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Curvature-induced geometric potential in strain-driven nanostructures

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We derive the effective dimensionally reduced Schrödinger equation for electrons in strain-driven curved nanostructures by adiabatic separation of fast and slow quantum degrees of freedom. The emergent strain-induced geometric potential strongly renormalizes the purely quantum curvature-induced potential and enhances the effects of curvature by several orders of magnitude. Applying this analysis to nanocorrugated thin films shows that this curvature-induced potential leads to strongly enhanced electron localization and the opening of substantial band gaps.

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I. INTRODUCTION

The experimental progress in synthesizing low-dimensional nanostructures with curved geometries—the next generation nanodevices[1–4]—has triggered the interest in the theory of quantum physics on bent two-dimensional manifolds. The theoretical description of the quantum motion of a particle constrained to a curved space has been a matter of controversy for a long time.[5–8] The problem arises because Dirac quantization on a curved manifold leads to operator-ordering ambiguities.[5] However, the thin-wall quantization procedure, introduced in the 1970s by Jensen and Koppe,[6] and generalized by da Costa (JKC),[7] circumvents this pitfall. It treats the quantum motion on a curved two-dimensional (2D) surface as the limiting case of a particle in three-dimensional (3D) space subject to lateral quantum confinement. Within the JKC method the surface curvature is eliminated from the Schrödinger equation at the expense of adding a potential term to it. This simplifies the problem substantially, as the quantum carriers now effectively live in a 2D space, in presence of a curvature-induced quantum geometric potential (QGP).

The quantum origin of the QGP—it is in magnitude proportional to $\hbar$—causes its physical consequences in condensed matter systems to be observable only on the nanoscale. In this realm the QGP can cause intriguing phenomena.[9–16] For instance, a quantum particle constrained to a periodically curved surface senses a periodic QGP acting as a topological crystal.[10] Likewise the QGP in spirally rolled-up nanostructures leads to winding-generated bound states.[17,18] However, the experimental realization and exploitation of such phenomena is hindered by the fact that in actual systems with curvature radii on the order of a few hundred nanometers, the QGP is still very weak and typically only comes into play on the sub-Kelvin energy scale.

In this work, we mitigate this problem by developing a thin-wall quantization procedure which explicitly accounts for the effect of the deformation potentials of the model-solid theory.[19,20] By employing a method of adiabatic separation of fast and slow quantum degrees of freedom, we show that the local variation of the strain induced by the curvature gives rise to a strain-induced geometric potential (SGP) that is of the same functional form as the QGP, but strongly (often gigantically) boosting it. This implies that on a phenomenological level one cannot distinguish between curvature-induced quantum effects and curvature-induced strain effects in nanosystems, in practice both are always present, contributing in different amount to the same geometric potential. The theoretical framework that we develop is immediately relevant for electronic nanodevices as the present-day nanostructuring method[1,2] is based on the tendency of thin films detached from their substrates to assume a shape yielding the lowest possible elastic energy. As a result, thin films can either roll up into tubes[21,22] or undergo wrinkling to form nanocorrugated structures.[3,23,24] A key property of such bent nanostructures is the nanoscale variation of the strain. This for instance leads to considerable band-edge shifts[25] with regions under tensile and compressive strain shifting in opposite direction. Strain is thus widely used and applied in nanosystems and here we put its coupling to the electronic structure of 2D curved manifolds on a formal basis. To do so one obviously needs to go beyond the JKC thin-wall quantization framework since strain variations intrinsically couple the transversal quantum degrees of freedom to the tangential quantum motion along the curved surface. The ensuing theoretical framework we apply to nanocorrugated thin films, analyzing the effect of the SGP on its electronic states and we establish a continuous crossover upon increasing strain from extended-like electronic states to states localized precisely at the points of maximum and minimum curvature.

II. ADIABATIC APPROXIMATION

In the thin-wall approach the lateral confinement raises quantum excitation energies in the normal direction far beyond those in the tangential direction. Hence one can safely neglect the quantum motion in the normal direction and derive an effective, dimensionally reduced, Schrödinger equation. As opposed to a classical particle, a quantum particle constrained to a curved surface retains some knowledge of the surrounding 3D space. In spite of the absence of interactions, it indeed experiences the well-known attractive QGP.[7] It has been shown that the JKC thin-wall quantization procedure to derive the effective Schrödinger equation is well founded, also in presence of externally applied electric and magnetic fields.[26,27] Empirical evidence for the validity of this approach is provided by the experimental realization of an optical analog of the curvature-induced geometric potential.[28] To develop a theoretical framework for SGPs we therefore use the conceptual framework of JKC. We start the mathematical description by defining a 3D curvilinear coordinate system (see Fig. 1) for a generic bent nanostructure. The stress-free surface

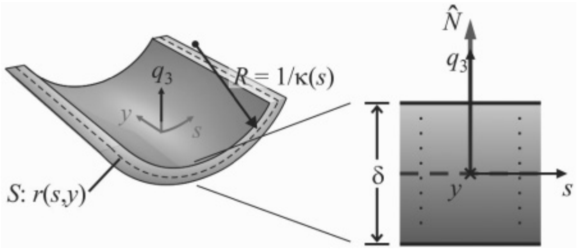

FIG. 1. Schematics of the three-dimensional coordinate system for a strain-driven bent nanostructure with positive radius of curvature R and total thickness δ. The $q_3 = 0$ surface $\mathcal{S}$ corresponds to the stress-free surface. Regions with $q_3 > 0$ ($q_3 < 0$) are under compressive (tensile) strain.

$\mathcal{S}$ is parametrized as $\mathbf{r} = \mathbf{r}(s,y)$, where y is the coordinate along the translational invariant direction of the thin film and s is the arc length along the curved direction of the surface $\mathcal{S}$ measured from an arbitrary reference point. Nothing prevents the thin film to be also deflected along the y direction, but in the remainder we will neglect this effect for simplicity. The 3D portion of space of the thin film can be then parametrized as $\mathbf{R}(s,y,q_3) = \mathbf{r}(s,y) + q_3 \hat{N}(s)$ with $\hat{N}(s)$ the unit vector normal to $\mathcal{S}$. We can evaluate the strain distribution in the thin film by assuming the plane strain condition[29] $\epsilon_y \equiv 0$. This assumption is well justified whenever the dimension of the structure in the y coordinate is very large as compared to the structural dimension in the other coordinates. It is well known[30] that the strain in the direction along the surface varies linearly across the thin film as $\epsilon_s = -q_3 \kappa(s)$, where $\kappa(s)$ is the principal curvature of the surface $\mathcal{S}$. The strain in the normal direction can be related to ϵ_s by means of the Poisson relation $\epsilon_{q_3} = -[\nu/(1-\nu)]\,\epsilon_s$ with ν the Poisson ratio. From the linear deformation potential theory[19] we know there is a strain-induced shift of the conduction band corresponding to a local potential for the conducting electrons $\mathcal{V}_\epsilon(s,q_3) = \gamma\, q_3 \kappa(s)$ with $\gamma > 0$, yielding an attraction toward regions under tensile strain (cf. Fig. 1). The characteristic energy scale γ which can be explicitly computed in the different conduction valleys of the nanostructure is proportional to the shear and the hydrostatic deformation potentials and typically lies in the electron volt scale for conventional semiconductors.[19] By adopting Einstein summation convention, the Schrödinger equation for the quantum carriers in the effective mass approximation then takes the following compact form[26,27]:

$$-\frac{\hbar^2}{2m^\star} G^{ij}\,\mathcal{D}_i\,\mathcal{D}_j\,\psi + \mathcal{V}_\epsilon(s,q_3)\,\psi = E\,\psi. \qquad (1)$$

G^{ij} corresponds to the 3D metric tensor of our coordinate system, the covariant derivative $\mathcal{D}_i$ is defined as $\mathcal{D}_i = \partial_i v_j - \Gamma_{ij}^{k} v_k$ with v_j the covariant components of a generic 3D vector field, and the Γ_{ij}^{k} are the Christoffel symbols. By expanding Eq. (1) by covariant calculus[26,27] we get

$$E\,\psi = \left[-\frac{\hbar^2}{2m^\star H_S}\partial_s\left(\frac{1}{H_S}\partial_s\right) - \frac{\hbar^2}{2m^\star H_S}\partial_{q_3}\left(H_S\,\partial_{q_3}\right) - \frac{\hbar^2}{2m^\star}\partial_y^2 + \mathcal{V}_\epsilon(s,q_3) + \mathcal{V}_\lambda(q_3)\right]\psi, \qquad (2)$$

where we defined $H_S = 1 - \kappa(s)\,q_3$, and we introduced a squeezing potential in the normal direction $\mathcal{V}_\lambda(q_3)$. In the following it will be considered as given by two infinite step potential barriers at $\pm\delta/2$, where δ is the total thickness of the thin film. However, our results can be straightforwardly generalized to other types of squeezing potential, for example, harmonic traps.

In the same spirit of the thin-wall quantization procedure[7] we next introduce a new wave function χ for which the surface density probability is defined as $\int |\chi(s,y,q_3)|^2 dq_3$. Conservation of the norm requires $\chi = \psi \times H_S^{1/2}$. The resulting Schrödinger equation is then determined by the Hamiltonian

$$\begin{aligned}\mathcal{H} = &-\frac{\hbar^2}{2m^\star}\partial_y^2 - \frac{\hbar^2}{2m^\star}\frac{\partial_s^2}{H_S^2} + \frac{\hbar^2}{m^\star}\frac{\partial_s H_S\,\partial_s}{H_S^3} - \frac{\hbar^2}{2m^\star}\partial_{q_3}^2 \\ &- \frac{\hbar^2}{2m^\star}\left[\frac{5}{4}\frac{(\partial_s H_S)^2}{H_S^4} - \frac{\partial_s^2 H_S}{2\,H_S^3}\right] - \frac{\hbar^2}{2m^\star}\frac{\left(\partial_{q_3} H_S\right)^2}{4\,H_S^2} \\ &+ \mathcal{V}_\lambda(q_3) + \mathcal{V}_\epsilon(s,q_3). \end{aligned} \qquad (3)$$

Assuming the thickness of the thin film δ to be small compared to the local radius of curvature $R(s) = \kappa(s)^{-1}$, the Hamiltonian Eq. (3) can be expanded as $\mathcal{H} = \sum_k q_3^k\,\mathcal{H}_k$. At the zeroth order in q_3 we recover precisely the effective JKC Hamiltonian[6,7] which disregards the strain-induced shifts of the conduction band and guarantees the separability of the tangential motion from the transverse one. Thus in this case the effect of the curvature results in the well-known QGP, $\mathcal{V}_g(s) = -\hbar^2\kappa(s)^2/(8\,m^\star)$. Strain effects can be explicitly monitored by retaining terms linear in q_3 in which case we obtain the effective Hamiltonian

$$\begin{aligned}\widetilde{\mathcal{H}} = &-\frac{\hbar^2}{2m^\star}\left(\partial_y^2 + \partial_s^2 + \partial_{q_3}^2\right) + \mathcal{V}_g(s) + \mathcal{V}_\lambda(q_3) + \mathcal{V}_\epsilon(s,q_3) \\ &- \frac{\hbar^2}{4m^\star}\left[\partial_s^2\kappa(s) + \kappa(s)^3\right]q_3 - \frac{\hbar^2}{m^\star}q_3\,\partial_s[\kappa(s)\partial_s]. \end{aligned} \qquad (4)$$

The strong size quantization along the normal direction allows us to employ the adiabatic approximation and solve the Schrödinger equation for the effective Hamiltonian Eq. (4) considering the ansatz for the wave function $\chi(s,y,q_3) = \chi^N(s,q_3) \times \chi^T(s,y)$, where the normal wave function χ^N solves at fixed s the one-dimensional Schrödinger equation for the "fast" normal quantum degrees of freedom

$$\left[-\frac{\hbar^2}{2m^\star}\partial_{q_3}^2 + \widetilde{\gamma}(s)\kappa(s)q_3 + \mathcal{V}_\lambda(q_3)\right]\chi_i^N = E_i^N(s)\chi_i^N. \qquad (5)$$

Here i indicates the transversal subband index and $\widetilde{\gamma}(s) = \gamma - \hbar^2[\kappa(s)^2 + \partial_s^2\kappa(s)/\kappa(s)]/(4m^\star)$ corresponds to the typical energy scale of the deformation potential locally renormalized by curvature effects. The latter term yields an attraction toward regions under compressive strain (where the local curvature is higher) competing with the dominant strain-induced attraction toward the tensile regions of the nanostructure [cf. Fig. 2(a)]. The Hamiltonian for the slow tangential quantum motion can be found by first integrating out the q_3 quantum degree of freedom and then performing the additional rescaling of the tangential wave function $\chi^T \rightarrow \chi^T \times \sqrt{1 + 2\kappa(s)\langle\chi^N|q_3|\chi^N\rangle}$.

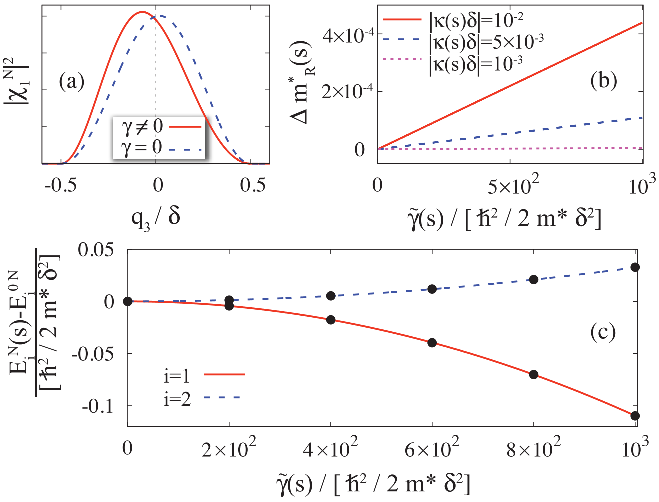

FIG. 2. (Color online) (a) Schematics of the electron density probability in the lowest normal eigenstate as a function of the coordinate q_3 measured in units of the thin film thickness δ for a positive value of the local curvature in a strain-free ($\gamma = 0$) and a strained ($\gamma \neq 0$) curved nanostructure. The vertical dashed line indicates the stress-free surface $q_3 = 0$. (b) Deviation of the locally renormalized effective mass $\Delta m^\star_R(s) = [m^\star_R(s) - m^\star]/m^\star$ as a function of the typical energy scale $\tilde{\gamma}(s)$ for different values of the expansion parameter $\kappa(s)\delta$. (c) Behavior of the adiabatic potentials $E^N(s)$ for the first two transversal subband measured from the quantum well levels $\hbar^2\pi^2 i^2/(2m^\star\delta^2)$ for $\kappa(s)\delta = 10^{-2}$ as a function of $\tilde{\gamma}(s)$. The continuous lines indicate the exact behavior, whereas the points are the results of the perturbation theory approximation.

The final form of the dimensionally reduced tangential Hamiltonian is as follows:

$$\mathcal{H}^T = -\frac{\hbar^2}{2m^\star_R(s)}\partial_s^2 - \frac{\hbar^2}{2m^\star}\partial_y^2 - \frac{\hbar^2}{8m^\star}\kappa(s)^2 + E^N(s) + \cdots, \tag{6}$$

where the $\cdots$ indicate the diagonal adiabatic corrections and we introduced the locally renormalized effective mass $m^\star_R(s) = m^\star/[1 + 2\kappa(s)\langle\chi^N|q_3|\chi^N\rangle]$. Figure 2(b) shows the deviation of the locally renormalized effective mass from its bare value for different values of the expansion parameter $\kappa(s)\delta$. The strain-induced localization of the normal wave function in the tensile regions of the nanostructure leads to an heavier effective local mass in the curved direction which is enhanced at the points of maximum curvature. This is contrary to the lighter local effective mass one would find in the absence of strain effects. Even for values of the local energy scale $\tilde{\gamma}(s)$ much larger than the characteristic energy of the normal quantum well energy $\hbar^2/(2m^\star\delta^2)$, this local renormalization of the effective mass is so small that for all practical purposes the use of the isotropic bare effective mass in Eq. (6) is justified. More rigorously one can show the reliability of this approximation in the regime $\tilde{\gamma}(s)\,\kappa(s)\,\delta \leqslant \hbar^2/(2m^\star\delta^2)$ where the strain-induced linear potential appearing in the fast Schrödinger Eq. (5) can be treated perturbatively. Since such a condition is typically satisfied in conventional semiconducting nanostructures with a total thickness in the nanometer scale, we will limit ourselves to this regime from here onwards.

In Fig. 2(c) we show the behavior of the adiabatic potentials in the first two transversal subband measured from the normal quantum well levels $E_i^{0\,N}$. The characteristic quadratic dependence on the local energy scale $\tilde{\gamma}(s)$ is well reproduced by the analytical formula $E_i^N(s) = E_i^{0\,N} + 2\,m^\star\,\delta^4\,\tilde{\gamma}(s)^2/\hbar^2 \times f_i\,\kappa(s)^2$ with the numerical constants that can be calculated using second-order perturbation theory as $f_1 \sim -10^{-3}$, $f_2 \sim 3 \times 10^{-4}$, etc. From this it also follows that the distance among the potential energy surfaces $E_2^N(s) - E_1^N(s) > E_2^{0\,N} - E_1^{0\,N}$ thereby guaranteeing the reliability of the adiabatic approximation in the regime $\kappa(s)\delta \ll 1$. As a result, we then find the effective Hamiltonian for the electronic motion along the curved nanostructure which in the first transversal subband reads

$$\begin{aligned}\mathcal{H}^T = & -\frac{\hbar^2}{2m^\star}\left(\partial_y^2 + \partial_s^2\right) - \frac{\hbar^2\kappa(s)^2}{8m^\star}v_R \\ & + |f_1|\,\gamma\,\delta^4\,\kappa(s)\left[\kappa(s)^3 + \partial_s^2\kappa(s)\right] \\ & - \frac{\hbar^2\delta^4|f_1|}{8m^\star}\left[\kappa(s)^3 + \partial_s^2\kappa(s)\right]^2,\end{aligned} \tag{7}$$

where we left out the constant energy term $\hbar^2\pi^2/(2m^\star\delta^2)$ and we neglected the diagonal adiabatic corrections. The second term in Eq. (7) corresponds to the QGP whose strength is renormalized by the SGP as $v_R = 1 + 4|f_1|(2m^\star\delta^2\gamma/\hbar^2)^2$. Remarkably we find this renormalization to become extremely large in case of the natural hierarchy of energy scales

$$\gamma \gg \frac{\hbar^2}{2m^\star\delta^2} \gg \frac{\hbar^2}{2m^\star R(s)^2}. \tag{8}$$

Considering for instance a value of $\gamma \sim 10$ eV, a characteristic quantum well energy $\hbar^2/(2m^\star\delta^2) \sim 5$ meV and the typical tangential kinetic energy $\hbar^2/[2m^\star R(s)^2] \sim 1\ \mu$eV, we find an enhancement of the curvature-induced potential by $\sim 10^4$. As we show below, this gigantic renormalization of the geometric potential has profound consequences on the electronic properties of low-dimensional nanostructures with curved geometry. It is worth noting that in absence of strain effects ($\gamma \to 0$), Eq. (7) corresponds to the effective JKC tangential Hamiltonian augmented with an higher order curvature-induced geometric potential $\propto \kappa(s)^6$ arising as a consequence of the finite thickness of the thin-film nanostructure.

III. NANOCORRUGATED THIN FILMS

We now use this theoretical framework to analyze the influence of the SGP on the electronic states of a nanocorrugated thin film with period $2\pi/q$ and total thickness δ [cf. Fig. 3(a)]. The stress-free surface can be parametrized in the Monge gauge as $q_3(x) = A\,\cos q\,x$ where A is the amplitude of the corrugation. In the shallow deformation limit $Aq \ll 1$, we can express the arc length of the layer $s \simeq x$, whereas the local curvature of the stress free surface $\kappa(s) \simeq \partial_s^2 q_3(s) \simeq -A\,q^2\cos(q\,s)$. Thus the problem reduces to the "flat" motion of free electrons embedded in a curvature-induced periodic potential. It is straightforward to obtain the energy spectrum of the "slow" tangential motion of Hamiltonian Eq. (7) in the first transversal subband for a thin film thickness much smaller than the corrugation wavelength

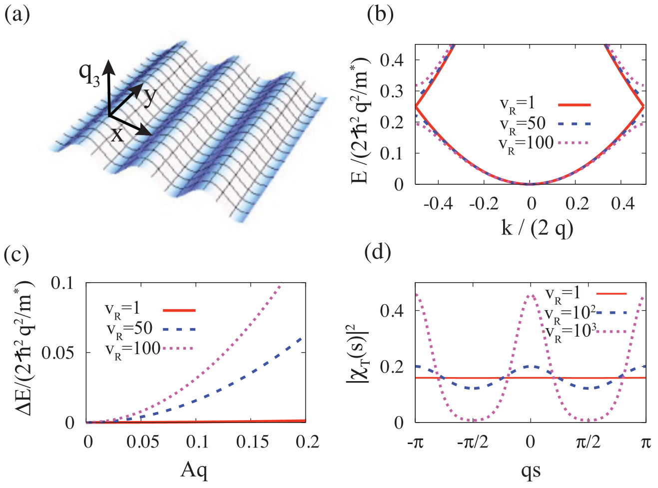

FIG. 3. (Color online) (a) Sketch of the stress-free surface of a nanocorrugated thin film. (b) Band structure of a nanocorrugated film with $Aq \equiv 0.2$ and different values of the geometric potential renormalization factor v_R. We show only the first two bands close to the bottom of the conduction band. (c) Behavior of the topological band gap as a function of the dimensionless parameter Aq for different values of v_R. (d) Tangential ground state density probability for $Aq \equiv 0.2$ and different values of the renormalization strength of the geometric potential.

as in this case the last two terms in Eq. (7) can be neglected. Figure 3(b) shows the behavior of the first two bands for different values of v_R. The zero of the energy has been chosen as the bottom of the conduction band. The qualitative behavior of the band structure is maintained when curvature effects are taken into account, but now with a curvature-induced gap[31] ΔE at momenta $k = \pm q$. These gaps increase quadratically in magnitude with the deformation potential γ, as $\Delta E \sim v_R \hbar^2 A^2 q^4/(16m^\star)$, in agreement with the numerical analysis [cf. Fig. 3(c)]. In Fig. 3(d) we show the ground state electron density for different values of v_R. By increasing strain effects, one finds a continuous crossover from extended-like states to electronic states localized precisely at the points of maximum and minimum curvature, which is in accordance with the results of a purely numerical approach.[32]

IV. CONCLUSIONS

We have derived, in conclusion, a dimensionally reduced Schrödinger equation in electronically two-dimensional, strain-driven nanostructures by employing a method of adiabatic separation of fast and slow quantum degrees of freedom. The strain effects render an often gigantic renormalization of the curvature-induced quantum geometric potential which has very significant consequences for the electronic properties of these materials. Applying our theoretical framework to the case of nanocorrugated thin films we find an enhanced electron localization and the opening of substantial band gaps on an experimentally relevant energy scale. It can also be applied to, for instance, 2D nanotubes rolled up in the shape of an Archimedean spiral, where the effect of the geometric quantum potential leads to shallow bound states whose number coincides with the winding number.[18] The inclusion of strain effects should lead to a very substantial deepening of such bound states, which will strongly affect the electronic and transport properties of such rolled-up nanostructures.

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