Absence of anomalous couplings in the quantum theory of constrained electrically charged particles

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The experimental progress in synthesizing low-dimensional nanostructures where carriers are confined to bent surfaces has boosted the interest in the theory of quantum mechanics on curved two-dimensional manifolds. It was recently asserted that constrained electrically charged particles couple to a term linear in A_3M, where A_3 is the transversal component of the electromagnetic vector potential and M is the surface mean curvature, thereby making a dimensional reduction procedure impracticable in the presence of fields. Here we resolve this apparent paradox by providing a consistent general framework of the thin-wall quantization procedure. We also show that the separability of the equation of motions is not endangered by the particular choice of the constraint imposed on the transversal fluctuations of the wave function, which renders the thin-wall quantization procedure well-founded. It can be applied without restrictions.

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Introduction. A proper understanding of quantum physics on surfaces in ordinary three-dimensional (3D) space has become immediate due to the present drive in constructing low-dimensional nanostructures such as sheets and tubes that can be bent into curved, deformable objects such as tori[1,2] and spirals.[3–5] The current theoretical paradigm relies on a thin-wall quantization method of the two-dimensional (2D) manifold introduced by Da Costa.[6] The quantum motion in the 2D surface is treated as a limiting case of a particle in an ordinary 3D space subject to a confining force acting in the normal direction to its 2D manifold. Because of the lateral confinement, quantum excitation energies in the normal direction are raised far beyond those in the tangential direction. Henceforth the quantum motion in the normal direction can be safely neglected. On the basis of this, one then deduces an effective dimensionally reduced Schrödinger equation. The thin-wall quantization procedure has been widely employed since.[7–14] From the experimental point of view, the realization of an optical analog of the curvature-induced geometric potential can be taken as empirical evidence for the validity of Da Costa's squeezing procedure.[15]

But in spite of its immediate relevance to constrained nanosctructures, the thin-wall quantization procedure is still theoretically debated,[16,17] particularly in the presence of externally applied electric and magnetic field.[18] Indeed, it has been asserted[16] that a charged particle of charge Q couples to a term linear in QA_3M with A_3 the transverse component of the electromagnetic potential and M the mean curvature of the 2D manifold. Even more, it was argued in Ref. 16 that, independent of the size of the charge Q, the essence of the thin-wall quantization procedure, i.e., the decoupling of the transversal quantum fluctuations from the motion along the surface, is necessarily undermined when constraints different from Dirichlet ones are imposed on the normal quantum degrees of freedom. In this Brief Report, we resolve this paradoxical situation and show that (i) there is no coupling between the mean surface curvature and the external electromagnetic field, independently of the gauge choice[18] and (ii) the thin-wall quantization procedure is well founded and can be safely applied even when non-Dirichlet-type constraints are considered for the transversal motion of the quantum particle.

Schrödinger equation. To derive the thin-wall quantization in the presence of externally applied electromagnetic field we follow the procedure of Refs. 16 and 18 and start out with the Schrödinger equation minimally coupled with the four-component vector potential in a generic curved three-dimensional space. Adopting the Einstein summation convention and tensor covariant and contravariant components, we have

$$i\hbar\left[\partial_t - \frac{iQA_0}{\hbar}\right]\psi = -\frac{\hbar^2}{2m}G^{ij}\left[\mathcal{D}_i - \frac{iQA_i}{\hbar}\right] \times \left[\mathcal{D}_j - \frac{iQA_j}{\hbar}\right]\psi \tag{1}$$

where Q is the particle charge, G^{ij} is the inverse of the metric tensor G_{ij} and A_i are the covariant components of the vector potential $\mathbf{A}$ with the scalar potential defined by $V = -A_0$. The covariant derivative $\mathcal{D}_i$ is, as usual, defined as $\mathcal{D}_i v_j = \partial_i v_j - \Gamma^k_{ij} v_k$, where v_j are the covariant components of a 3D vector field $\mathbf{v}$ and Γ^k_{ij} is the affine connection related to the 3D metric tensor by

$$\Gamma^k_{ij} = \frac{1}{2}G^{kl}[\partial_j G_{li} + \partial_i G_{lj} - \partial_l G_{ij}].$$

The gauge invariance of Eq. (1) can be made explicit[18] by considering the gauge transformations $A_j \to A_j + \partial_j\omega$, $A_0 \to A_0 + \partial_t\omega$ and $\psi \to \psi\exp(iQ\omega/\hbar)$ with ω a scalar function. To proceed further, it is useful to define a coordinate system. As in Refs. 6, 16, and 18 we consider a surface $\mathcal{S}$ with parametric equations $\mathbf{r} = \mathbf{r}(q_1,q_2)$. The portion of the 3D space in the immediate neighborhood of $\mathcal{S}$ can be then parametrized as $\mathbf{R}(q_1,q_2) = \mathbf{r}(q_1,q_2) + q_3\hat{N}(q_1,q_2)$ with $\hat{N}(q_1,q_2)$ the unit vector normal to $\mathcal{S}$. We then find, in agreement with previous studies,[6,16,18] the relations among G_{ij} and the covariant components of the 2D surface metric tensor g_{ij} to be

$$G_{ij} = g_{ij} + [\alpha g + (\alpha g)^T]_{ij}q_3 + (\alpha g\alpha^T)_{ij}q_3^2 \qquad i,j = 1,2,$$
$$G_{i,3} = G_{3,i} = 0 \qquad i = 1,2; \qquad G_{3,3} = 1,$$

where α indicates the Weingarten curvature tensor of the surface $\mathcal{S}$.[6,18] We recall that the mean curvature M and the

Gaussian curvature K of the surface $\mathcal{S}$ can be related to the Weingarten curvature tensor by

$$\begin{cases} M = \dfrac{\mathrm{Tr}(\alpha)}{2} \\ K = \mathrm{Det}(\alpha). \end{cases}$$

Now we can apply the thin-layer procedure introduced by Da Costa[6] and take into account the effect of a confining potential $V_\lambda(q_3)$, where λ is a squeezing parameter that controls the strength of the confining potential. When λ is large, the total wave function will be localized in a narrow range close to $q_3 = 0$. This allows one to take the $q_3 \to 0$ limit in the covariant derivative appearing in Schrödinger equation Eq. (1). From the structure of the metric tensor, it is straightforward to show the following limiting relations for the affine connection to hold:

$$\lim_{q_3\to 0} G^{ij}\Gamma^3_{ij} \equiv -2M,$$
$$\lim_{q_3\to 0} G^{ij}\Gamma^k_{ij} \equiv g^{ij}\gamma^k_{ij},$$

where we introduced γ^k_{ij}, the affine connection related to the 2D surface metric tensor g_{ij}. With this, the effective Schrödinger equation in the portion of the 3D space close to the surface $\mathcal{S}$ is

$$\begin{aligned} i\hbar\left[\partial_t - \frac{iQA_0}{\hbar}\right]\psi &= -\frac{\hbar^2}{2m}g^{ij}\left[d_i - \frac{iQA_i}{\hbar}\right]\left[d_j - \frac{iQA_j}{\hbar}\right]\psi \\ &\quad -\frac{\hbar^2}{2m}\left[\partial_3 - \frac{iQA_3}{\hbar}\right]^2\psi - \frac{\hbar^2}{m}M\partial_3\psi + \frac{iQ\hbar}{m}MA_3\psi, \end{aligned} \tag{2}$$

where we left out the confining potential term and defined the 2D covariant derivatives of the surface metric g_{ij} as $d_i v_j = \partial_i v_j - \gamma^k_{ij}v_k$ where v_i now indicates the covariant components of a generic 2D vector field. In the equation above, the term $M\partial_3\psi$ yields a coupling among the transversal fluctuations of the wave function and the surface curvature. Similarly, the linear coupling between the A_3 component of the vector potential and the mean curvature of the surface through the term QMA_3 yields an anomalous curvature contribution to the orbital magnetic moment of the charged particle.[16] Now we show that both these terms vanish by considering the effective Schrödinger equation for a well-defined surface wave function. In agreement with Ref. 18, we subsequently find that for arbitrary gauge, there is no coupling between an external magnetic field and the curvature of the surface, independent of the shape of the surface.

In order to find a surface wave function with a definable surface density probability,[6] we are led to introduce a new wave function $\chi(q_1,q_2,q_3)$ for which in the event of separability the surface density probability is $|\chi_\parallel(q_1,q_2)|^2\int dq_3|\chi_N(q_3)|^2$. Conservation of the norm requires

$$\psi(q_1,q_2,q_3) = \left[1 + 2Mq_3 + Kq_3^2\right]^{-1/2}\chi(q_1,q_2,q_3).$$

In the immediate neighborhood of the surface ($q_3 \to 0$) the original wave function and its corresponding derivatives in the normal direction are related to the new wave function χ by

$$\begin{cases} \lim_{q_3\to 0}\psi = \chi \\ \lim_{q_3\to 0}\partial_3\psi = \partial_3\chi - M\chi \\ \lim_{q_3\to 0}\partial_3^2\psi = \partial_3^2\chi - 2M\partial_3\chi + 3M^2\chi - K\chi. \end{cases}$$

With the relations above, the effective Schrödinger equation Eq. (2) takes the following form:

$$\begin{aligned} i\hbar\partial_t\chi &= -\frac{\hbar^2}{2m}g^{ij}\left[d_i - \frac{iQA_i}{\hbar}\right]\left[d_j - \frac{iQA_j}{\hbar}\right]\chi \\ &\quad + \left[QV - \frac{\hbar^2}{2m}\left(M^2 - K\right)\right]\chi \\ &\quad - \frac{\hbar^2}{2m}\left[\partial_3 - \frac{iQA_3}{\hbar}\right]^2\chi. \end{aligned} \tag{3}$$

The purely quantum potential $\propto \hbar^2$ in the equation above corresponds to the curvature induced geometric potential originally found by Da Costa.[6] Apart from that, Eq. (3) represents the gauge invariant Schrödinger equation minimally coupled to the four-component vector potential in a curved three-dimensional space with metric tensor[18]

$$\widetilde{G} = \begin{pmatrix} g_{11} & g_{12} & 0 \\ g_{21} & g_{22} & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{4}$$

We therefore obtain a mapping of the original metric tensor G_{ij} into $\widetilde{G}_{ij}$ preserving the gauge invariance. If we now choose to fix the gauge, the new metric tensor Eq. (4) has to be taken into account. For instance, by imposing the Lorentz gauge,[16,17] the condition reads

$$\nabla\cdot\mathbf{A} \equiv \nabla_\parallel\cdot\mathbf{A}_\parallel + \partial_3 A_3 \equiv 0.$$

It is then clear that independent of the electromagnetic gauge, a quantum charged particle does not couple to the mean surface curvature and the gauge choice is free of pathologies. This allows us to apply a gauge transformation to Eq. (3) such as to cancel A_3,[18] thereby reaching a separability of the dynamics along to direction normal to the surface $\mathcal{S}$ from the tangential one.

General action. Next, we reinforce our conclusions by analyzing in the same spirit of Refs. 16, 19, and 20 a gauge invariant canonical action for the Schrödinger field in the embedding space,

$$\begin{aligned} S = \int \frac{\hbar^2}{2m}&\left[\left(\mathcal{D}^j - \frac{iQA^j}{\hbar}\right)\psi\right]^\dagger\left(\mathcal{D}_j - \frac{iQA_j}{\hbar}\right)\psi \\ &- i\hbar\psi^\star\left(\partial_t - \frac{iQA_0}{\hbar}\right)\psi. \end{aligned} \tag{5}$$

By performing an integration by parts we can separate a volume integral contribution

$$\begin{aligned} S_V = \int -\frac{\hbar^2}{2m}&\psi^\star\left(\mathcal{D}^j - \frac{iQA^j}{\hbar}\right)\left(\mathcal{D}_j - \frac{iQA_j}{\hbar}\right)\psi \\ &- i\hbar\psi^\star\left(\partial_t - \frac{iQA_0}{\hbar}\right)\psi \end{aligned} \tag{6}$$

and a total spatial derivative term

$$\int \frac{\hbar^2}{2m}\mathcal{D}^j\left[\psi^\star\left(\mathcal{D}_j - \frac{iQA_j}{\hbar}\right)\psi\right]. \tag{7}$$

By varying S_V alone, we can easily reach the gauge invariant Schrödinger equation Eq. (1). It is also clear that under confinement the volume integral Eq. (6) transforms to

$$\mathcal{S}_V = \int -i\hbar\chi^\star\left(\partial_t - \frac{iQA_0}{\hbar}\right)\chi - \frac{\hbar^2}{2m}\chi^\star\left(\widetilde{\mathcal{D}}^j - \frac{iQA^j}{\hbar}\right) \times\left(\widetilde{\mathcal{D}}_j - \frac{iQA_j}{\hbar}\right)\chi - \frac{\hbar^2}{2m}\chi^\star(M^2-K)\chi,$$

where we have introduced the covariant derivative $\widetilde{\mathcal{D}}$ related to the metric tensor $\widetilde{G}_{ij}$ and to conserve the norm we are considering the rescaled scalar field χ. Variation of the action written above gives precisely the confined Schrödinger equation of Eq. (3). Since the dynamical Schrödinger equation comes entirely from a volume contribution, it directly follows that the total derivative term Eq. (7) acts as a boundary condition which is stipulated by the vanishing of the three-dimensional field

$$\psi^\star\left(D_j - \frac{iQA_j}{\hbar}\right)\psi$$

along the surface $\partial\Omega$ of the region of integration. As pointed out in Ref. 16, this boundary condition is fulfilled by construction if the wave function ψ identically vanishes on $\partial\Omega$—Dirichlet-type constraints are imposed. This can be achieved by considering a squeezing potential $V_\lambda(q_3)$ in the form of an infinite potential well. This assumption, however, seems not to be the most physically sound one since under confinement ($q_3 \to 0$) it would break the natural limits set by the uncertainty principle. That the wave function should vanish along the surface of integration is too restrictive a condition. In the confinement procedure, indeed, it is natural to consider regions of integration that are symmetrical to the 2D manifold $\mathcal{S}$ in the normal direction. Therefore the boundary condition reads

$$\lim_{\epsilon\to 0}\left[(\psi^\star\partial_3\psi)_\epsilon - (\psi^\star\partial_3\psi)_{-\epsilon}\right] \equiv 0, \tag{8}$$

where we have considered a region of integration with a 2ϵ width in the normal direction and we have set the transversal component of the electromagnetic field $A_3 \equiv 0$. By referring to the rescaled scalar field χ, Eq. (8) becomes

$$\lim_{\epsilon\to 0}\left[(\chi^\star\partial_3\chi - M|\chi|^2)_\epsilon - (\chi^\star\partial_3\chi - M|\chi|^2)_{-\epsilon}\right] \equiv 0. \tag{9}$$

This implies that the smoothness of the rescaled wave function and of its first derivative as they pass through the curved surface are enough to fulfill the canonical action boundary condition. With this, other types of squeezing potentials can also be considered in the thin-wall quantization scheme. As an example, we can consider a harmonic trap $V_\lambda(q_3) = m\lambda^2 q_3^2/2$. Since, after gauge fixing, the variation of the canonical action leads to the separable Schrödinger equation Eq. (3), we may write the rescaled wave function as

$$\chi(q_1,q_2,q_3) = \chi_\parallel(q_1,q_2) \times \left(\frac{m\lambda}{\pi\hbar}\right)^{1/4} e^{-(m\lambda/2\hbar)q_3^2}, \tag{10}$$

which readily satisfies Eq. (9). It is worth noticing that the harmonic trap potential corresponds to the Neumann-type boundary conditions for which a coupling of the quantum particle to the mean surface curvature was put forward.[16]

Conclusions. Here we have provided a consistent framework of the thin-wall quantization procedure for charged particles in the presence of externally applied electric and magnetic field. Contrary to previous claims,[16] we have shown that the mean surface curvature does not couple to the transversal component of the vector potential, either explicitly in the effective dimensionally reduced Schrödinger equation[16] or implicitly in the gauge fixing procedure.[17] We have also considered a canonical Schrödinger action and shown that the thin-wall quantization procedure is not endangered by the particular constraints imposed on the transverse fluctuations of the wave function. Therefore Da Costa's method is well founded and can be applied without restrictions.

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