More on effective potentials of quantum strip waveguides

1998 J. Phys. A: Math. Gen. 31 2103

(http://iopscience.iop.org/0305-4470/31/8/020)

J. Phys. A: Math. Gen. **31** (1998) 2103–2107. Printed in the UK PII: S0305-4470(98)88852-5

ADDENDUM

More on effective potentials of quantum strip waveguides

Iain J Clark†

Department of Mathematics and Statistics, The University of Edinburgh, James Clerk Maxwell Building, The King's Buildings, Mayfield Road, Edinburgh EH9 3JZ, UK

Received 30 October 1997

Abstract. We investigate further the dynamics of a particle constrained to move on a curved quantum strip waveguide embedded in 3-space, subject to Dirichlet boundary conditions. An earlier calculation of the dependence of the effective potential upon torsion and twisting is modified to yield a corrected expression, by use of the 'straightening-out' transformation.

In [1], an expression was derived for the effective potential of a quantum strip waveguide, embedded with twisting and torsion in 3-space:

$$V_{\text{eff}}(q_1, q_2) \approx \frac{\hbar^2}{2m^*}\left(-\frac{1}{4}[\kappa(q_1)\cos[\theta(q_1)]]^2 + \frac{1}{2}[\tau(q_1) - \theta'(q_1)]^2\right) \tag{1}$$

where q_2 is constrained to assume values either (c1) between 0 and d, or (c2) between $-d/2$ and $d/2$. However, it was pointed out that (1) could not be correct as it stands: for example, when $\tau(q_1)$ and $\theta'(q_1)$ vanish, one has different values of V_{eff} for waveguides with different orientations $\theta(q_1)$ in the limit as $d \to 0$. Physically, however, one would expect these values of V_{eff} to coincide. It was subsequently found [2] that the correct expression for (1) was given by

$$V_{\text{eff}}(q_1, q_2) \approx \frac{\hbar^2}{2m^*}\left(-\frac{1}{4}[\kappa(q_1)]^2 + \frac{1}{2}[\tau(q_1) - \theta'(q_1)]^2\right). \tag{2}$$

This addendum provides a derivation of this result.

Consider a strip Ω of uniform width d embedded with torsion in 3-space. As in [1], we define a right-handed orthonormal triad $\{\boldsymbol{t}(q_1), \boldsymbol{n}(q_1), \boldsymbol{b}(q_1)\}$ of vectors along a reference curve $\mathcal{C} = \{\boldsymbol{r}(q_1) : q_1 \in \mathbb{R}\}$. We then take linear combinations of $\boldsymbol{n}$ and $\boldsymbol{b}$, the relative proportions given at each point along $\mathcal{C}$ by a scalar function $\theta(q_1)$, obtaining new vectors $\boldsymbol{n}_2(q_1)$ and $\boldsymbol{n}_3(q_1)$. This allows the construction of a surface S containing Ω; the points in the surface S are given by

$$\boldsymbol{S}(q_1, q_2) = \boldsymbol{r}(q_1) + q_2\boldsymbol{n}_2(q_1). \tag{3}$$

It is straightforward to see that $\boldsymbol{n}_3(q_1)$ is normal to S where $q_2 = 0$; the extension of this to obtain a vector normal to S for *any* q_2 proceeds as in [1], and we obtain

$$\boldsymbol{N}(q_1, q_2) = h^{-1}(-q_2T\boldsymbol{t} + K\boldsymbol{n}_3) \tag{4}$$

† E-mail address: iclark@maths.ed.ac.uk

where $\boldsymbol{T}(q_1) = \tau(q_1) - \theta'(q_1)$ and $\boldsymbol{K}(q_1, q_2) = 1 - q_2\kappa(q_1)\cos(\theta(q_1))$, and

$$h(q_1, q_2) = \sqrt{K^2 + q_2^2 T^2}. \tag{5}$$

This allows points near Ω to be expressed as $\boldsymbol{R}(q_1, q_2, q_3) = \boldsymbol{S}(q_1, q_2) + q_3\boldsymbol{N}(q_1, q_2)$.

However, the argument in [1], taking the limit as $q_3 \to 0$, fails to account for the partial derivatives with respect to q_3. A more careful treatment of this limiting process yields the corrected expression for $V_{\rm eff}$. We use the following, from [3].

Proposition (Straightening-out transformation). Suppose the metric tensor $\mathbf{G}$, with components g_{ij} and determinant g, is invertible. Let the components of $\mathbf{G}^{-1}$ be denoted by g^{ij} in the standard manner. Then with the substitution $\psi = g^{-1/4}\chi$, the Laplace–Beltrami operator ∇^2 acting on ψ can be expressed as

$$\nabla^2\psi = f^{-1/4}(\nabla_0^2\chi + K_0\chi + V_0\chi) \tag{6}$$

where

$$K_0\chi = (g^{ij} - \delta^{ij})\partial_{ij}\chi + (\partial_j\chi)(\partial_i g^{ij}) \tag{7}$$

and

$$U_0\chi = -\tfrac{1}{4}[g^{-1/4}\partial_i(g^{ij}g^{-3/4}\partial_j g)]\chi. \tag{8}$$

□

We construct the metric tensor $\mathbf{G}$ in question. The partial derivatives of $\boldsymbol{R}$ with respect to q_1, q_2 and q_3 are given by

$$\begin{aligned}
\partial_1\boldsymbol{R} &= \partial_1\boldsymbol{S} + q_3\partial_1\boldsymbol{N}\\
\partial_2\boldsymbol{R} &= \partial_2\boldsymbol{S} + q_3\partial_2\boldsymbol{N}\\
\partial_3\boldsymbol{R} &= \boldsymbol{N}.
\end{aligned} \tag{9}$$

The metric tensor will, therefore, depend upon the partial derivatives of $\boldsymbol{N}$ and $\boldsymbol{S}$, which we express in terms of the basis vectors $\boldsymbol{t}$, $\boldsymbol{n}_2$ and $\boldsymbol{n}_3$, obtaining

$$\begin{aligned}
\partial_1\boldsymbol{N} &= h^{-1}T\boldsymbol{n}_2 - [h^{-1}\kappa\sin\theta - h^{-3}q_2M][K\boldsymbol{t} + q_2T\boldsymbol{n}_3]\\
\partial_2\boldsymbol{N} &= -h^{-3}T(K\boldsymbol{t} + q_2T\boldsymbol{n}_3)\\
\partial_1\boldsymbol{S} &= K\boldsymbol{t} + q_2T\boldsymbol{n}_3\\
\partial_2\boldsymbol{S} &= \boldsymbol{n}_2
\end{aligned} \tag{10}$$

where $M = T\partial_1K - K\partial_1T$. These partial derivatives are easily expressed in terms of an orthonormal triad of vectors $\boldsymbol{m}_1$, $\boldsymbol{m}_2$ and $\boldsymbol{m}_3$:

$$\begin{aligned}
\boldsymbol{m}_1 &= h^{-1}[K\boldsymbol{t} + q_2T\boldsymbol{n}_3]\\
\boldsymbol{m}_2 &= \boldsymbol{n}_2\\
\boldsymbol{m}_3 &= h^{-1}[-q_2T\boldsymbol{t} + K\boldsymbol{n}_3].
\end{aligned} \tag{11}$$

This allows (4) and (10) to be more conveniently expressed as

$$\begin{aligned}
\boldsymbol{N} &= \boldsymbol{m}_3 & \partial_1\boldsymbol{N} &= h^{-1}T\boldsymbol{m}_2 - \Xi\boldsymbol{m}_1\\
\partial_2\boldsymbol{N} &= -h^{-2}T\boldsymbol{m}_1 & \partial_1\boldsymbol{S} &= h\boldsymbol{m}_1\\
\partial_2\boldsymbol{S} &= \boldsymbol{m}_2
\end{aligned} \tag{12}$$

where

$$\Xi = \kappa\sin\phi - h^{-2}q_2M. \tag{13}$$

We then construct the metric tensor $\mathbf{G}$ by expanding the differential $\mathrm{d}\boldsymbol{R}$ in terms of $\mathrm{d}q_1$, $\mathrm{d}q_2$ and $\mathrm{d}q_3$, yielding the following expressions for the components of $\mathbf{G}$:

$$\begin{aligned}
g_{11} &= h^2 + 2q_3([\partial_1 \boldsymbol{S}]\cdot[\partial_1 \boldsymbol{N}]) + q_3^2\|\partial_1 \boldsymbol{N}\|^2\\
g_{22} &= 1 + 2q_3([\partial_2 \boldsymbol{S}]\cdot[\partial_2 \boldsymbol{N}]) + q_3^2\|\partial_2 \boldsymbol{N}\|^2\\
g_{33} &= 1\\
g_{12} &= g_{21} = q_3(([\partial_1 \boldsymbol{S}]\cdot[\partial_2 \boldsymbol{N}]) + ([\partial_2 \boldsymbol{S}]\cdot[\partial_1 \boldsymbol{N}])) + q_3^2([\partial_1 \boldsymbol{N}]\cdot[\partial_2 \boldsymbol{N}])\\
g_{13} &= g_{31} = q_3([\partial_1 \boldsymbol{N}]\cdot \boldsymbol{N})\\
g_{23} &= g_{32} = q_3([\partial_2 \boldsymbol{N}]\cdot \boldsymbol{N}).
\end{aligned}\tag{14}$$

We investigate the terms in (14) which are made up of scalar products of $\boldsymbol{N}$, the partial derivatives of $\boldsymbol{N}$ and the partial derivatives of $\boldsymbol{S}$. With Ξ as in (13), we have

$$\begin{aligned}
&([\partial_1 \boldsymbol{N}]\cdot \boldsymbol{N}) = 0 \qquad ([\partial_2 \boldsymbol{N}]\cdot \boldsymbol{N}) = 0\\
&([\partial_1 \boldsymbol{S}]\cdot[\partial_1 \boldsymbol{N}]) = -h\,\Xi \qquad \|\partial_1 \boldsymbol{N}\|^2 = h^{-2}T^2 + \Xi^2\\
&([\partial_2 \boldsymbol{S}]\cdot[\partial_2 \boldsymbol{N}]) = 0 \qquad \|\partial_2 \boldsymbol{N}\|^2 = h^{-4}T^2\\
&([\partial_1 \boldsymbol{S}]\cdot[\partial_2 \boldsymbol{N}]) = -h^{-3}T \qquad ([\partial_2 \boldsymbol{S}]\cdot[\partial_1 \boldsymbol{N}]) = h^{-1}T\\
&([\partial_1 \boldsymbol{N}]\cdot[\partial_2 \boldsymbol{N}]) = -h^{-2}T\,\Xi.
\end{aligned}\tag{15}$$

This leads to the desired metric tensor

$$\mathbf{G} = \begin{bmatrix} g_{11} & g_{12} & 0\\ g_{21} & g_{22} & 0\\ 0 & 0 & 1\end{bmatrix} = \begin{bmatrix} (h-\Xi_3)^2 + 2h^{-2}T_3^2 & (h^{-1}-h^{-3})T_3 & 0\\ (h^{-1}-h^{-3})T_3 & 1+h^{-4}T_3^2 & 0\\ 0 & 0 & 1\end{bmatrix}\tag{16}$$

where we use the dimensionless variables T_3 and Ξ_3 obtained by scaling T and Ξ by q_3, that is, $T_3 = q_3 T$ and $\Xi_3 = q_3\,\Xi$.

The determinant of $\mathbf{G}$ is given by $g = g_{11}g_{22} - g_{12}^2$, which we express as

$$g = h^{-2}[(h^2 - h^{-2}T_3^{-2})(h-\Xi_3)^2 + h^{-2}T_3^{-2}(1-h^{-2}T_3^{-2})].\tag{17}$$

This gives the inverse $\mathbf{G}^{-1}$ of $\mathbf{G}$,

$$\mathbf{G}^{-1} = \begin{bmatrix} g^{11} & g^{12} & 0\\ g^{21} & g^{22} & 0\\ 0 & 0 & 1\end{bmatrix} = \begin{bmatrix} g_{22}/g & -g_{12}/g & 0\\ -g_{12}/g & g_{11}/g & 0\\ 0 & 0 & 1\end{bmatrix}.\tag{18}$$

We now are ready to apply the 'straightening-out' transformation. Because the Hamiltonian is given by multiplying ∇^2 by $-\hbar^2/(2m^*)$, the effective potential is given by

$$V_{\text{eff}}(q_1,q_2,q_3)\chi = \frac{-\hbar^2}{2m^*}U_0\chi.\tag{19}$$

We now go back to (8), and with (14) and (17) we obtain

$$V_{\text{eff}}(q_1,q_2,q_3) = \frac{\hbar^2}{8m^*}\left[g^{-1/4}\sum_{i,j=1}^{2}\partial_i(g^{-3/4}g^{ij}\partial_j g) + f^{-1}\partial_3^2 f - \frac{3}{4}f^{-2}[\partial_3 f]^2\right].\tag{20}$$

Note that V_{eff} also depends on q_3. It is now that we take the limit as $q_3 \to 0$, since we have been careful to include the extra terms depending on $\partial_3^2 g$ and $\partial_3 g$ terms. We put $g_\Omega = h^2$, obtaining

$$V_{\text{eff}}(q_1,q_2) = \frac{\hbar^2}{8m^*}\left[h^{-1/2}\frac{\partial}{\partial q_1}(h^{-7/2}\partial_1 g_\Omega) + h^{-1/2}\frac{\partial}{\partial q_2}(h^{-3/2}\partial_2 g_\Omega) - h^{-2}\,\Xi^2\right].\tag{21}$$

It is easier to evaluate the partial derivatives of g_Ω than of h. Hence, we express (21) in terms of g_Ω, obtaining

$$V_\Omega = \frac{\hbar^2}{8m^*}\left[g_\Omega^{-2}\partial_1^2 g_\Omega - \frac{7}{4}g_\Omega^{-3}[\partial_1 g_\Omega]^2 + g_\Omega^{-1}\partial_2^2 g_\Omega - \frac{3}{4}g_\Omega^{-2}[\partial_2 g_\Omega]^2 - g_\Omega^{-1}\Xi^2\right]. \quad (22)$$

Note that (22) is a corrected version of the effective potential result given in equation (24) of [1]; the Ξ-dependent term was inadvertently neglected in [1].

Suppose d is small compared with a length L over which curvature and torsion vary in the longitudinal direction. The same dimensionless variables x and y in equation (44) in [1] are used, i.e. $q_1 = xL$ and $q_2 = yd$. Henceforth, the variables θ, M and Ξ are taken to be functions of x and y, the correspondence being made in the natural manner. We find it easier to transform $\Xi(q_1, q_2)$ into

$$\hat{\Xi}(x, y) = \hat{\kappa}(x)\sin\theta + g_\Omega^{-1}\epsilon y\left[\hat{T}\epsilon y\frac{\partial A}{\partial x} + (1-\epsilon y A)\frac{\mathrm{d}\hat{T}}{\mathrm{d}x}\right] \quad (23)$$

where

$$\hat{T}(x) = \hat{\tau}(x) - \frac{\mathrm{d}\phi}{\mathrm{d}x} \qquad \text{and} \qquad A(x) = \hat{\kappa}(x)\cos[\phi(x)]. \quad (24)$$

This satisfies $\Xi = \hat{\Xi}/L$. From the effective potential $V_{\mathrm{eff}}(q_1, q_2)$, we define a dimensionless effective potential $\mathcal{V}(x, y)$:

$$V_{\mathrm{eff}}(q_1, q_2) = \mathcal{V}(x, y)E_d. \quad (25)$$

The expression for g_Ω can then be expressed as

$$g_\Omega(x, y) = 1 - 2\epsilon y A(x) + \epsilon^2 y^2 B(x) \quad (26)$$

where $B(x) = A^2(x) + \hat{T}^2(x)$. After some simple algebra, (22) becomes

$$V_{\mathrm{eff}}(q_1, q_2) = \frac{\hbar^2}{8m^* d^2}\left[g_\Omega^{-1}\frac{\partial^2 g_\Omega}{\partial y^2} - \frac{3}{4}g_\Omega^{-2}\left[\frac{\partial g_\Omega}{\partial y}\right]^2 + \epsilon^2 g_\Omega^{-2}\frac{\partial^2 g_\Omega}{\partial x^2} - \frac{7}{4}\epsilon^2 g_\Omega^{-3}\left[\frac{\partial g_\Omega}{\partial x}\right]^2 \right.$$
$$\left. -\epsilon^2 g_\Omega^{-1}\hat{\Xi}^2\right]. \quad (27)$$

From (25), we have

$$\mathcal{V}(x, y) = \frac{1}{4}g_\Omega^{-1}\frac{\partial^2 g_\Omega}{\partial y^2} - \frac{3}{16}g_\Omega^{-2}\left[\frac{\partial g_\Omega}{\partial y}\right]^2 + \epsilon^2\left[\frac{1}{4}g_\Omega^{-2}\frac{\partial^2 g_\Omega}{\partial x^2} - \frac{7}{16}g_\Omega^{-3}\left[\frac{\partial g_\Omega}{\partial x}\right]^2 - \frac{1}{4}g_\Omega^{-1}\hat{\Xi}^2\right]. \quad (28)$$

Using (26) to express g_Ω as a quadratic, and collecting terms in ϵ, we have

$$\mathcal{V}(x, y) = \epsilon^2[\tfrac{1}{2}B - \tfrac{3}{4}A^2 - \tfrac{1}{4}\hat{\Xi}^2] + \mathrm{O}(\epsilon^3). \quad (29)$$

We then ignore the higher-order terms in ϵ and use (23) to obtain the asymptotic expansion to second order in ϵ:

$$\mathcal{V}(x, y) \approx \epsilon^2\left[-\frac{1}{4}[\hat{\kappa}(x)]^2 + \frac{1}{2}\left[\hat{\tau}(x) - \frac{\mathrm{d}\phi(x)}{\mathrm{d}x}\right]^2\right] \quad (30)$$

or in terms of q_1 and q_2,

$$V_\Omega(q_1, q_2) \approx \frac{\hbar^2}{2m^*}\left[-\frac{1}{4}[\kappa(q_1)]^2 + \frac{1}{2}[\tau(q_1) - \theta'(q_1)]^2\right]. \quad (31)$$

This agrees with (2), concluding this work.

The author is grateful to P Exner for pointing out that (1) could not be correct as it stands, and to Anthony J Bracken for all his help with the author's PhD project.

References

[1] Clark I J and Bracken A J 1996 *J. Phys. A: Math. Gen.* **29** 339–48
[2] Clark I J 1996 *PhD Thesis* The University of Queensland, Brisbane, Australia
[3] Clark I J 1998 *Appl. Math. Lett.* to appear