Quantum Hall-like effect on strips due to geometry

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In this Letter we present an exact calculation of the effective potential which appears on a helicoidal strip. This potential leads to the appearance of localized states at a distance $\xi_0$ from the central axis. The twist $\omega$ of the strip plays the role of a magnetic field and is responsible for the appearance of these localized states and an effective transverse electric field thus this is reminiscent of the quantum Hall effect. At very low temperatures the twisted configuration of the strip may be stabilized by the electronic states.

PACS numbers: 03.65.Ge, 73.43.Cd

The appearance of nanostructures has boosted the interest in quantum strip waveguides and in tubular quantum waveguides. Of special interest is the appearance of bound states in these structures. For a thin tubular waveguide the binding potential is [1]

$$V_{eff} \approx -\frac{k^2} {2m} \frac{k^2} {4}$$  

where $k$ is the curvature of the axis of the tube, viewed as a space curve. In the case of a quantum strip the effective potential is [2]

$$V_{eff} \approx \frac{\hbar^2} {2m} \left( -\frac{k^2} {4} + \frac{1} {2} [\tau - \theta_s]^2 \right)$$  

where $\tau$ is the torsion of the strip axis and $\theta$ is the twist angle around the axis. Here the subscript $s$ stands for $\frac{ds}{dx}$, where $s$ is the arc-length of the curve. Usually these results are valid for thin tubes and narrow strips and the curvature $k$ should be small. [1]. The curvature $k$ is responsible for the appearance of bound states in both types of waveguides.

In this Letter we evaluate the sole effect of twisting of a strip and show that a pure twist may cause localization and play the role of an applied magnetic field.

We consider a strip whose edge is a straight line along the $x$-axis and whose other edge follows a helix around the $x$-axis. The surface represents a helicoid and is given by the following equation:

$$r = x e_x + \xi [\cos(\omega x) e_y + \sin(\omega x) e_z],$$  

where $\omega = 2\pi/L$, $L$ is the total length of the strip and $n$ is the number of $2\pi$-twists.

$$(e_x, e_y, e_z)$$ is the usual orthonormal triad in $R^3$ and $\xi \in [0, D]$, where $D$ is the width of the strip. Let $dr$ be the displacement

$$dr = dx e_x + [\cos(\omega x) e_y + \sin(\omega x) e_z] d\xi +$$  

$$+ [-\omega \xi \sin(\omega x) e_y + \omega \xi \cos(\omega x) e_z] dx$$

and therefore we have:

$$|dr|^2 = (1 + \omega^2 \xi^2) dx^2 + d\xi^2 = h_1^2 dx^2 + h_2^2 d\xi^2,$$  

where $h_1 = \sqrt{1 + \omega^2 \xi^2}$ and $h_2 = 1$ are the Lamé coefficients of the induced metric (from $R^3$) on the strip. Now the Hamiltonian for a free particle on the strip is given by:

$$H = -\frac{\hbar^2} {2m} \frac{1} {h_1} \left[ \left( \frac{\partial}{\partial \xi} h_1 \frac{\partial}{\partial \xi} \right) + \frac{1} {4} \frac{h_1^2} {h_2^2} \left( \frac{\partial h_1}{\partial \xi} \right)^2 + \frac{\partial^2}{\partial \xi^2} \right]$$  

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After rescaling the wave function $\psi \mapsto \frac{1}{\sqrt{h_1}} \psi$ (because we require the wave function to be normalized with respect to the area element $dx d\xi$) and after some algebra we arrive at the following expression for the Hamiltonian:

$$H = -\frac{\hbar^2} {2m} \frac{1} {h_1} \frac{\partial^2}{\partial \xi^2} + V_{eff}(\xi) - \frac{\hbar^2} {2m} \frac{1} {h_1^2} \frac{\partial^2}{\partial x^2},$$  

where $V_{eff}(\xi)$ is the effective potential. The appearance of these localized states and an effective transverse electric field thus this is reminiscent of the quantum Hall effect.

FIG. 1: Helicoidal Surface

This Hamiltonian may be rewritten in a more transparent form:

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where the effective potential in the \( \xi \) direction is given by:

\[
V_{\text{eff}}(\xi) = -\frac{\hbar^2}{2m} \left[ -\frac{1}{2h_1} \left( \frac{\partial^2 h_1}{\partial \xi^2} \right) + \frac{1}{4} \frac{1}{h_1} \left( \frac{\partial}{\partial \xi} \right)^2 \right]
\]

Note that in \([\text{1}]\) and \([\text{2}]\) the effective potential is longitudinal. In the present case there is no longitudinal effective potential. After insertion of \( h_1 = \sqrt{1 + \omega^2 \xi^2} \) the effective potential becomes:

\[
V_{\text{eff}}(\xi) = \frac{\omega^2 \hbar^2}{4m} \frac{1}{(1 + \omega^2 \xi^2)^2} \left[ 1 - \frac{\omega^2 \xi^2}{2} \right]. \quad (8)
\]

This effective potential is of pure quantum-mechanical origin because it is proportional to \( \hbar \). Note that this expression is exact and is valid not only for small \( \xi \): here no expansions in small parameter has been used. On the axis of the helicoid \( \xi = 0 \) we get the following value of the repulsive potential \( V_{\text{eff}}(0) = 4\omega^2 \xi^2 \) which corresponds to the expression for the effective potential found in \([\text{2}]\) for \( k = 0 \) and \( \tau = 0 \) and \( \theta = \omega \). \( V_{\text{eff}}(0) \) represents a local maximum of the potential. The local minimum is reached for \( \xi_0 = \frac{\pi L}{\tau} \) and \( V_{\text{eff}}(\xi_0) = -\frac{1}{2} \frac{\omega^2 \hbar^2}{4m} \).

Now we may write the time-independent Schrödinger equation as:

\[
\left[ \frac{\hbar^2}{2m} \frac{\partial^2}{\partial \xi^2} + V_{\text{eff}}(\xi) \right] \psi - \frac{\hbar^2}{2m} \frac{1}{h_1} \frac{\partial \psi}{\partial \xi} = E \psi \quad (9)
\]

Using the ansatz: \( \psi(x, \xi) = \phi(x) f(\xi) \):

\[
\left[ \frac{\hbar^2}{2m} \frac{1}{f(\xi)} \frac{\partial^2 f(\xi)}{\partial \xi^2} + \left( V_{\text{eff}}(\xi) - E \right) \frac{1}{h_1^2} \frac{\partial^2 \phi(x)}{\partial x^2} \right] = 0
\]

we get two differential equations:

\[
\frac{\hbar^2}{2m} \frac{\partial^2 \phi(x)}{\partial x^2} = -E\phi(x), \quad (11)
\]

and

\[
-\frac{\hbar^2}{2m} \frac{\partial^2 f(\xi)}{\partial \xi^2} + \left[ V_{\text{eff}}(\xi) + \frac{E_0}{h_1^2(\xi)} \right] f(\xi) = E, \quad (12)
\]

With \( \phi(x) = e^{ik_x x} \) in eq(11) we have \( E_0 = \frac{k_x^2 \hbar^2}{2m} \) where \( k_x \) is the partial momentum in \( x \)-direction.

It is clear from eq(8) that for \( \xi \) close to 0, \( V_{\text{eff}} \) represents a repulsive potential and the twist \( \omega \) works “against” the appearance of localized states \([\text{2}]\). However, for \( \xi \geq \frac{\sqrt{2}}{\omega} = \frac{\sqrt{2} \pi L}{n} = \xi_0 \) (there are no restrictions on \( \xi \) in eq.(8)) \( V_{\text{eff}} \leq 0 \) and there will be localized states. Physically one may understand the appearance of localized states away from the central axis using the Heisenberg uncertainty principle: for greater \( \xi \) a particle on the strip will dispose with more “space” along the corresponding helix and therefore the corresponding momentum and hence energy will be smaller than for a particle closer to the central axis. Thus the twist \( \omega \) will “push” the electrons towards the outer edge of the strip and create an effective electric field between the central axis and the helix. The depth of the potential minimum depends on \( \omega \). Thus the number of localized states (and their existence) will depend on the width of the strip and on the twist. The minimum of the potential in eq(12) is reached for \( \xi = \xi_0 \) and is given by:

\[
U_{\text{min}} = \frac{\hbar^2}{6m} \left[ k_x^2 - \frac{\omega^2}{16} \right].
\]

For small \( k_x \) i.e. \( k_x \leq \frac{\omega}{4} \), \( E_{\text{min}} \leq 0 \) and there is a possibility for having localized states with negative energy levels. For very low temperatures most of the \( k_x \)'s will be well below \( \frac{\omega}{4} \) (\( \frac{\sqrt{2} \pi L}{n} \sim k_B T \), where \( k_B \) is the Boltzmann constant and \( T \) is the temperature). For a strip of width at least \( D = \xi_0 \), the twisting the strip will increase its elastic energy (the elastic energy density per unit length is \( \frac{1}{4} C^* \omega^2 \), where \( C^* \) is the torsional constant) but on the other hand will create localized states with negative energy levels which will diminish the total electronic energy and for rather soft materials it may favor the twisted configuration against that of the flat strip.

Eq(12) represents the motion in the direction \( \xi \) with a net potential

\[
U(\xi) = \frac{\omega^2}{4} \left\{ \frac{4C^2 - 1}{(1 + \omega^2 \xi^2)^2} + \frac{3}{(1 + \omega^2 \xi^2)^2} \right\}
\]

where \( C = \frac{k_x}{\omega} \). This potential is a sum of two contributions, a repulsive part: \( \frac{3}{(1 + \omega^2 \xi^2)^2} \) and a variable part which is repulsive for \( C^2 \geq \frac{1}{4} \) and attractive for \( C^2 \leq \frac{1}{4} \).

If \( C \leq \frac{1}{2} \) the \( U(\xi) \) becomes negative for \( \omega \xi \geq \sqrt{\frac{2 + 4C^2}{1 - 4C^2}} \) and one expects bound states with negative energy eigenvalues in this potential well. The finite size of the width \( D \) determines the cut-off of \( U(\xi) \) and hence the probability for a particle to be “pushed” to the boundary of the strip.

Equation of motion (12) may take the remarkable normal form of the equation of a confluent Heun function \([\text{3}]\): let’s call \( f(\xi) = H(\omega^2 \xi^2) = H(z) \). Then putting \( e = \frac{k_x}{\omega} \), we get an equation for the function \( H(z) \):

\[
-z H''(z) - \frac{1}{2} \frac{z}{H'}(z) + \frac{1}{16} \left\{ \frac{4C^2 - 1}{1 + z} + \frac{3}{(1 + z)^2} \right\} H(z) = -e H(z).
\]

A further change of function \( H(z) = z^{1/4} L(z) \) leads to:

\[
-z L'' - \frac{3}{16} L + \frac{1}{16} \left\{ \frac{4C^2 - 1}{1 + z} + \frac{3}{(1 + z)^2} \right\} L = -e L.
\]
Now define $\zeta = 1 + z$ and set $L(z) = M(\zeta)$, the equation satisfied by $M(\zeta)$ is of the form:

$$M''(\zeta) + Q(\zeta)M(\zeta) = 0. \quad (16)$$

with

$$Q(\zeta) = -\left( e + \frac{4C^2 - 1}{16} \right) \frac{1}{\zeta - 1} + \frac{4C^2 + 2}{16\zeta} + \frac{3}{16\zeta^2} \quad (17)$$

This is to be compared to the normal form of a confluent Heun equation:

$$y'(x) + \left\{ A + \frac{B}{x} + \frac{C}{x - 1} + \frac{D}{x^2} + \frac{E}{(x - 1)^2} \right\} y(x) = 0.$$ 

Thus eq(16) is really a confluent Heun equation with

$$A = 0, \quad B = \frac{4C^2 + 2}{12}, \quad C = -\left( e + \frac{4C^2 - 1}{16} \right),$$

$$D = \frac{3}{16}, \quad E = 0$$

which all depend on $C = \frac{k}{\omega}$ representing the ratio of straight propagation in the $x$-direction over the geometric twist. As the properties of confluent Heun functions are not extensively known, e.g. zeros have not yet been completed, we shall not dwell on it.

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