Quantum dot–ring nanostructure — A comparison of different approaches

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It has been shown recently that a nanostructure composed of a quantum dot (QD) surrounded by a quantum ring (QR) possesses a set of very unique characteristics that make it a good candidate for future nanoelectronic devices. Its main advantage is the ability to easily tune transport properties on demand by so-called “wavefunction engineering”. In practice, the distribution of the electron wavefunction in the nanostructure can be controlled by, e.g., electrical gating. In order to predict some particular properties of the system, one has to know the exact wavefunctions for different shapes of the confining potential that defines the structure.

In this paper, we compare three different methods that can be used to determine the energy spectrum, electron wavefunctions and transport properties of the system under investigation. In the first approach, we utilize the cylindrical symmetry of the confining potential and solve only the radial part of the Schrödinger equation; in the second approach, we discretize the Schrödinger equation in two dimensions and find the eigenstates with the help of the Lanczös method; in the third approach, we use package Kwant to solve a tight-binding approximation of the original system. To study the transport properties in all these approaches, we calculate microscopically the strength of the coupling between the nanosystem and leads. In the first two approaches, we use the Bardeen method, in the third one calculations are performed with the help of package Kwant.

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1. Introduction

In the recent years advances in nanofabrication have led to a growing interest in complex semiconducting nanostructures.¹ Such complex systems are highly controllable objects. By utilizing their peculiar properties, one can design devices with additional functionalities.
In this paper, we consider a quasi two-dimensional nanostructure in the form of a quantum dot (QD) surrounded by a quantum ring (QR), named as a dot–ring nanostructure (DRN). It has been shown\textsuperscript{2–7} that by changing the confinement potential, e.g., by electrical gating, one can change many physical characteristics such as spin relaxation, optical absorption and conduction. All these features are strongly related to the spatial distribution of the electron wavefunctions in a DRN.

In particular, conduction through a DRN depends crucially on the coupling strength of its states to the leads, which is largely dependent on the position of the electron wavefunctions: states located in a QD (QR) are weakly (strongly) coupled. By changing the confinement potential this distribution can be modified so that the ground and excited states move over between the inner (dot) and the outer (ring) part of the DRN.

Transport through a DRN separated from the source and drain leads by the tunneling barriers can be studied by various model calculations. In this paper, we want to compare results of a few different approaches. In the first one we assume a weak coupling between the DRN and leads. It means that the electron states in the DRN and in the leads do not change when the leads are attached to the nanosystem. They can be calculated separately and then used to determine the tunneling rates for tunneling between the DRN and the leads. In this case, we use the Bardeen approach\textsuperscript{8–12} to calculate microscopically the coupling strength. The wavefunctions of an electron in the DRN are calculated by solving numerically the time-independent Schrödinger equation. To this end, we apply two methods:

1. We exploit the cylindrical symmetry of the confining potential and numerically solve the equation for the radial part of the electron wavefunction,
2. We discretize the Schrödinger equation in two dimensions and then use the Lanczöss method to find the low-lying eigenstates.

As expected, for a sufficiently fine discretization the energy spectrum and the shape of the wavefunctions obtained in both approaches are very similar in the physically relevant regime.\textsuperscript{13} As a result, the transport properties in both cases are also similar.

In the second approach, we release the requirement of a weak coupling between the DRN and the leads. Then, when the leads are attached, the wavefunctions change their original shape and the Bardeen approach cannot be used anymore. Instead, we use a wavefunction-based approach to compute transport properties in a tight-binding system. Namely, we perform calculations with the help of an open-source software package Kwant.\textsuperscript{14} It allows one to define the nanosystem together with the leads, so in this approach we are able to control the coupling. By comparing results of both methods, one can determine the range of coupling strengths for which the Bardeen approximation is valid.

Within the framework of both methods, we calculate the energy spectra, spatial distributions of the ground and excited state wavefunctions and transport characteristics for different shapes of the DRN confining potential.
2. Dot–Ring Nanostructure

We consider a two-dimensional, circularly symmetric DRN defined by a confinement potential $V(r)$. Such a structure which conserves the circular symmetry\textsuperscript{15} has been recently fabricated with the help of the droplet epitaxy method.\textsuperscript{16,17} The DRN is composed of a QD surrounded by a QR with a potential barrier $V_0$ between these parts. The height of the barrier is that it allows the electron tunneling in such a way between the dot and ring parts of the DRN. The overall view of the DRN confining potential with explanation of symbols used throughout the text is presented in Fig. 1.

The confining potential is modeled by the function $V(r)$ given by

$$V(r) = \begin{cases} V_{\text{QD}} + (V_0 - V_{\text{QD}}) \exp[-0.018(r - r_B)^2] & \text{for } r < r_B, \\ V_1 \{1 - \exp[-(r/r_0)^{30}]\} + V_0 \exp[-0.018(r - r_B)^2] & \text{for } r > r_B. \end{cases} \quad (1)$$

Throughout this paper, we assume the radius of the DRN $r_0 = 60$ nm, the position of the internal barrier $r_B = (1/2)r_0 = 30$ nm and the height of the external barrier $V_1 = 90$ meV. The bottom of the QR potential is zero, whereas the bottom of the QD potential and the height of the internal barrier are parameters which are varied. In real experiments, $V_{\text{QD}}$ can be controlled by applying voltage to a gate located close to the center of the DRN. By changing $V_{\text{QD}}$, one can modify the distribution of the electron wavefunction. For example, if $V_{\text{QD}} \ll V_{\text{QR}}$ the ground state is located in the QD, whereas for $V_{\text{QD}} \gg V_{\text{QR}}$ the ground state is in the QR. Such manipulations can drastically affect the conductance through the ground state: on the one hand, if the wavefunction is in QD, the overlap with states in...
lead is negligible and the conductance is close to zero. On the other hand, if the wavefunction is in QR, its overlap with the lead states will be much larger and so is the conductance.

The energy spectrum of the original “continuous” system, i.e., before any discretization, consists of a set of discrete energies $E_{nl}$ due to radial motion with radial quantum numbers $n = 0, 1, 2, \ldots$, and rotational motion with angular momentum quantum numbers $l = 0, \pm 1, \pm 2, \ldots$. The single particle orbital wavefunction is of the form

$$\Psi_{nl}(r) = R_{nl}(r) \exp(il\phi),$$

with the radial part $R_{nl}(r)$.

3. Distribution of Electron Wavefunctions in a Dot–Ring Nanostructure

The energy spectra and wavefunctions have been calculated in three different models of the DRN:

1. A “continuous” system that conserves the cylindrical symmetry, without leads. The Schrödinger equation is solved only for the radial part of the wavefunction.
2. The Schrödinger equation is discretized in two dimensions. Then, the Lanczos method is used to find the ground and low-lying excited states. No leads.
3. The tight-binding version of the Hamiltonian with attached two leads is solved with the help of the Kwant package.

In approach No. 1, we assume the wavefunctions in the form given by Eq. (2). To find the radial part $R_{nl}(r)$, we apply the Numerov algorithm\textsuperscript{18} and the shooting method. In approach No. 2 the two-dimensional Schrödinger equation is cast in a matrix form where a discrete basis is used instead of the continuous real-space position basis. Then, the low-lying states and corresponding energies are found by diagonalizing the matrix with the help of the Lanczos method. In the last approach, Kwant program is used. It is a free software package that uses the Python programming language. It is available at http://kwant-project.org/. Kwant can be used for numerical calculations related to transport in quantum systems. One can use it to calculate conductivity, scattering matrix, wavefunctions and Green’s functions. This package can be used to perform simulation of metals, semiconductors, topological insulators, superconductors, etc. One can use various lattice types, e.g., square, triangular or honeycomb lattice. In our approach, we define a tight-binding model on a square lattice with only nearest-neighbor hoppings and the on-site potential given by Eq. (1). We have infinite leads attached to both sides of the DRN. By changing the positions of the leads, we can control the strength of the coupling between the leads and the nanosystem. Figure 2 shows the geometry in the cases of weak and strong coupling. With the possibility of controlling of the DRN-lead coupling, we can study how the energy spectrum and the wavefunctions are affected.
by attaching the leads. This is important because the wavefunctions are needed to calculate microscopically the tunneling matrix element between states in the DRN \( \Psi_{nl} \) and in leads \( \psi_k \)

\[
t_{nlk} = \frac{\hbar^2}{2m^*} \int [\Psi_{nl}^*(\mathbf{r}) \nabla \psi_k(\mathbf{r}) - \psi_k^*(\mathbf{r}) \nabla \Psi_{nl}(\mathbf{r})] \cdot \mathbf{dS},
\]

where the integration is performed over a surface separating the DRN and the leads.

Within the Bardeen approach\(^8\)-\(^12\) it is assumed that \( \Psi_{nl} \) and \( \psi_k \) are eigenfunctions of the DRN and the leads, respectively. However, when the coupling gets stronger, the real wavefunctions are modified and the Bardeen approach is not valid any more. Below we will show how increasing coupling affects the wavefunctions and how it affects conductivity.

But first we want to demonstrate the possibility of wavefunction engineering in a DRN. By this term we mean the ability to control the spatial distribution of the electron wavefunction by changing the shape of the confining potential. It is possible to control many of the potential parameters but here we will show the effect of tuning of the position of the QD potential \( V_{QD} \). It can be realized by electrical gating below or above the central part of the DRN. Figure 3 shows the distribution of the ground state wavefunction for three different values of \( V_{QD} \). With increasing...
position of the bottom of the QD potential the wavefunction is moved over from the QD part to the QR part of the DRN.

The wavefunctions have been calculated within the approach No. 1, i.e., by solving the Schrödinger equation only for the radial part $R_{nl}(r)$. For all values of $V_{QD}$ the state with $n = 0$ and $l = 0$ is the ground state. One can see that for $V_{QD} = 0$ the ground state wavefunction is located in the QD part of the DRN. Then, the wavefunction is pushed towards the ring part of the DRN with rising the bottom of the QD potential. The ground state wavefunction has a constant phase and its shape is exactly the same in all three mentioned above approaches. The situation can be different for excited states. Moreover, the spatial distribution of the wavefunctions can be significantly affected by even a very weak coupling to leads. We start the comparison of the wavefunctions calculated within different approaches with the case without leads. Since the ground state in all these methods is almost exactly the same, we start with the excited states. In Fig. 4 one can see the first ($\Psi_{10}$), the second ($\Psi_{01}$) and the third ($\Psi_{0,-1}$) excited states (the second and third are degenerated) calculated within approach no. 1, where the full (complex) wavefunction is given by Eq. (2). These states were calculated for $V_0 = 30$ meV and $V_{QD} = 0$. By comparing with Fig. 3(a) one can infer that these states can be

![Fig. 4](image-url)
located in a different part of the DRN than the ground state. As a result the matrix element between these states and the ground state is small and in Ref. 2 and 3, we have demonstrated that this feature can be used to increase the relaxation time for a spin qubit built on a DRN.

Figure 5 shows the same states calculated by solving the Schrödinger equation discretized in two dimensions and then diagonalized with the help of the Lanczos method (approach No. 2). In this case, the wavefunctions are real. In this approach, the cylindrical symmetry is broken by the discretization of the Schrödinger equation. Therefore, $n$ and $l$ are not good quantum numbers anymore. Of course, the second and the third excited states are still degenerated. One can check that these wavefunctions can be expressed as a linear combination of $\Psi_{0,1}$ and $\Psi_{0,-1}$ (up to a phase factor, see Figs. 4(b), 4(e) and 4(c), 4(f):

$$\Psi_{\text{Fig. 5(b), (e)}} = \frac{1}{\sqrt{2}} (\Psi_{0,1} + \Psi_{0,-1}) , \quad \Psi_{\text{Fig. 5(c), (f)}} = \frac{1}{\sqrt{2i}} (\Psi_{0,1} - \Psi_{0,-1}).$$  (4)

Excited states calculated from the tight-binding model (approach No. 3) are presented in Fig. 6. The wavefunctions are complex (like in approach No. 1), but the cylindrical symmetry of the Hamiltonian is broken (like in approach No. 2). The first excited state, which possesses (at least approximately) the cylindrical symmetry is the same in all the approaches. However, in the next two states, the amplitude of the wavefunctions is angle-dependent, but the modulation is much weaker than in
Fig. 6. The same as in Fig. 4, but calculated within approach No. 3.

approach No. 2. Namely, the wavefunctions do not have nodes in any direction and therefore their phase cannot change discontinuously as in approach No. 2. What is interesting, this holds true only for an insulated system. If the system is even very weakly coupled to leads, the wavefunctions become real with nodes, as in approach No. 2. Such situation is presented in Fig. 7.

If the coupling is very weak, it only breaks the underlying cylindrical symmetry of the original Hamiltonian but the character of the states remains unaffected. The degeneracy of the second and the third excited states shown in Fig. 7 corresponds to the degeneracy of states $\Psi_{01}$ and $\Psi_{0,-1}$. However, when the coupling increases the change of the geometry becomes important and the spatial distribution of the wavefunctions changes as well. The changes are pronounced mainly for states which are located in the ring part of the DRN, i.e., close to the areas where the leads are attached. Figure 8 demonstrates how the ground state for $V_{QD} = 6$ meV (which even in the absence of coupling to leads is located entirely in the QR) evolves with increasing coupling.

One can see there that in the case of strong coupling the wavefunctions are completely different from these in an insulated system and therefore in this regime the Bardeen approach cannot be valid. In order to determine the regime where this approximation can be used, in the next section we compare the coupling constants and conductivities calculated within the Bardeen approach and with the help of the Kwant package for a tight-binding model.
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Fig. 7. The same as in Figs. 6(b), 6(e), 6(c) and 6(f), but for a system very weakly coupled to leads.

Fig. 8. The ground state wavefunction for $V_{\text{QD}} = 6$ meV in the case of (a) weak, (b) average and (c) strong coupling between the DRN and the leads.

4. The Dot–Ring Nanostructure with Leads

In this section, we study a system composed of the DRN and weakly coupled source and drain leads with $\Gamma_S$ and $\Gamma_D$ as the subsequent tunneling rates. We focus here on the case of equal tunnel barriers, i.e., $\Gamma_S = \Gamma_D = \Gamma$. Within the first method, we calculate the tunnel rate for tunneling through state $\Psi_{nl}(r)$ as

$$\Gamma_{nl}(\varepsilon) = 2\pi \sum_k |t_{nlk}|^2 \delta(\varepsilon - \varepsilon_k),$$

(5)
Fig. 9. A fit of the Breit–Wigner formula to a conductance peak for the ground state calculated with the help of Kwant for $V_{QD} = -1$ meV. In this case, the ground state is located in the QD part of the DRN and therefore is very weakly coupled to the leads. Additionally, the leads are relatively far from the center of the DRN in the position presented in Fig. 2(a).

where $t_{nlk}$ is given by Eq. (3). In the following, we restrict our study only to tunneling through the ground state ($n = 0, l = 0$) and skip the indices "00" in $\Gamma_{00}$. Note that the situation where only the ground state is in the bias window $\mu_S - \mu_D$ not always can be realized because for some values of $V_{QD}$ energy levels cross.

Since package Kwant does not allow one to calculate the tunneling rates $\Gamma$ directly, we use the Breit–Wigner formula\textsuperscript{19–21} for the energy-dependent transmission that gives the half-width-at-half-maximum of the conductance peak equal to $\Gamma$:

$$G(\omega) = \frac{e^2}{\hbar} \frac{\Gamma^2}{(\omega - E_0)^2 + \Gamma^2}.$$  \hspace{1cm} (6)

This fit, however, works only for separate peaks in a system with relatively weakly coupled leads. Figure 9 shows how well the Breit–Wigner formula describes the conductance peak in this regime. For a stronger coupling, when the peak broadening is so large that adjoining peaks overlap with each other, this formula does not give good results.

In Fig. 10, we show a comparison of the tunneling rate $\Gamma$ between a lead and the ground state calculated with the help of the Bardeen approach [Eqs. (3) and (5)] and determined from the width of the conductance peak. One can see there that as far as $V_{QD}$ is small, the ground state wavefunction is located in the QD part of the DRN (situation presented in Fig. 3(a) and there is no coupling to the leads. When the bottom of the QD potential is sufficiently high, the wavefunction moves over towards the QR part [Fig. 3(b)] and the coupling increases. For $V_{QD} \approx 5$ meV the wavefunction is entirely in the QR and further increase of $V_{QD}$ does not affect its...

\textsuperscript{a}Our studies are restricted to low temperatures $kT \ll \Gamma$ so the thermal broadening of the conductance peak can be neglected.
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Fig. 10. Comparison of the tunneling rate between the lead and the ground state as a function of $V_{QD}$. The solid line and the stars represent results of the Bardeen approach and Kwant, respectively.

Fig. 11. (Color online) The cross-section of the confining potential with a weakly attached lead for $V_{QD} = 0$. The red arrow illustrates the tunneling between the DRN and the lead. This setup corresponds to the situation presented in Fig. 2(a). The thick dashed green line in the inset shows the position of the cross-section.

shape [Fig. 3(c)]. As a result $\Gamma$ saturates. In the case presented in Fig. 10, the leads where attached at a finite distance from the DRN [see Fig. 2(a)] so the height of the barrier between the nanosystem and the lead was almost $V_1$. Figure 11 shows the cross-section of the confining potential along the $x$-axis. For such a high barrier, the coupling is weak independently of the distribution of the wavefunction. Figure 10 shows that even if $V_{QD}$ is so large that the wavefunction is located only in the outer (QR) part of the DRN, $\Gamma$ calculated within the framework of the Bardeen approach remains in a good agreement with the tight-binding model that takes into account modifications of the wavefunction shape due to attached leads.

However, as the distance between the lead and the DRN decreases, the tunneling barrier becomes smaller and the DRN energy spectrum and shape of the wavefunctions change. Figure 12 presents how the spectrum changes when the lead
is shifted towards the DRN. The energy levels in some regimes linearly increase with increasing $V_{\text{QD}}$ and in others are almost constant. Since $V_{\text{QD}}$ describes the confining potential only in the QD part of the DRN, whereas its shape in the QR parts is constant, states with energies that depend on $V_{\text{QD}}$ are located mostly in the central QD. Figure 12 shows that the energies of these states are not affected by attaching leads, even if the coupling is relatively strong. On the other hand, the
states with energies independent of $V_{QD}$ are located in the QR, where their matrix elements with states in the leads are finite and increase with increasing coupling. As a result their energies do depend on the position of the leads. As shown in Fig. 8, not only the energies, but also the shapes of the wavefunctions are modified in this regime. Both the effects, i.e., the reduction of the tunnel barrier between the DRN and the leads together with the change of the distribution of the wavefunction, lead to a dramatic increase of the coupling between the states in the DRN and in the leads. The resulting change of the tunneling rates is presented in Fig. 13.

5. Summary

Combined quantum structures are highly relevant to new technologies in which the control and manipulations of electron spin and wavefunctions play an important role. In contrast to real atoms, DRNs allow for flexible control over the confinement potential which gives rise to wavefunction engineering. We have shown that the peculiar structure of a DRN allows us to use an electrical gating to manipulate the confinement potential so that the coupling between states in the DRN and in the leads can be changed by orders of magnitude. As a result, by applying the gate voltage one can easily control the conductance of a DRN. The difference between the “traditional” single electron transistor\(^22\) and the DRN is that in our case the Coulomb blockade is not used. Instead, the gate voltage is used to switch it by coupling/decoupling of the DRN to/from the leads.\(^23\)

We have shown that in the case of weakly coupled leads the approximate cylindrical symmetry of the confining potential can be utilized and the Schrödinger equation for only the radial part of the wavefunction can be solved numerically. Then, the Bardeen method can be used to calculate microscopically the geometry-dependent transport properties. However, when the coupling to leads is stronger, the cylindrical symmetry of the wavefunctions is broken and other computational methods must be used. In this paper, we have demonstrated that one of the possibilities is package Kwant, which allows one to do the required calculations relatively easily.

In this paper, we have presented the case of sequential tunneling with only a single state in the bias window. From Fig. 12 one can infer that for some shapes of the confining potential energy levels are very close and such an assumption cannot be fulfilled. When more than one state is in the bias window and all the states are coupled to the leads, charge transport can take place through many states. Then, even if we still assume a single electron transport (the Coulomb blockade does not allow for more than one occupied state to be in the bias window), one has to take into consideration the relaxation processes between different states. Such situation has been analyzed in Ref. 5. The situation becomes much more complicated when more than one electron can occupy the DRN. In this case the Coulomb interaction and the spin degrees of freedom come into play, which gives a possibility to control other properties of the nanosystem. Then, a DRN may turn out to be useful also in
spintronics. The work along this line is in progress and the results will be published elsewhere.\textsuperscript{24}

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**References**