Quantum confinement in mesoscopic annular regions with C_{1v} and $C_{\infty v}$ symmetries

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(Received 31 January 2002; revised manuscript received 19 August 2002; published 14 March 2003)

The single-electron energy spectrum is studied, highlighting axial-symmetry-breaking ($C_{\infty v} \rightarrow C_{1v}$) aspects, in annular two-dimensional and three-dimensional mesoscopic finite-potential wells. The closed analytical forms for the elements of the matrix utilized in calculations are those obtained after satisfying the effective-mass boundary conditions exactly at both the interfaces. The limiting cases when the barrier heights or the effective-mass discontinuities become infinite are analyzed and it is observed that they produce just opposite effects on the finite-well eigenvalues. Also, these cases require the well region wave function to satisfy respectively the Dirichlet and Neumann boundary conditions analogous to the longitudinal fields of the transverse magnetic and transverse electric modes in electromagnetic waveguides with perfect metallic boundaries. The consideration of a "massive wall" thus unveils interesting physics and establishes one-to-one correspondence between electron and electromagnetic waveguides. Moreover, the general trend for doublet splittings when $C_{\infty v} \rightarrow C_{1v}$ in our study under the Dirichlet condition is in conformity with recent experimental observations [Dembowski *et al.*, Phys. Rev. Lett **84**, 867 (2000)].

DOI: 10.1103/PhysRevB.67.113304 PACS number(s): 73.21.−b, 73.61.−r

It is possible to study many salient features of condensed-matter systems through classical (acoustic or electromagnetic wave) analog studies and vice versa.[1,2] A model of the optical waveguide considering light waves in it as though they were electrons trapped in a square potential well was constructed by Tien,[3] and Black and Ankiewicz[4] have presented a unified connection of the fiber optics with the quantum mechanics. The similarity between the free-electron wave functions satisfying hard-wall boundary conditions (BC's) in two-dimensional channels or wires and the electric fields of the TE modes in electromagnetic (EM) waveguides constructed from such systems has been thoroughly investigated by Carini *et al.*[5] both theoretically and experimentally to gain information regarding the electron waveguides through the study of the properties of the EM waveguides. On the other hand, the ideas of electronic band structure and electron localization have been pushed into the realm of electromagnetics wherein the concepts like photonic band structure and light localization have been introduced and have become a dynamic area of research.[2] However, notwithstanding these similarities, there is no one-to-one correspondence between the problems so far as the electron and EM waveguides are concerned: the metallic waveguides[6] can support both TM and TE modes whose longitudinal fields satisfy, respectively, Dirichlet and Neumann BC's whereas the infinite potential wells for electrons give rise to the Dirichlet BC only. Furthermore, the counterparts of the TM and TE modes in optical waveguides are, in general, the hybrid modes[7] containing longitudinal components of both magnetic and electric fields. Hence in order to have larger symbiotic enrichment through conceptual unification in the studies of EM and quantum-mechanical systems, there is a need to discuss the physical situation across the interface boundaries that would entertain Neumann BC in latter systems as well.

The finite band offset between the well and barrier materials in semiconductor heterostructures creates soft-wall confinement (SWC). The continuity of the electron wave function as well as the quantity $\nabla\psi(\mathbf{r})/m^*(\mathbf{r})$ across the interfaces in such systems constitutes the effective-mass BC (EMBC),[8] with $m^*(\mathbf{r})$ as the space-dependent effective mass. The theoretical investigations of electronic properties are generally carried out also by considering a hard-wall condition (HWC). However, there is possibility of an alternative limiting situation by considering a very large discontinuity in the effective mass of an electron across the well-barrier interface boundary giving rise to a massive-wall condition (MWC).[9,10] It is found that the MWC appearing as the limiting offshoot of the SWC for square, spherical or cylindrical well satisfies zero-slope condition whereas the HWC requires vanishing of $\psi(\mathbf{r})$ at an interface boundary. The former and the latter are typically akin to the BC satisfied, respectively, by the TE and TM modes in perfect metallic waveguides. Thus the consideration of MWC together with HWC ensures one-to-one correspondence between electron and perfect metallic waveguides. This unveiling of interesting symmetry constitutes the first purpose of this paper.

The cylindrical quantum wires—simply connected,[11–13] nested structures,[10,14,15] and double-wire systems[16]—have attracted a lot of interest in recent years for the study of a variety of physical phenomena. Also, the realization by Kim *et al.*[15] that the curvature can be regarded as a geometric degree of freedom in nanosystems has gained support in recent studies[17,18] since the presence of a curved geometry exhibits some physical properties which do not exist in the corresponding flat or untwisted structures. We were wondering regarding the role that the topology of the nested structures in conjugation with the MWC could play and hence the analysis of these aspects through the study of the single-electron energy spectrum in eccentric annular nanoregions constitutes to be our second purpose. The EMBC (Ref. 8) have been satisfied[19] exactly at each of the interfaces making use of the Graf's addition theorems[20] for the cylindrical Bessel functions. The theorem helps in shifting the origin of

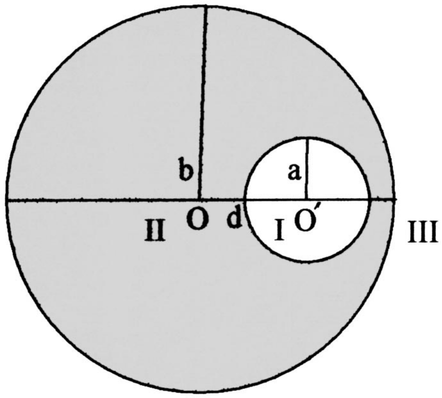

FIG. 1. Cross-sectional view of an eccentric annular well. The radii of inner and outer circles are a and b; eccentricity $OO'=d$.

the wave function from one point to the other in the considered two-center problem with C_{1v} symmetry. The analysis leads to a doubly infinite determinantal equation whose zeros give the energy eigenvalues of the system. The expressions for the elements of the determinant are in closed analytical forms which show correct behavior for various limiting cases and reproduce the results obtained earlier by us[10] and also by other workers.[12–14]

We consider a system wherein an electron is free to move along the axial direction, assumed to be parallel to the z axis of the cylindrical polar coordinates (ρ, ϕ, z), in an annular potential well (region II) lying between two cylindrically symmetric barriers (regions I and III). The radii of the cross-sectional interface boundaries of I-II and II-III are, respectively, a and b whereas region III extends up to infinity. We introduce a parameter d, the separation between the centers O and O' of these two circular cross-sectional boundaries (Fig. 1), as eccentricity of region I such that $0\leqslant d\leqslant(b-a)$. The nonzero value of d corresponds to the geometrical symmetry breaking giving rise to the topological aspect and resulting into a two-center problem when the complete axial symmetry $C_{\infty v}$ of the system reduces to C_{1v}.

The transverse motion of an electron is size quantized due to a regionwise constant potential profile taken to be of the form $U_\ell(\mathbf{r})=(1-\delta_{\ell,2})V_\ell$, where $\delta_{\ell,2}$ is the Kronecker delta function and ℓ=1, 2, and 3 represent regions I, II, and III, respectively. The solutions of the effective-mass Schrödinger equation in the three regions with the origin at O' of the cylindrical coordinates (ρ', ϕ', z') can be written as $\Psi_{\rm I}=\Sigma_{m=0}^{\infty}A_m I_m(k_1\rho')\chi_m$, $\Psi_{\rm II}=\Sigma_{m=0}^{\infty}[B_m J_m(k_2\rho')+C_m Y_m(k_2\rho')]\ \chi_m$, and $\Psi_{\rm III}=\Sigma_{m=0}^{\infty}D_m K_m(k_3\rho')\ \chi_m$, where $\chi_m=\sin(m\phi'+\phi_o)\exp(i\beta z')$, $J_m(x)$ and $Y_m(x)$ are the cylindrical Bessel functions of the first and second kinds, $I_m(x)$ and $K_m(x)$ are their modified counterparts, β is the axial wave number, and ϕ_o is $\pi/2$ (zero) for even (odd) parity states. Also, we have $k_\ell^2=(-1)^\ell[2m_\ell^*(E-U_\ell)/\hbar^2-\beta^2]$, where m_ℓ^* is the effective mass in the ℓth region and E denotes electronic energy. The choice β=0 corresponds to the solutions for the eccentric annular circular regions.

The EMBC can be satisfied straightway at I-II interface where $\rho'=a$ but in order to apply the same at II-III interface $\Psi_{\rm II}$ and $\Psi_{\rm III}$ are needed explicitly in terms of ρ and ϕ defined with respect to O. This has been achieved using the addition theorems[20] expressed[21,22] as

$$K_m(k_3\rho')\sin(m\phi'+\phi_o)=\sum_{p=-\infty}^{\infty}K_p(k_3\rho)I_{p-m}(k_3d)\sin(p\phi+\phi_o)\quad(1)$$

and

$$Z_m(k_2\rho')\sin(m\phi'+\phi_o)=\sum_{p=-\infty}^{\infty}Z_p(k_2\rho)J_{p-m}(k_2d)\sin(p\phi+\phi_o),\quad(2)$$

with $Z_m(x)$ standing for $J_m(x)$ or $Y_m(x)$. We thus obtain ultimately, after satisfying the EMBC at the II-III interface, an infinite set of linear homogeneous equations whose nontrivial solutions require that det$|P_{mn}^{\rm SWC}|=0$, where

$$P_{mn}^{\rm SWC}=[F_m(k_1,k_2)S_n(k_2,k_3)+G_m(k_1,k_2)T_n(k_2,k_3)]W_{mn}(k_2d)\quad(3)$$

with

$$W_{mn}(k_2d)=J_{n-m}(k_2d)+(-1)^{m+1}\cos2\phi_oJ_{n+m}(k_2d),\quad(4)$$

$$F_m(k_1,k_2)=\frac{\pi a}{2m_1^*}[k_2m_1^*I_m(k_1a)Y_m'(k_2a)-k_1m_2^*I_m'(k_1a)Y_m(k_2a)],\quad(5)$$

$$G_m(k_1,k_2)=\frac{\pi a}{2m_1^*}[k_1m_2^*I_m'(k_1a)J_m(k_2a)-k_2m_1^*I_m(k_1a)J_m'(k_2a)],\quad(6)$$

$$S_n(k_2,k_3)=m_2^*k_3K_n'(k_3b)J_n(k_2b)-m_3^*k_2K_n(k_2b)J_n'(k_3b),\quad(7)$$

and

$$T_n(k_2,k_3)=m_2^*k_3K_n'(k_3b)Y_n(k_2b)-m_3^*k_2K_n(k_2b)Y_n'(k_3b).\quad(8)$$

If we consider the limiting cases $V_1=V_3\to\infty$ and $m^*\equiv m_1^*/m_2^*=m_3^*/m_2^*\to\infty$ which correspond to HWC and MWC, respectively, we get

$$P_{mn}^{\rm HWC}=[J_m(k_2a)Y_n(k_2b)-J_n(k_2b)Y_m(k_2a)]W_{mn}(k_2d)\quad(9)$$

and

$$P_{mn}^{\rm MWC}=[J_m'(k_2a)Y_n'(k_2b)-J_n'(k_2b)Y_m'(k_2a)]W_{mn}(k_2d)\quad(10)$$

which have the forms identical with those obtained[23] for the propagation of TM and TE modes in an off-centered annular cylindrical EM waveguide with perfect metallic boundaries. The substitution $d=0$ in Eq. (9) yields expression studied by Masale *et al.*[13] in the context of coaxial quantum wires. The

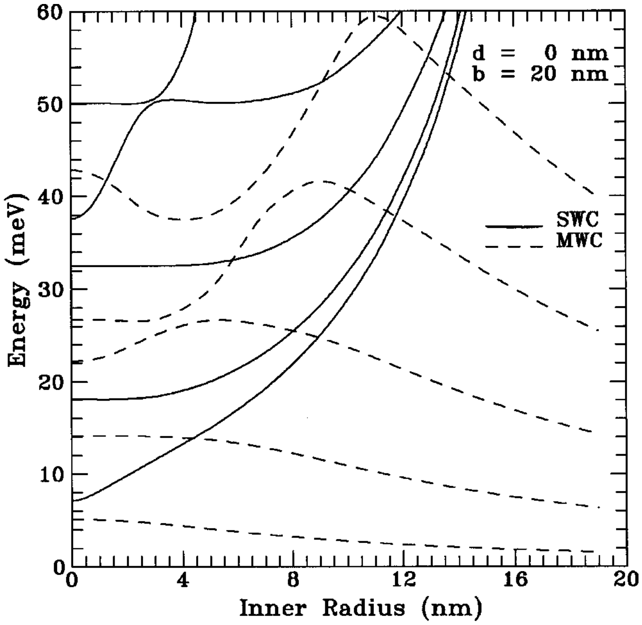

FIG. 2. Comparison between SWC and MWC eigenenergies as a function of inner radius in a concentric annular region.

expression $P_{mn}^{\mathrm{HWC}}(d=0)$ together with $P_{mn}^{\mathrm{MWC}}(d=0)$ were analyzed by us too in Ref. 10. The substitution $a=d=0$ yields $P_{mn}^{\mathrm{HWC}}=J_m(k_2b)\,\delta_{mn}$ and $P_{mn}^{\mathrm{MWC}}=J_m'(k_2b)\,\delta_{mn}$ which arise[6] also in the study of metallic cylindrical waveguides and the former one was utilized by Constantinou and co-workers[12,13] for simply connected cylindrical quantum wires.

The calculations have been performed for a system consisting of GaAs in region II and $Ga_{0.7}Al_{0.3}As$ in regions I and III. We have set $\beta=0$ and $b=20$ nm, and have taken $V_1=V_3=190$ meV, $m_2^*=5.73\times10^{-32}$ kg, and $m_1^*=m_3^*=1.4m_2^*$. Figure 2 compares variation in energy of five low-lying states as a function of a in a coaxial, i.e., $C_{\infty v}$, system under SWC and MWC. It can be seen that any MWC state has lower (just opposite to the known HWC) eigenvalue as compared to the corresponding SWC state. Although the curves for both SWC and HWC (not plotted) continuously rise with increase in a, each of the plots of MWC excited levels shows a peak which becomes more and more pronounced and shifts towards higher value of a as the level becomes higher and higher.

Figure 3(a) shows that twofold degenerate levels separate into even and odd parity states for $C_{\infty v}\to C_{1v}$, i.e., when $d>0$. For $d\ll b$, the system tends to behave like a coaxial annular structure whereas for $d\to(b-a)$, i.e., when the inner region almost touches the outer interface boundary, the system is nearly the same as a simply connected system since we have taken $a=0.05b$. Thus for both the limiting locations of the inner barrier we get results almost identical with $C_{1v}\to C_{\infty v}$ under all the three confining situations. It is worth mentioning here that recently Dembowski *et al.*[24] have extracted information regarding the quasidoublet splittings from their experiments for chaos-assisted tunneling in a microwave annular billiard, a structure corresponding to our C_{1v} system under HWC. Although it is not possible to compare directly our numerical values with their reported results

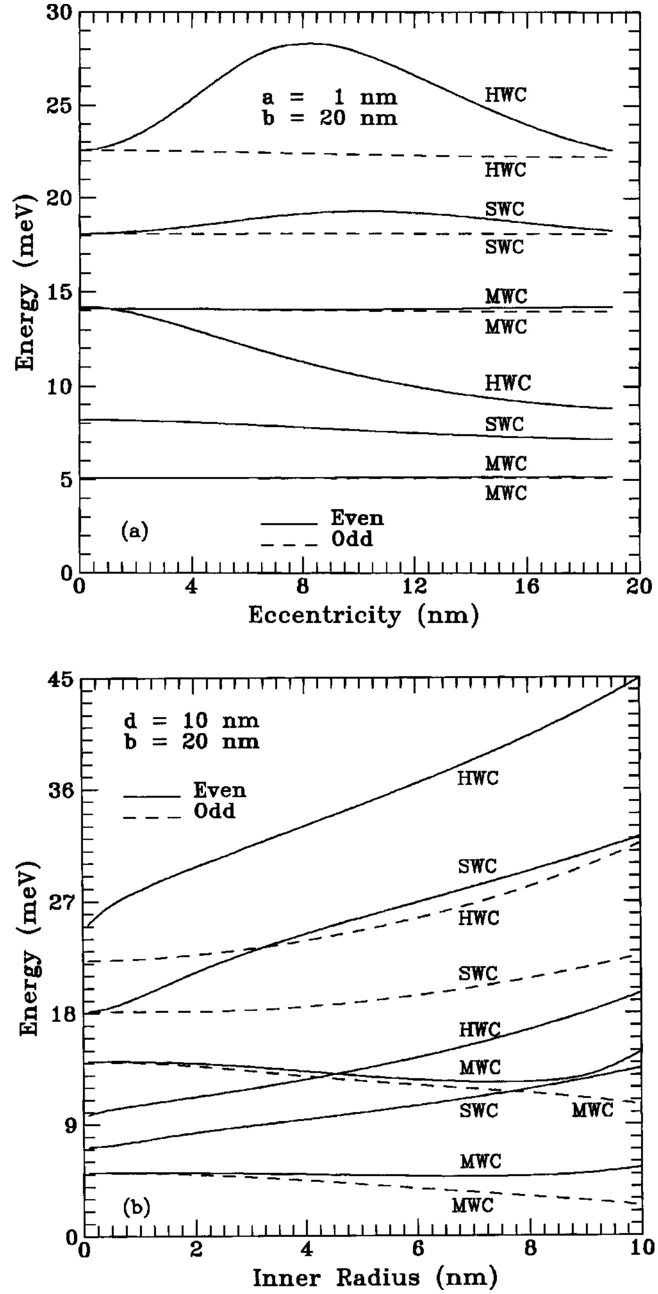

FIG. 3. Variation of eigenenergies as a function of (a) eccentricity for a fixed inner radius and (b) inner radius for a fixed eccentricity.

but our calculations are in confirmity with their general findings for the eigenvalues so far as small quasidoublet splittings and ultimate systematic destruction of the doublet structures with continuous increase in eccentricity are concerned.

We find in Fig. 3(b) that the energies increase with increase in a both for SWC and HWC as expected. However, one observes that for MWC the energies of the odd parity states decrease with increase in a. Also, the eigenvalues of even and odd parity states for MWC have different trends unlike SWC and HWC where both the parities show almost identical behavior. Finally, Fig. 4 depicts that increase in m^*,

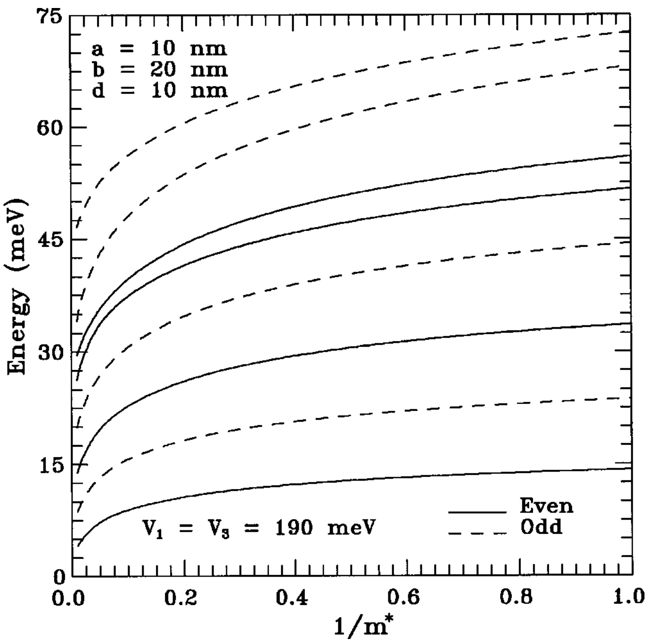

FIG. 4. Effect of barrier-to-well effective mass on eigenenergies in an eccentric annular well.

the barrier-to-well effective mass, for fixed barrier heights leads to decrease in the eigenvalues, a trend which is just opposite to that wherein increase in confining potentials for any fixed m^* is known to show monotonic increase in the eigenenergies. It seems pertinent to mention that variation in m^* for a fixed value of the barrier height does not have *a priori* justification and the study of the effect of a massive wall is on the same footing as consideration of a hard wall for any fixed value of m^*.

Thus it is observed that decrease in the size of the well or increase in the height of the barrier potential pushes the energy levels upwards, as expected, but the levels get pushed downwards as one moves toward the MWC. The decrease in the symmetry from $C_{\infty v}$ to C_{1v} leads to bifurcation of even and odd parity states and the separation of the levels depends on the value of the eccentricity. Hence an appropriate choice of various geometrical and physical parameters would provide a recipe to have the separation between a pair of given levels around a desired value. Furthermore, the approach utilized here can be extended to deal with the energy spectrum for a structure wherein *n* cylindrical wires could be arranged on a ring such that the system as a whole possesses C_{nv} symmetry, particularly coupled[16] quantum wires with C_{2v} symmetry, and our group-theoretic analysis[22] would be helpful in such an endeavor.

In summary, the role of topology and the effect of massive-wall condition on the eigen-spectrum together with one-to-one correspondence between electron and EM waveguides have been elaborated. Our calculations under the Dirichlet BC for the quasidoublet splittings when $C_{\infty v} \rightarrow C_{1v}$ are in confirmity with the experimentally observed[24] trends. The fast convergence characteristics of our semianalytical approach would make it ideally suited for investigating the behavior of higher excited states too in broken axial-symmetry situations.

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