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Effective potentials of quantum strip waveguides and their dependence upon torsion

Iain J Clark† and Anthony J Bracken

Department of Mathematics, The University of Queensland, Brisbane, Qld 4072, Australia

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Abstract. We investigate the dynamics of a particle constrained to move on a curved quantum strip waveguide embedded in three-space, subject to Dirichlet boundary conditions. By establishing a coordinate system which allows a more general formulation of the dynamics, we demonstrate consistency with previous results and provide evidence that the presence of torsion introduces a further effective potential term. This result has implications for nanostructure device engineering.

1. Introduction

Recent advances in semiconductor physics have enabled the fabrication of nanostructure devices which have the four properties described by Duclos and Exner [6]:

(p1) nanoscale dimension (typically between 5 and 500 nm)
(p2) high purity with an electron mean free path greater than 1 micron
(p3) crystalline structure of the semiconductor lattice
(p4) suppression of the wavefunction at boundaries between different materials.

Buot [2] and Sundaram *et al* [15] discuss methods for fabrication of such nanostructures, and the nature of the mesoscopic physics which describes the interaction of such nanoscale systems with macroscopic experimental apparatus.

Because of the regularity of the lattice, we can describe the motion of an electron in the semiconductor lattice as that of a free particle of effective mass m^*, subject to Dirichlet boundary conditions. What distinguishes mesoscopic physics from most previous applications of quantum mechanics is that it becomes important to consider explicitly the nature and effect of boundary conditions for Schrödinger's equation. The small size of the nanostructure, in combination with the large mean free path, indicate that the particles exist in the ballistic regime, and thus we can neglect scattering processes.

Hence the physical problem is, for such structures, modelled by considering the Helmholtz equation on a configuration space subject to Dirichlet boundary conditions, which we shall transform into a more complicated differential equation (including an effective potential term) on a simple rectangular strip of infinite length and width d.

† E-mail address: ijc@maths.uq.oz.au

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2. The coordinate system

Consider a two-dimensional strip Ω of infinite length and uniform width d, embedded in three-space, subject to regularity conditions:

(r1) Ω is not self-intersecting, and
(r2) the two curves which are equivalent to $\partial\Omega$ are infinitely smooth.

We shall investigate the dynamics of a particle which is free to move on this strip, with appropriate Dirichlet boundary conditions.

To this end, we construct a coordinate system in which the motion of the particle both *along* and *across* the strip is most simply described in terms of curvilinear coordinates q_1 and q_2.

However, a complicating factor is that, because we are dealing with the embedding of a two-dimensional manifold in three-space, we have to adopt initially a canonical coordinate system (q_1,q_2,q_3)—where Ω lies in the surface S defined by $q_3 = 0$, and q_3 corresponds to the displacement of an arbitrary point P from this surface S—and then consider the dynamics of the particle upon the surface S, subject to suitable boundary conditions to restrict the particle to move on $\Omega \subset S$. This fixes the embedding of the manifold Ω in $\mathbb{R}^3$.

Depending on the geometry of Ω, we choose as a reference curve $\mathcal{C}$ either (c1) an edge, or (c2) the central axis of the strip. We describe $\mathcal{C}$ by a vector valued function $\boldsymbol{r}(q_1)$ of an arc length parameter q_1, where $\boldsymbol{r} \in C^\infty(\mathbb{R})$:

$$\mathcal{C} = \{\boldsymbol{r}(q_1) : q_1 \in \mathbb{R}\}. \tag{1}$$

Because the strip Ω is of uniform width d, the coordinate q_2 will assume values either (c1) between 0 and d, or (c2) between $-d/2$ and $d/2$, while q_1 can be any real number.

Along this reference curve $\mathcal{C}$, the unit tangent vector is given by the first derivative of $\boldsymbol{r}$

$$\boldsymbol{t}(q_1) = \frac{\boldsymbol{r}'(q_1)}{||\boldsymbol{r}'(q_1)||} = \boldsymbol{r}'(q_1) \tag{2}$$

noting that this choice of q_1 as arc length requires $||\boldsymbol{r}'(q_1)|| = 1$, and the second derivative of $\boldsymbol{r}$ yields the unsigned curvature† of the curve

$$\kappa(q_1) = ||\boldsymbol{r}''(q_1)||. \tag{3}$$

Unit normal and binormal vectors $\boldsymbol{n}(q_1)$ and $\boldsymbol{b}(q_1)$ are then defined along $\mathcal{C}$ in the usual manner [5]

$$\boldsymbol{n}(q_1) = \frac{\boldsymbol{t}'(q_1)}{\kappa(q_1)} \tag{4}$$

$$\boldsymbol{b}(q_1) = \boldsymbol{t}(q_1) \wedge \boldsymbol{n}(q_1) \tag{5}$$

so that the set of vectors $\{\boldsymbol{t}, \boldsymbol{n}, \boldsymbol{b}\}$ forms a right-handed orthonormal triad.

The intrinsic torsion $\tau(q_1)$ of $\mathcal{C}$ is then given by one of the Frenet–Serret formulae

$$\boldsymbol{b}'(q_1) = -\tau(q_1)\boldsymbol{n}(q_1) \tag{6}$$

which describes the tendency for the curve to twist out of the osculating plane (the plane of $\boldsymbol{t}$ and $\boldsymbol{n}$). Following da Costa [3, 4], we introduce a new coordinate system by taking linear

† We explicitly attach the label 'unsigned' to this usual measure of curvature, in order to differentiate this quantity from Exner's signed curvature [7], which will be discussed below.

combinations of the normal and binormal vectors—the relative proportions determined by a scalar function $\theta(q_1)$—giving new vectors

$$\begin{pmatrix} \boldsymbol{n}_2 \\ \boldsymbol{n}_3 \end{pmatrix} = \begin{bmatrix} \cos(\theta(q_1)) & -\sin(\theta(q_1)) \\ \sin(\theta(q_1)) & \cos(\theta(q_1)) \end{bmatrix} \begin{pmatrix} \boldsymbol{n}(q_1) \\ \boldsymbol{b}(q_1) \end{pmatrix} \tag{7}$$

where the set $\{\boldsymbol{t}, \boldsymbol{n}_2, \boldsymbol{n}_3\}$ forms a right-handed orthonormal triad also. Then, the Frenet–Serret formulae relating unit vectors and their derivatives become

$$\begin{pmatrix} \boldsymbol{t}' \\ \boldsymbol{n}_2' \\ \boldsymbol{n}_3' \end{pmatrix} = \begin{bmatrix} 0 & \kappa\cos\theta & \kappa\sin\theta \\ -\kappa\cos\theta & 0 & T \\ -\kappa\sin\theta & -T & 0 \end{bmatrix} \begin{pmatrix} \boldsymbol{t} \\ \boldsymbol{n}_2 \\ \boldsymbol{n}_3 \end{pmatrix} \tag{8}$$

where

$$T(q_1) = \tau(q_1) - \theta'(q_1). \tag{9}$$

The surface S of interest is then described by the points

$$\boldsymbol{S}(q_1, q_2) = \boldsymbol{r}(q_1) + q_2\boldsymbol{n}_2(q_1). \tag{10}$$

We now construct a unit normal vector $\boldsymbol{N}(q_1, q_2)$, perpendicular to S for all values of q_1 and q_2. It is easy to see that we can take $\boldsymbol{N}(q_1, 0) = \boldsymbol{n}_3(q_1)$. Introducing a q_2 dependent term and imposing the condition that $\partial\boldsymbol{S}/\partial q_i$ is orthogonal to $\boldsymbol{N}$ for $i = 1, 2$ gives

$$\boldsymbol{N}(q_1, q_2) = \frac{1}{\sqrt{K^2 + q_2^2T^2}}(-q_2T\boldsymbol{t} + K\boldsymbol{n}_3) \tag{11}$$

where

$$K(q_1, q_2) = 1 - q_2\kappa(q_1)\cos(\theta(q_1)). \tag{12}$$

Note that (r2) requires that the denominator of (11) must never vanish. Hence, there must not exist a point $\boldsymbol{S}(q_1, q_2)$ on $\mathcal{S}$ for which $[K(q_1, q_2)]^2 + q_2^2T^2 = 0$. In the specific case where $T = 0$, which is the case surveyed by the literature to date, this requires that K must not vanish. Where $T \neq 0$, however, there is no need of such a restriction.

Following Martinez [11], an arbitrary point $\boldsymbol{R}$ in the vicinity of S can now be described by a suitable choice of the three canonical coordinates q_1, q_2, q_3

$$\boldsymbol{R}(q_1, q_2, q_3) = \boldsymbol{S}(q_1, q_2) + q_3\boldsymbol{N}(q_1, q_2). \tag{13}$$

Constructing the metric tensor G by expanding the differential $\mathrm{d}\boldsymbol{R}$ in terms of $\mathrm{d}q_1$, $\mathrm{d}q_2$ and $\mathrm{d}q_3$ and using the equation

$$||\mathrm{d}\boldsymbol{R}||^2 = \begin{pmatrix} \mathrm{d}q_1 & \mathrm{d}q_2 & \mathrm{d}q_3 \end{pmatrix} G \begin{pmatrix} \mathrm{d}q_1 \\ \mathrm{d}q_2 \\ \mathrm{d}q_3 \end{pmatrix} \tag{14}$$

we get an expression for G on $\mathcal{S}$ by taking the limit as $q_3 \to 0$, giving

$$G = \begin{bmatrix} K^2 + q_2^2T^2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} g & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{15}$$

where $g = \det(G) = K^2 + q_2^2T^2$.

Since we are constructing the Hamiltonian for the particle which is closely bound to the surface $q_3 = 0$, we will approximate the Laplace–Beltrami operator in an ϵ-neighbourhood of the surface S by constructing the Laplace–Beltrami operator using the above expression for the metric tensor on the surface S. It is possible, but beyond the scope of this paper, to examine the conditions under which the sequence of Laplacians on increasingly thin ϵ-neighbourhoods of S converge in the sense of unbounded operators to this approximation.

This expression for the metric tensor allows us to construct the Hamiltonian for the particle. More importantly, because of the diagonal structure of G, we can decompose the dynamical equations of motion for the particle into two equations—one describing the motion of the particle upon the surface S, and the other describing the motion of the particle along the q_3 coordinate.

3. Construction and analysis of the Hamiltonian

We are considering the case of the quantum particle of effective mass m^* free to move on a strip Ω, but nevertheless bound to the surface of the strip.

We approach this situation by expressing the Hamiltonian for a free particle in terms of our canonical coordinates $\{q_1, q_2, q_3\}$, using the Laplace–Beltrami operator

$$\nabla^2 = g^{-1/2} \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{\partial}{\partial q_i} g^{1/2} \left[G^{-1} \right]_{ij} \frac{\partial}{\partial q_j}. \tag{16}$$

Because of the form of G, we have

$$\nabla^2 = \frac{1}{\sqrt{g}} \left[\frac{\partial}{\partial q_1} g^{-1/2} \frac{\partial}{\partial q_1} + \frac{\partial}{\partial q_2} g^{1/2} \frac{\partial}{\partial q_2} \right] + \frac{\partial^2}{\partial q_3^2} \tag{17}$$

and we write the time-independent Schrödinger equation for the free particle in the form

$$(\nabla^2 + k^2)\psi(q_1, q_2, q_3) = 0 \qquad (q_1, q_2, q_3) \in \Omega. \tag{18}$$

The complication comes from the fact that now we wish to introduce Dirichlet boundary conditions—and of course the boundary of a two-dimensional manifold Ω embedded in three-space is the manifold itself. Accordingly, we need to approach the imposition of boundary conditions upon the solution of the free particle Schrödinger equation with some care, because it is not possible to introduce directly Dirichlet boundary conditions. Several authors [9, 12] have considered approaches that can be taken to circumvent this problem; the method we shall use here is to introduce a family of suitable *infinitesimal confining potentials* V_λ which approximate a quantum well of infinitesimal width and infinitely steep walls as $\lambda \to \infty$, and therefore restrict the domain of the wavefunction to the lesser dimensional configuration manifold embedded in $\mathbb{R}^3$. Since we seek to confine the particle to the surface $q_3 = 0$, V_λ need only be a function of q_3. We will use the scaled confining potential $U_\lambda(q_3) = [2m^* V_\lambda(q_3)]/\hbar^2$ for brevity below.

Hence the problem to consider is in fact

$$\left(\nabla^2 + k^2 - U_\lambda(q_3)\right) \psi(q_1, q_2, q_3) = 0 \qquad (q_1, q_2, q_3) \in \Omega. \tag{19}$$

It is this imposition of suitable confining potentials and the associated limiting process, that is the key to solving the problem of the dimensional reduction of the Hamiltonian.

In the coordinate system (q_1, q_2, q_3), the volume elements $\mathrm{d}V$ scale in size as the square root of g. Because we require the wavefunctions to be normalized with respect to the volume element $\mathrm{d}q_1\mathrm{d}q_2\mathrm{d}q_3$, we introduce new wavefunctions $\chi_s(q_1, q_2)$ and $\chi_n(q_3)$, the product of which is dimensionally scaled by the fourth root of g, and make the substitution

$$\psi(q_1, q_2, q_3) = g^{-1/4}\chi_s(q_1, q_2)\chi_n(q_3). \tag{20}$$

Then equation (19) reduces to

$$\frac{1}{\sqrt{g}}\left[\frac{\partial}{\partial q_1}g^{-1/2}\frac{\partial}{\partial q_1}\left(\frac{\chi_s}{g^{1/4}}\right) + \frac{\partial}{\partial q_2}g^{1/2}\frac{\partial}{\partial q_2}\left(\frac{\chi_s}{g^{1/4}}\right)\right]\chi_n$$
$$+\chi_s\frac{\mathrm{d}^2\chi_n}{\mathrm{d}q_3^2} + \left[k^2 - U_\lambda(q_3)\right]\chi_s\chi_n = 0. \tag{21}$$

This decomposes into the pair of equations

$$\frac{\partial}{\partial q_1}\left(g^{-1}\frac{\partial\chi_s}{\partial q_1}\right) + \frac{\partial^2\chi_s}{\partial q_2^2} - \frac{2m^*}{\hbar^2}V_{\mathrm{eff}}(q_1, q_2)\chi_s + k_s^2\chi_s = 0 \tag{22}$$

and

$$\chi_n'' + k_n^2\chi_n - U_\lambda(q_3)\chi_n = 0 \tag{23}$$

where the effective potential is given by

$$V_{\mathrm{eff}}(q_1, q_2) = \frac{-\hbar^2}{2m^*}\left[-\frac{1}{4g^2}\frac{\partial^2 g}{\partial q_1^2} + \frac{7}{16g^3}\left(\frac{\partial g}{\partial q_1}\right)^2 - \frac{1}{4g}\frac{\partial^2 g}{\partial q_2^2} + \frac{3}{16g^2}\left(\frac{\partial g}{\partial q_2}\right)^2\right] \tag{24}$$

and $k^2 = k_s^2 + k_n^2$.

Equation (23) describes the confinement of the particle to an ϵ-neighbourhood of the surface $q_3 = 0$. However (22) is of much greater interest to us, since it describes the dynamics of a particle moving on the surface S under the influence of an effective potential

$$V_{\mathrm{eff}}(q_1, q_2) = \frac{-\hbar^2}{2m^*} \times \left[\begin{array}{c} -\frac{1}{2g^2}\left[\left(\frac{\partial K}{\partial q_1}\right)^2 + K\frac{\partial^2 K}{\partial q_1^2} + q_2^2\left(TT'' + [T']^2\right)\right] + \frac{7}{4g^3}\left[K\frac{\partial K}{\partial q_1} + q_2^2 TT'\right]^2 \\ -\frac{1}{2g}\left[\left(\frac{\partial K}{\partial q_2}\right)^2 + T^2\right] + \frac{3}{4g^2}\left[K\frac{\partial K}{\partial q_2} + q_2 T^2\right]^2 \end{array}\right]. \tag{25}$$

In the remainder of this section, we will separately recover the effective potential results of da Costa [3] and of Exner and Šeba [7], and then give an indication of why the twisting of an otherwise linear quantum strip can modify the effective potential both across and along the strip.

3.1. Particle tightly bound to a curve in three-space

Following da Costa [3], we consider firstly the case of a particle constrained to move along a reference curve $\mathcal{C}$. This is, of course, an example of a system with only one degree of freedom, but the technique is illustrative and relevant to this work.

Because of the physical symmetry with respect to arbitrary rotations around the axis tangent to the curve, we are able to choose the rate at which the coordinate system twists around $\mathcal{C}$ in order to simplify the analysis. The optimal choice of such a twisting factor is given by integrating the torsion $\tau(q_1)$ along the curve $\mathcal{C}$, thus satisfying

$$\theta'(q_1) = \tau(q_1). \tag{26}$$

Then we have $T = 0$. Substituting this into (11) causes (13) to take the form

$$\boldsymbol{R}(q_1, q_2, q_3) = \boldsymbol{r}(q_1) + q_2\boldsymbol{n}_2(q_1) + q_3\boldsymbol{n}_3(q_1). \tag{27}$$

Using equation (14), we see that the metric tensor becomes

$$G = \begin{bmatrix} (1-\kappa[q_2\cos\theta + q_3\sin\theta])^2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{28}$$

Note that in the limit as $q_3 \to 0$, this reduces to (15), since $T = 0$.

We then impose a scaled confining potential $U_\lambda(q_2, q_3)$ which has the property that the equipotential surfaces can be described as a family of space curves which are obtainable from $\mathcal{C}$ by a Combescure transformation [14]—thus ensuring that points with the same values of the coordinates q_2 and q_3, but different values of q_1, will have the same potential. The simplest example of such a potential is

$$U_\lambda(q_2, q_3) = \lambda\left(q_2^2 + q_3^2\right) \tag{29}$$

but other potentials with non-circular equipotential curves are possible, depending on the nature of the torsion and curvature of $\mathcal{C}$. With such an effective potential, the time-independent Schrödinger equation can be expressed as

$$\frac{1}{\sqrt{g}}\left(\frac{\partial}{\partial q_1}\frac{1}{\sqrt{g}}\frac{\partial}{\partial q_1} + \sum_{i=2}^{3}\frac{\partial}{\partial q_i}\sqrt{g}\frac{\partial}{\partial q_i} + k^2 - U_\lambda(q_2, q_3)\right)\psi(q_1, q_2, q_3) = 0. \tag{30}$$

Applying the substitution (20), we separate (30) into the pair of equations

$$\frac{\mathrm{d}^2\chi_t}{\mathrm{d}q_1^2} - \frac{2}{\sqrt{g}}\frac{\partial\sqrt{g}}{\partial q_1}\frac{d\chi_t}{\mathrm{d}q_1} + \left[\frac{5}{4g}\left(\frac{\partial\sqrt{g}}{\partial q_1}\right)^2 - \frac{1}{2\sqrt{g}}\frac{\partial^2\sqrt{g}}{\partial q_1^2} + \frac{1}{4}\kappa^2 + k_t^2\right]\chi_t = 0 \tag{31}$$

and

$$\frac{\partial^2\chi_n}{\partial q_2^2} + \frac{\partial^2\chi_n}{\partial q_3^2} + \left[k_n^2 - U_\lambda(q_2, q_3)\right]\chi_n = 0. \tag{32}$$

Now equation (32) describes the confinement of the particle to an tubular ϵ-neighbourhood of $\mathcal{C}$. Hence in (31) we can take the limit as both q_2 and q_3 tend to zero due to the effect of V_λ. In this limit $g = 1$, yielding

$$\frac{\mathrm{d}^2\chi_t}{\mathrm{d}q_1^2} + \left[\frac{1}{4}\kappa^2 + k_t^2\right]\chi_t = 0. \tag{33}$$

This gives, in agreement with da Costa, an effective potential term

$$V_{\mathrm{eff}}(q_1) = \frac{-\hbar^2[\kappa(q_1)]^2}{8m^*}. \tag{34}$$

Physically, this means that it is possible for quantum wires to have bound states localized around regions of curvature. Such bound states appear as resonances when they are observed by coupling macroscopic electrodes to a finite length quantum waveguide. This has been experimentally observed by Timp *et al* [16] for the case of right-angled bends.

Note, however, that if we attempt to model the dynamics of the particle moving along $\mathcal{C}$ by constructing a strip Ω which follows the curve $\mathcal{C}$, and twists at such a rate so as to make T identically vanish everywhere, equation (25) yields an effective potential term $V_{\text{eff}}(q_1) = -\hbar^2\kappa^2\cos^2\theta/(8m^*)$. The error here is due to the discrepancy between the metric tensor (28), and the approximation (15) which holds for small values of q_3. However, since we are considering a limiting process in which q_2 and q_3 tend to zero at the same rate, we cannot neglect q_3 terms while still considering q_2 terms.

This demonstrates the need for caution in considering the quantum mechanics of constrained systems, and in particular suggests that with regard to dimensionally reduced systems, arguments which appeal to the vanishing of tangential components of the force† may require a certain amount of caution.

3.2. Particle confined to a strip of uniform width in two-space

In the preceding section, we derived an expression for the effective potential that is only dependent upon the longitudinal coordinate q_1. In this section we reconstruct the analysis of Exner and Šeba [7], in which they derive additional potential terms that depend also upon the transverse coordinate q_2, for the case of a quantum waveguide of uniform‡ width d existing upon a flat two-dimensional surface.

In this case, we choose one edge of the strip Ω to be the reference curve $\mathcal{C}$, which will be taken to lie on the surface of the plane $q_3 = 0$, and can be described as

$$\mathcal{C} = \{r_x(q_1)\boldsymbol{i} + r_y(q_1)\boldsymbol{j} : q_1 \in \mathbb{R}\}. \tag{35}$$

Such a curve will naturally have $\tau(q_1) = 0$. We shall only consider the case of a *simply bent* strip, in which the signed curvature γ of $\mathcal{C}$ does not change, where

$$\gamma(q_1) = r_x''(q_1)r_y'(q_1) - r_x'(q_1)r_y''(q_1). \tag{36}$$

Note that the absolute value of γ is equal to the curvature of $\mathcal{C}$, from

$$\gamma^2 = (r_x''r_y' - r_x'r_y'')^2 = ||\boldsymbol{r}''||^2 - (\boldsymbol{r}' \cdot \boldsymbol{r}'')^2 = \kappa^2 \tag{37}$$

because $\boldsymbol{r}' \perp \boldsymbol{r}''$. However, because of Exner and Šeba's sign convention, the case where positive values of q_2 correspond to points within Ω is given by the case in which $\gamma < 0$. We therefore put

$$\kappa(q_1) = -\gamma(q_1). \tag{38}$$

Now having fixed the location of the curve $\mathcal{C}$, we describe the entire quantum strip by allowing q_2 to range between 0 and d. Note that we wish the strip itself to lie *in* the plane also, and hence we require that $\theta(q_1) = 0$. This means that $T = 0$, and that points in the vicinity of $\mathcal{C}$ can be expressed by

$$\boldsymbol{R}(q_1, q_2, q_3) = \boldsymbol{r}(q_1) + q_2\boldsymbol{n}_2(q_1) + q_3\boldsymbol{n}_3(q_1) \tag{39}$$

after the fashion of (13), where

$$\boldsymbol{n}_2(q_1) = \boldsymbol{n}(q_1) = \frac{\gamma(q_1)}{|\gamma(q_1)|}\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}\boldsymbol{r}'(q_1) \tag{40}$$

† The force on a quantum particle in this coordinate system being given by the gradient of the effective potential, as discussed by da Costa [3].

‡ Andrews and Savage [1] consider the case of a planar quantum strip of non-uniform width.

and

$$\boldsymbol{n}_3(q_1) = \boldsymbol{k}. \tag{41}$$

From this, we can see that since $T = 0$, the effective potential (25) can be expressed using $K = 1 - \kappa q_2$ as

$$V_{\mathrm{eff}}(q_1, q_2) = \frac{-\hbar^2}{2m^*}\left[\frac{5}{4}\frac{q_2^2(\kappa')^2}{(1-\kappa q_2)^4} + \frac{1}{2}\frac{\kappa'' q_2}{4(1-\kappa q_2)^3} + \frac{\kappa^2}{4(1-\kappa q_2)^2}\right] \tag{42}$$

Note that this reduces to (34) in the limit $q_2 \to 0$. Furthermore, using equation (38), this becomes the same expression as that given in equation (3.9) of Exner and Šeba [7]:

$$V_{\mathrm{eff}}(q_1, q_2) = \frac{-\hbar^2}{2m^*}\left[\frac{5}{4}\frac{q_2^2(\gamma')^2}{(1+\gamma q_2)^4} - \frac{1}{2}\frac{\gamma'' q_2}{4(1+\gamma q_2)^3} + \frac{\gamma^2}{4(1+\gamma q_2)^2}\right]. \tag{43}$$

3.3. Particle confined to a strip of uniform width embedded with torsion in three-space

Previous authors [10, 3, 17, 8, 9, 13] have considered the case of a quantum particle which is constrained to move upon a curved two-dimensional manifold embedded in three-space, and derived an effective potential which is dependent upon the extrinsic curvature of the manifold. However, because Exner and Šeba model the dynamics upon a flat surface, this effect vanishes in their work [7] since a planar surface has no extrinsic curvature. Thus, from the results of the previous section, it is apparent that in general, the effective potential must arise from the *mesoscopic confinement process* which constrains the particle to move in a region of width d across the strip, in addition to the *infinitesimal confinement process* which ensures that the particle moves upon the surface of the manifold.

Consider now a strip of uniform width d embedded with torsion in three-space, in the situation where d is small compared with a typical length scale L over which the relevant quantities of curvature and torsion vary in the longitudinal q_1 direction.

In order to see the relative importance of the different terms in (24), we transform all variables into dimensionless form, setting

$$\epsilon = d/L \ll 1 \qquad E_d = \hbar^2/(2m^* d^2)$$

$$q_1 = xL \qquad q_2 = yd \tag{44}$$

$$\kappa(q_1) = \hat{\kappa}(x)/L \qquad \tau(q_1) = \hat{\tau}(x)/L$$

$$V_{\mathrm{eff}}(q_1, q_2) = \mathcal{V}(x, y)E_d \tag{45}$$

and

$$\phi(x) = \theta(q_1). \tag{46}$$

With this, the expression for the Jacobian transforms to

$$\hat{g}(x, y) = 1 - 2\epsilon y A(x) + \epsilon^2 y^2 B(x) \tag{47}$$

where

$$\begin{aligned} A(x) &= \hat{\kappa}(x)\cos[\phi(x)] \\ B(x) &= A^2(x) + \left[\hat{\tau}(x) - \phi'(x)\right]^2 \end{aligned} \tag{48}$$

and equation (24) becomes

$$\mathcal{V}(x, y) = \frac{1}{4\hat{g}}\frac{\partial^2\hat{g}}{\partial y^2} - \frac{3}{16\hat{g}^2}\left(\frac{\partial\hat{g}}{\partial y}\right)^2 + \epsilon^2\left[\frac{1}{4\hat{g}^2}\frac{\partial^2\hat{g}}{\partial x^2} - \frac{7}{16\hat{g}^3}\left(\frac{\partial\hat{g}}{\partial x}\right)^2\right]. \tag{49}$$

Then we have, from (47),

$$\mathcal{V}(x, y) = \epsilon^2 \left[\tfrac{1}{2} B(x) - \tfrac{3}{4} A^2(x)\right] + \mathrm{O}(\epsilon^4). \tag{50}$$

Ignoring the terms of order ϵ^4, we get

$$\mathcal{V}(x, y) \approx \epsilon^2 \left[-\tfrac{1}{4}\left[\hat{\kappa}(x)\cos\phi(x)\right]^2 + \tfrac{1}{2}\left[\hat{\tau}(x) - \phi'(x)\right]^2\right] \tag{51}$$

or, in terms of the original variables,

$$V_{\mathrm{eff}}(q_1, q_2) = \frac{\hbar^2}{2m^*}\left(-\tfrac{1}{4}\big[\kappa(q_1)\cos[\theta(q_1)]\big]^2 + \tfrac{1}{2}\big[\tau(q_1) - \theta'(q_1)\big]^2\right). \tag{52}$$

From this, it can be seen firstly that the introduction of any twisting of a planar strip with given curvature reduces the attractive strength of the effective potential in the longitudinal direction, and hence the tendency for bound states to occur, because $|\cos\theta| \leqslant 1$ in the attractive term in (52). This factor corresponds physically to the projection of the strip onto the osculating plane.

More interesting is the repulsive term proportional to $[\tau(q_1) - \theta'(q_1)]^2$ which occurs in (52). In particular, we would expect no binding at all in the longitudinal direction if V_{eff} is everywhere repulsive, i.e. if

$$\sqrt{2}|\tau(q_1) - \theta'(q_1)| > |\kappa(q_1)\cos(q_1)| \tag{53}$$

for all values of q_1.

Geometrically, the twisting of a strip requires particles on it to deviate from motion in the osculating plane, and the energy required to perturb the particle motion to force this to occur explains the extra terms in the effective potential. We can conjecture that a similar result holds for two-dimensional quantum waveguides of any cross sectional shape in which one dimension is markedly larger than the other.

We hope to return elsewhere to a more detailed analysis of specific geometric examples, using equation (49).

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