trapping potential, ν_0. This observation has already been reported in Ref. 19. In addition to a strong electron trapping at $\varepsilon\approx\nu_0$, we can have the exact localization of an electron in the quantum dot if the potential, ν_0, satisfies a special condition. Namely, we can see from Eq. (8) that if the potential strength, ν_0, is the root of the Bessel function of the order $(m-1/2)$, i.e., $J_{m-1/2}(\nu_0)=0$, then there is a solution of eigenvalue equation, $\varepsilon=\nu_0$, with *zero imaginary part*, and the electron at this level is strongly localized. Therefore, the strongly localized state of the electron in the quantum dot exists only if the potential satisfies the condition

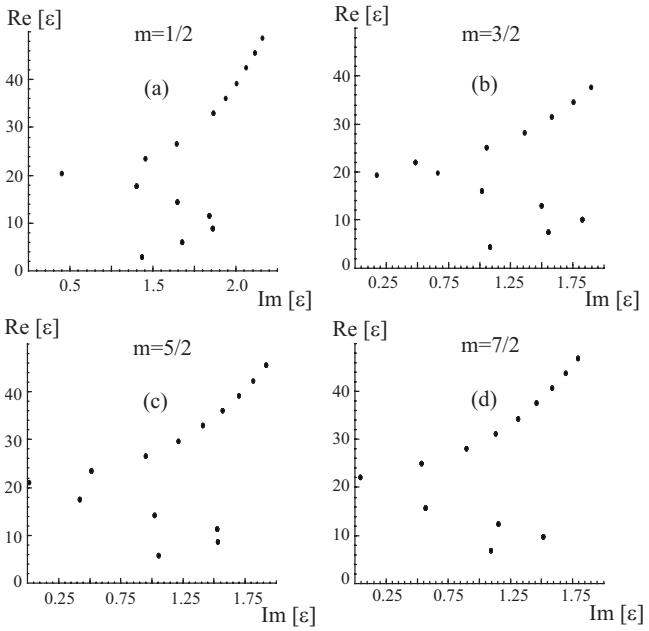

FIG. 1. The energy spectra of an electron in the graphene quantum dot are shown for different angular momenta m (as indicated) in the complex energy plane. For all the panels $\nu_0=20$.

$$\nu_0=\lambda_{n,i}, \tag{9}$$

where $\lambda_{n,i}$ is the ith root of the Bessel function of the order $n=0,1,2,\cdots$ and n is related to the angular momentum: $n=m-1/2$. We can rewrite expression (9) in the original units. Taking into account that the unit of the energy is γ/R, we obtain

$$V_0=\frac{\gamma}{R}\lambda_{n,i}. \tag{10}$$

For example, for $R=50$ nm and $\gamma=645$ meV nm we have

$$V_0=12.9\lambda_{n,i}\ \text{(meV)}. \tag{11}$$

Then for each n we can find the set of the heights of the confinement potential, at which an electron can be strongly localized. In Table I we show these heights for a few lowest values of n and i.

Any violation of the condition $\nu_0=\lambda_{n,i}$ introduces an escape of electron from the quantum dot. In this relation we need to address the following question: How large is the trapping time of an electron in the quantum dot if the condition of localization is weakly violated, i.e., $\delta_\nu\equiv\nu_0-\lambda_{m-1/2,i}$ is small and nonzero. We expect that in this case the escape rate from the quantum dot and correspondingly the imaginary part of the energy is small. To find the imaginary part of

TABLE I. The heights of the confinement potential V_0, at which the electron that can be strongly localized is shown for a few lowest values of n and i. The potential satisfies Eq. (11). The potential strength is in units of meV. The radius of the quantum dot is $R=50$ nm.

i/n	1	2	3	4	5	6	7
0	31	71	112	152	193	233	274
1	50	91	131	172	213	253	294
2	66	109	150	191	232	272	313
3	82	126	168	209	250	291	332
4	98	143	185	227	269	310	351
5	113	159	203	245	287	328	369

the energy $\varepsilon \approx \nu_0 \approx \lambda_{m-1/2,i}$ of the almost localized state we consider $\delta_\nu = \nu_0 - \lambda_{m-1/2,i}$ as a small parameter and then from Eq. (8) obtain the first nonzero corrections to $\mathrm{Im}[\varepsilon]$. The details of calculations are presented in Appendix. The final results are the following.

If the energy of the state is close to $\nu_0 \approx \lambda_{m-1/2,i}$, then the imaginary part of the energy has the form

$$\mathrm{Im}[\varepsilon] = \frac{\pi}{[2^m(m-1/2)!]^2}\left[1-\frac{1}{2m}\right]^{2m+1}\delta_\nu^{2m} \tag{12}$$

for $m > 1/2$ and

$$\mathrm{Im}[\varepsilon] = \frac{\pi}{2}\left(\frac{\delta_\nu}{\ln \delta_\nu}\right) \tag{13}$$

for $m=1/2$. We can see from Eq. (12) that the imaginary part of the energy has exponential dependence on m of the quasilocalized state: $\mathrm{Im}[\varepsilon] \propto \exp[-2m|\ln \delta_\nu|]$. Therefore, the states with large angular momentum can be trapped for a longer time than the states with small values of m. At the same time the imaginary part of the energy has a weak power-law dependence on δ_ν. Another interesting fact about expressions (12) and (13) is that the coefficients in these expressions depend only on the angular momentum, m, but not on the value of $\lambda_{m-1/2,i}$.

Since $\nu_0 = RV_0/\gamma$, the condition of strong localization can be expressed in terms of the original parameters of the confinement potential, i.e., the strength of the potential, V_0, and R,

$$RV_0 = \gamma \lambda_{n,i}, \tag{14}$$

where $n=0,1,2,\cdots$ and $i=1,2,\cdots$. From Eqs. (12)–(14) we can estimate the trapping time of the quasilocalized states for the quantum dots with spatially fluctuating parameters. For example, if the radius of the quantum dot varies within the range δR, then from Eq. (12) we can find that the escape rate, i.e., imaginary part of the energy, from quasilocalized state of the dot is proportional to $(\delta R/R)^{2m}$.

One of the manifestations of the strongly trapped state in the quantum dot is a sharp peak in the electron density of states, which can be measured in the resonant tunneling experiments or in the resonant scattering experiments. The density of states can be expressed through the real part of the energy and the imaginary part of the energy, which now becomes the width of the resonance, by the following equation:[24]

$$g(\varepsilon) = \frac{1}{\pi}\sum_j \frac{\mathrm{Im}(\varepsilon_j)}{[\varepsilon - \mathrm{Re}(\varepsilon_j)]^2 + [\mathrm{Im}(\varepsilon_j)]^2}, \tag{15}$$

where the density is expressed in the dimensionless units. The density of states for $\nu_0=20$ and $m=3/2$ is shown in Fig. 2. We can clearly see the sharp maximum at the energy close to ν_0. This maximum corresponds to the highly trapped state of electron within quantum dot.

The existence of a highly trapped state of electron in the quantum dot, i.e., the state with small imaginary part of the energy, is due to interference effect. It means that the imaginary part of the energy of such state is very sensitive to the exact profile of the confinement potential. The deviation from the boxlike shape of the confinement potential of quantum dot [see Eq. (1)] can increase or decrease the escape rate from the quantum dot, i.e., increase or decrease the imaginary part of the energy. To illustrate this behavior we consider quantum dot with an additional hole at the center of the dot, i.e., quantum ring. We show below that by varying the size of the hole we can tune the trapping time of the quasilocalized state of an electron in the quantum dot.

IV. MAIN EQUATIONS: QUANTUM RING

The quantum ring is shown schematically in Fig. 3(a) and is described by the following confinement potential:

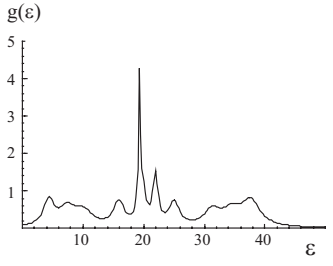

FIG. 2. The density of states, $g(\varepsilon)$ as a function of ε [for panel (b) in Fig. 1], where $\nu_0=20$ and $m=3/2$.

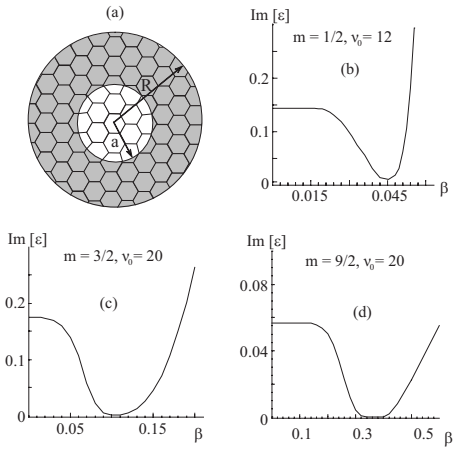

FIG. 3. The imaginary part of the energy, Im[ε], of the quasilocalized state as a function of $\beta(\beta=a/R)$ for a graphene quantum ring for different values of angular momentum, m, and different strength of confinement potential, ν_0 (as indicated). Panel (a) shows the geometry of the graphene ring with the outer radius R and the inner radius a.

$$V(r)=\begin{cases} V_0 & \text{if } r<a \\ 0 & \text{if } a<r<R \\ V_0 & \text{if } r>R, \end{cases} \tag{16}$$

where R is the external radius of the ring and a is the internal radius of the ring. The quantum ring can also be considered as a quantum dot of radius R with an additional hole of radius a at the center of the dot.

Now we have three different regions, within which the confinement potential is constant and the functions χ_1 or χ_2 satisfy the corresponding Bessel equations. Similar to the quantum dot system we consider only the positive values of angular momentum, $m=1/2,3/2,\cdots$. Then the general solution of the system of Eqs. (4) and (5) has the following form:

$$\begin{pmatrix}\chi_1(r)\\ \chi_2(r)\end{pmatrix}=A\begin{pmatrix}J_{m-1/2}([\varepsilon-\nu_0]r/R)\\ iJ_{m+1/2}([\varepsilon-\nu_0]r/R)\end{pmatrix} \tag{17}$$

for $r<a$,

$$\begin{pmatrix}\chi_1(r)\\ \chi_2(r)\end{pmatrix}=B\begin{pmatrix}H^{(1)}_{m-1/2}(\varepsilon r/R)\\ iH^{(1)}_{m+1/2}(\varepsilon r/R)\end{pmatrix}+C\begin{pmatrix}H^{(2)}_{m-1/2}(\varepsilon r/R)\\ iH^{(2)}_{m+1/2}(\varepsilon r/R)\end{pmatrix} \tag{18}$$

for $a<r<R$, and

$$\begin{pmatrix}\chi_1(r)\\ \chi_2(r)\end{pmatrix}=D\begin{pmatrix}H^{(1)}_{m-1/2}([\varepsilon-\nu_0]r/R)\\ iH^{(1)}_{m+1/2}([\varepsilon-\nu_0]r/R)\end{pmatrix} \tag{19}$$

for $r>R$. Here $H^{(2)}_n$ is the Hankel function of the second kind. In these expressions we took into account that the wave function should be finite at $r=0$ and outside the quantum ring we have outgoing waves.

From the continuity of the wave functions at $r=a$ and $r=R$ we obtain the energy eigenvalue equation

$$\frac{\alpha_1 H^{(1)}_{m+1/2}(\beta\varepsilon)-H^{(1)}_{m-1/2}(\beta\varepsilon)}{\alpha_1 H^{(2)}_{m+1/2}(\beta\varepsilon)-H^{(2)}_{m-1/2}(\beta\varepsilon)}=\frac{\alpha_2 H^{(1)}_{m+1/2}(\varepsilon)-H^{(1)}_{m-1/2}(\varepsilon)}{\alpha_2 H^{(2)}_{m+1/2}(\varepsilon)-H^{(2)}_{m-1/2}(\varepsilon)}, \tag{20}$$

where we introduced the following notations: $\beta=a/R$ and

$$\alpha_1=\frac{J_{m-1/2}[\beta(\varepsilon-\nu)]}{J_{m+1/2}[\beta(\varepsilon-\nu)]},\quad \alpha_2=\frac{H^{(1)}_{m-1/2}(\varepsilon-\nu)}{H^{(1)}_{m+1/2}(\varepsilon-\nu)}. \tag{21}$$

In the limit of small β, $\beta\to 0$, Eq. (20) transforms into Eq. (8) for an ideal quantum dot.

V. QUANTUM RING: FINE TUNING OF THE TRAPPING TIME

In the case of the quantum ring, we are interested in the effect of an additional structure, i.e., a hole, in the quantum dot on the electron escape rate from the highly trapped state of the quantum dot. From Sec. III we know that for an ideal quantum dot the energy of highly trapped state is close to the confinement potential strength, $\varepsilon\approx\nu_0$. When the condition of localization [see Eq. (14)] is satisfied then the energy of localized state is exactly equal to ν_0 and the imaginary part of the energy is zero. When condition (14) is violated then the imaginary part of the energy is nonzero. Now we consider the effect of additional hole at the center of the quantum dot on the magnitude of the imaginary part of the energy of the highly trapped quasilocalized state. Therefore we study the dependence of the imaginary part of the energy on the parameter $\beta=a/R$ of the ring. This dependence can be found from Eq. (20).

The results of numerical solution of Eq. (20) are shown in Fig. 3, where the imaginary part of the energy of the quasilocalized state is shown as a function of β. We can clearly see that by increasing the inner radius of the ring we can strongly decrease the imaginary part of the energy of the quasilocalized state. This is valid for all values of m. Therefore the additional internal structure of the quantum dot can produce "constructive interference," which suppresses the electron escape rate from the highly trapped state of the quantum dot. In Fig. 3 we used different values for the heights of the confinement potential. The reason for this is that we need to choose the confinement potential height close to the value determined by the condition of strong localization [Eq. (9)]. Therefore in Fig. 3(b) we have $\nu_0=12$ and $|\nu_0-\lambda_{0,4}|=0.2$, in Fig. 3(c) we have $\nu_0=20$ and $|\nu_0-\lambda_{1,6}|=0.4$, and in Fig. 3(d) we have $\nu_0=20$ and $|\nu_0-\lambda_{4,5}|=0.6$. We can also see another property of confinement potential, which has already been discussed in Sec. III. Namely, with increasing the angular momentum, m, the imaginary part decreases.

We can also see from Fig. 3 that there is a general tendency in the dependence of the imaginary part on the inner radius of the quantum ring. Namely, the sensitivity of the imaginary part of the energy to the inner radius of the ring decreases with increasing the angular momentum of the state. We can see that the imaginary part of the energy remains constant at small values of β and we can see the changes in the imaginary part of the energy only at $\beta>0.02$ for $m=1/2$, at $\beta>0.03$ for $m=3/2$, and at $\beta>0.15$

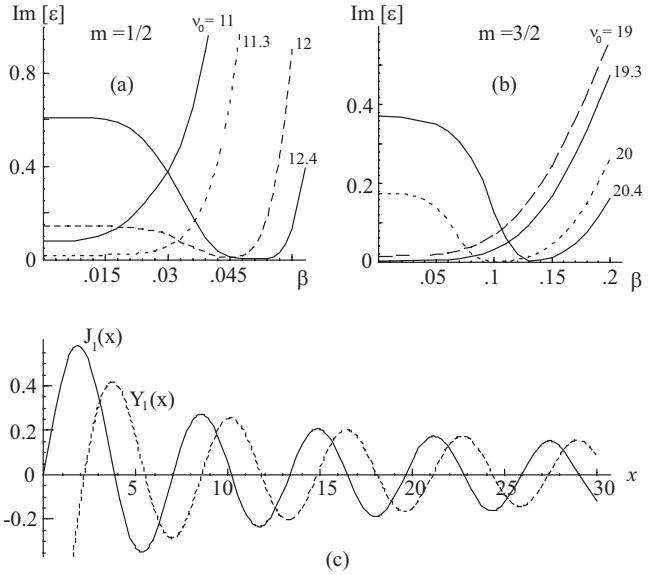

FIG. 4. The imaginary part of the energy, Im[ε], as a function of β for different values of ν_0 (as indicated). The angular momentum is $m=1/2$ for panel (a) and $m=3/2$ for panel (b). (c) The Bessel function, J_1, and the Neumann function, Y_1, of the first order.

for $m=9/2$. This behavior can be understood from the fact that with increasing the electron angular momentum, the corresponding wave function becomes more localized near the outer radius of the ring. In this case the energy of such wave function becomes less sensitive to the inner radius of the ring.

It happens that the dependence, shown in Fig. 3, can be observed only if the confinement potential, ν_0, is greater than the value corresponding to the condition of strong localization. It means that only if $\nu_0 > \lambda_{m,i}$ ($\nu_0 - \lambda_{m,i} \ll 1$) then the additional hole in the quantum dot suppresses the escape rate of an electron from the quantum dot. To illustrate this effect we show in Figs. 4(a) and 4(b) the dependence of Im[ε] on the parameter β for different values of ν_0. In Fig. 4(a) the data are shown for $m=1/2$. In this case the condition of strong localization is satisfied at $\nu_0 \approx 11.5$. We can see from Fig. 4(a) that if $\nu_0 > 11.5$ then the function Im[$\varepsilon(\beta)$] has a minimum, while if $\nu_0 < 11.5$ then the function Im[$\varepsilon(\beta)$] increases with increasing the inner radius of the ring, a. Similar behavior, which is shown in Fig. 4(b), is observed for $m=3/2$. Now the condition of strong localization for the quantum dot is satisfied at $\nu_0 \approx 19.5$.

We can understand this behavior from the analysis of the energy eigenequation (20). Similar to the quantum dot system we are looking for the real solution of this equation in the form $\varepsilon = \nu_0$. Under this condition we can easily obtain $\alpha_1 \to \infty$ and $\alpha_2 \to 0$. Then Eq. (20) becomes

$$\frac{H^{(1)}_{m+1/2}(\beta\nu_0)}{H^{(2)}_{m+1/2}(\beta\nu_0)} = \frac{H^{(1)}_{m-1/2}(\nu_0)}{H^{(2)}_{m-1/2}(\nu_0)}. \tag{22}$$

At a real argument the Hankel function of the second kind is complex conjugated to the Hankel function of the first kind. Then Eq. (22) becomes

$$\frac{J_{m+1/2}(\beta\nu_0)}{Y_{m+1/2}(\beta\nu_0)} = \frac{J_{m-1/2}(\nu_0)}{Y_{m-1/2}(\nu_0)}, \tag{23}$$

where Y_n is the Neumann function of the order n. From Eq. (23), at fixed value of potential strength, ν_0, we can find the β at which we have strongly localized state within the quantum ring, i.e., imaginary part of the energy of this state is zero. If the potential strength, ν_0, satisfies condition (9) then the solution of Eq. (23) is $\beta=0$.

Now we assume that there is a small violation of condition (9), i.e., $\delta_\nu = \nu_0 - \lambda_{m,i}$ is small, but it can be positive or negative. In this case, if the solution of Eq. (23) exists, then the corresponding value of β is small, i.e., $\beta\nu_0 \ll 1$. Then for small β the left-hand side of Eq. (23) becomes

$$-\frac{\pi(\beta\nu_0/2)^{2(m+1/2)}}{(m+1/2)\,!\,(m-1/2)!} = \frac{J_{m-1/2}(\nu_0)}{Y_{m-1/2}(\nu_0)}. \tag{24}$$

Since $\delta_\nu = \nu_0 - \lambda_{m,i}$ is small, we can rewrite the right-hand side of Eq. (24) in the following form:

$$-\frac{\pi(\beta\lambda_{m,i}/2)^{2(m+1/2)}}{(m+1/2)\,!\,(m-1/2)!} = \frac{J'_{m-1/2}(\lambda_{m,i})}{Y_{m-1/2}(\lambda_{m,i})}\delta_\nu, \tag{25}$$

where we take into account that $J_{m-1/2}(\lambda_{m,i})=0$. Then from Eq. (25) we can find β,

$$\beta = \Lambda_{m,i}\left(-\frac{J'_{m-1/2}(\lambda_{m,i})}{Y_{m-1/2}(\lambda_{m,i})}\delta\nu\right)^{1/2(m+1/2)}, \tag{26}$$

where we introduced the following notation:

$$\Lambda_{m,i} = \frac{2}{\lambda_{m,i}}\left(\frac{(m+1/2)\,!\,(m-1/2)!}{\pi}\right)^{1/2(m+1/2)}. \tag{27}$$

The solution of Eq. (26) exists only if

$$-\frac{J'_{m-1/2}(\lambda_{m,i})}{Y_{m-1/2}(\lambda_{m,i})}\delta_\nu > 0. \tag{28}$$

The typical behavior of the functions J_n and Y_n is shown in Fig. 4(c). Taking into account that $\lambda_{m,i}$ are zeros of the Bessel function $J_{m-1/2}$ we can conclude that for all values of $\lambda_{m,i}$ the ratio $J'_{m-1/2}(\lambda_{m,i})/Y_{m-1/2}(\lambda_{m,i})$ is negative. Then the solution of Eq. (26) and correspondingly the solution of Eq. (20) exist only for positive δ_ν, i.e., only if $\nu_0 > \lambda_{m,i}$. Therefore only for $\nu_0 > \lambda_{m,i}$ an additional hole at the center of the quantum dot can suppress the escape rate from the quasilocalized state of the dot.

VI. CONCLUSION

There are two different mechanisms of trapping of an electron in graphene quantum dot. The first one is due to generation of the trapping barrier, which is induced by the transverse momentum, i.e., by the angular momentum for cylindrically symmetric quantum dots. In this case the trapping time is determined by electron tunneling through the trapping barrier. The width of the trapping barrier depends on the slope of the confinement potential. Therefore the most efficient trapping of the electron is achieved for a smooth confinement potential.[18] Since the electron angular momen-

tum determines the height of the trapping barrier, then the trapping time has also strong exponential dependence on the magnitude of the angular momentum. For such mechanism of trapping the electron escape rate from the quantum dot is robust with respect to variations of the parameters of the confinement potential.

In this paper we discussed another mechanism of trapping. This mechanism occurs in a quantum dot with sharp boundary. In this case the width of the trapping barrier is very small, and the trapping is realized not only due to electron tunneling but also due to interference effects. Since the interference is very sensitive to the parameters of the confinement potential, then for a given electron angular momentum, m, a strong electron localization can occur only at one energy level. The energy of this level is equal to the strength of the confinement potential, ν_0. Therefore, the imaginary part of the energy of this level is zero and the electron trapping time at this level is infinitely large. In addition the potential should satisfy a special condition [Eq. (14)]. As a result, only a discrete but infinite set of values of the height of the confinement potential can produce a strongly localized electronic state.

Although it is more easier to create experimentally a confinement potential with smooth boundary, the quantum dots with sharp boundary are also important. As we have shown in the present paper, for the quantum dots with sharp boundaries there is a completely different mechanism of trapping. This trapping is due to interference effect and as a result, it can be observed for all values of angular momentum, even for a small m. For smooth boundary the trapping is due to a tunneling and can be achieved only for large values of angular momentum.[18] This shows the advantage of sharp boundaries of the quantum dots. Namely, if we choose the parameters of the confinement potential with sharp boundaries correctly, then the electrons with small values of m can be strongly localized. The finite width (say w) of the boundary of the quantum dot introduces an additional escape from the quantum dot due to violation of condition (14). Then the escape rate from such quantum dot can be estimated as $(w/R)^{2m}$.

When the electron trapping is due to interference effects any variation of the profile of the confinement potential strongly affects the trapping time. This opens a possibility of efficient tuning of the trapping properties of an electron in quantum dots by introducing an internal structure in the quantum dot and by varying the parameters of this structure. We illustrated this behavior for quantum rings, where the internal radius of the ring affects the trapping properties of the ring.

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APPENDIX

We introduce the following notations $\delta_\varepsilon \equiv \varepsilon - \nu_0$ and consider δ_ε and $\delta_\nu = \nu_0 - \lambda_{m,i}$ as small parameters. Then

$$\varepsilon = \lambda_{m,i} + \delta_\varepsilon + \delta_\nu \tag{A1}$$

and the right-hand side of Eq. (8) can be rewritten in the following form:

$$\frac{J_{m-1/2}(\varepsilon)}{J_{m+1/2}(\varepsilon)} = \frac{J_{m-1/2}(\lambda_{m,i} + \delta_\varepsilon + \delta_\nu)}{J_{m+1/2}(\lambda_{m,i} + \delta_\varepsilon + \delta_\nu)}. \tag{A2}$$

The left-hand side of Eq. (8) in these notations becomes

$$\frac{H^{(1)}_{m-1/2}(\varepsilon - \nu_0)}{H^{(1)}_{m+1/2}(\varepsilon - \nu_0)} = \frac{H^{(1)}_{m-1/2}(\delta_\varepsilon)}{H^{(1)}_{m+1/2}(\delta_\varepsilon)}. \tag{A3}$$

Then the eigenvalue equation [Eq. (8)] takes the form

$$\frac{J_{m-1/2}(\lambda_{m,i} + \delta_\varepsilon + \delta_\nu)}{J_{m+1/2}(\lambda_{m,i} + \delta_\varepsilon + \delta_\nu)} = \frac{H^{(1)}_{m-1/2}(\delta_\varepsilon)}{H^{(1)}_{m+1/2}(\delta_\varepsilon)}. \tag{A4}$$

The next step is to find the small-δ_ε and small-δ_ν expansions of the right- and left-hand sides of Eq. (A4). Since we are looking for the imaginary part of the energy then we need to find both the real and imaginary terms in Eq. (A4). The left-hand side of Eq. (A4) contains only the Bessel functions. For a real argument the expansion of the Bessel function is always real. Therefore the left-hand side of Eq. (A4) gives contribution only to the real terms in Eq. (A4). Keeping only the lowest-order corrections in the right-hand side of Eq. (A4), we obtain

$$(\delta_\varepsilon + \delta_\nu)\frac{J'_{m-1/2}(\lambda_{m,i})}{J_{m+1/2}(\lambda_{m,i})} = \frac{H^{(1)}_{m-1/2}(\delta_\varepsilon)}{H^{(1)}_{m+1/2}(\delta_\varepsilon)}. \tag{A5}$$

The left-hand side of Eq. (A5) contains the Hankel functions. Even for the real argument the expansion of the Hankel function contains both the real and imaginary terms. Finally, the imaginary terms will determine the imaginary part of the energy. The small argument expansion of the Hankel function depends on its order, i.e., on the value of m. Therefore we need to consider two cases: (i) $m > 1/2$ and (ii) $m = 1/2$.

Case (i): $m > 1/2$. For $m > 1/2$ the order of the Hankel function is greater then 0, then the small-δ_ε expansion of the right-hand side of Eq. (A5) is

$$\frac{H^{(1)}_{m-1/2}(\delta_\varepsilon)}{H^{(1)}_{m+1/2}(\delta_\varepsilon)} = \frac{\delta_\varepsilon}{2m-1} + i\frac{\pi\delta_\varepsilon^{2m}}{2^{2m}[(m-1/2)!]^2}, \tag{A6}$$

where we took into account both the real and imaginary terms. Combining Eqs. (A5) and (A6), we obtain the following equation for the correction, δ_ε, to the energy of the electronic state in the quantum dot:

$$\frac{2m}{2m-1}\delta_\varepsilon = -\delta_\nu - i\frac{\pi}{2^{2m}[(m-1/2)!]^2}\delta_\varepsilon^{2m}, \tag{A7}$$

where we used the relation $J'_{m-1/2}(\lambda_{m,i}) = -J_{m+1/2}(\lambda_{m,i})$. From this equation we can find both the real and imaginary parts of δ_ε,

$$\delta_\varepsilon = -\left(1 - \frac{1}{2m}\right)\delta_\nu - i\frac{\pi}{[2^m(m-1/2)!]^2}\left[1 - \frac{1}{2m}\right]^{2m+1}\delta_\nu^{2m}. \tag{A8}$$

Since $\mathrm{Im}\,\varepsilon = \mathrm{Im}\,\delta_\varepsilon$ then from Eq. (A8) we obtain Eq. (12).

Case (ii): $m = 1/2$. Now in Eq. (A5) we have Hankel functions of the zeroth order. Then the small-δ_ε expansion of the Hankel function contains the logarithm and the right-hand side of Eq. (A5) becomes

$$\frac{H_0^{(1)}(\delta_\varepsilon)}{H_1^{(1)}(\delta_\varepsilon)} = -\,\delta_\varepsilon \ln \delta_\varepsilon + i\frac{\pi}{2}\delta_\varepsilon. \tag{A9}$$

Taking into account that m in Eq. (A5) is equal to 1/2, we obtain the following equation for δ_ε:

$$(\delta_\varepsilon + \delta_\nu)\frac{J_0'(\lambda_{0,i})}{J_1(\lambda_{0,i})} = -\,\delta_\varepsilon \ln \delta_\varepsilon + i\frac{\pi}{2}\delta_\varepsilon. \tag{A10}$$

Since $\delta_\varepsilon \ln \delta_\varepsilon \gg \delta_\varepsilon$ then in the real part of Eq. (A10) we need to keep only $\delta_\varepsilon \ln \delta_\varepsilon$ term. Taking into account that $J_0'(\lambda_{0,i}) = -J_1(\lambda_{0,i})$, we obtain the final equation for δ_ε,

$$\delta_\varepsilon \ln \delta_\varepsilon = \delta_\nu + i\frac{\pi}{2}\delta_\varepsilon. \tag{A11}$$

We can solve this equation and find the imaginary part of the energy

$$\delta_\varepsilon = \frac{\delta_\nu}{\ln \delta_\nu} + i\frac{\pi}{2}\left(\frac{\delta_\nu}{\ln \delta_\nu}\right). \tag{A12}$$

Finally, we obtain Eq. (13) if we take into account that $\mathrm{Im}\,\varepsilon = \mathrm{Im}\,\delta_\varepsilon$.

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