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THE SHAPE-SCHRÖDINGER EQUATION ON AN ELASTIC MEMBRANE

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Виктор Атанасов. УРАВНЕНИЕТО НА ФОРМАТА-ШРЬОДИНГЕР ВЪРХУ ЕЛАСТИЧНА МЕМБРАНА

Тук демонстрираме еквивалентност между уравнението на формата на еластична мембрана и квантовомеханичното двумерно уравнение на Шрьодингер за (квази-) частица върху повърхността на мембрана. Кривината на повърхността е свързана с неочаквано статично формирование подобно на конформон: концентрация на плътността на вероятноста да се намери (квази-) частицата там, където е концентрирана еластичната енергия, или, с други думи, там, където кривината има максимум.

Victor Atanasov. THE SHAPE-SCHRÖDINGER EQUATION ON AN ELASTIC MEMBRANE

We demonstrate an equivalence between the elastic membrane shape equation and the quantum mechanical two dimensional Schrödinger equation for a (quasi-) particle on the surface of the membrane. Surface curvature is related to an unexpected static formation: the concentration of the expectation value to find a (quasi-) particle where the elastic energy is concentrated, namely where surface curvature has a maximum.

Keywords: membrane, shape equation, two dimensional Schrödinger equation, conformon
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Setting any of the coordinates of a quantum system to zero is an act prohibited by the Uncertainty Principle due to Werner Heisenberg, a cornerstone principle of a viable quantum mechanical theory. Therefore the correct quantum description of a (quasi-) particle on a two dimensional surface (which can be severely curved) has to account for the embedding. Setting the off-surface coordinate to zero is prohibited, therefore the (quasi-) particle's wave function would be able to probe the surface for bending through the embedding space. Consequently, a geometrically induced term appears in the surface Schrödinger equation. The complete quantum procedure producing the two dimensional quantum equation is realized by constraints (external potentials [1]) forcing the system to occupy less degrees of freedom available for the (quasi-) particle, namely in two-dimensional electron (or hole) systems (2DES) such as those of graphene and graphene oxide.

Thus the (quasi-) particle's wave function is separable into surface and normal (off-surface) components. However, absent a truly two dimensional system that can be easily bent, the effect of geometric potential on the electronic band structure has been justifiably ignored in device engineering up to now.

Graphene and its oxide represent a class of materials which can display the effects produced by the geometric potential due to bending of the surface.

Specifically, the two dimensional form of sp^3/sp^2 hybridized carbon, known as graphene oxide, is a flexible 1 nm thick soft membrane embedded in three dimensional space. This is an example of novel material which carriers are of Schrödinger type.

The quantum dynamics of a *nonrelativistic* (quasi-) particle constrained to an arbitrary orientable surface is well explored: the curvature of the surface induces an attractive (has a minimum where maximally curved) geometric potential due to da Costa [1]

$$V_G = -\frac{\hbar^2}{2m^*}\left(H^2 - K\right),$$

where $m^*$is the effective mass of the particle, $\hbar$ is the Planck's constant; $H = \frac{1}{2}\left(k_1 + k_2\right)$ and $K = k_1 k_2$ are the Mean and the Gaussian curvature of the surface, respectively. Here k_1,k_2 are the two position-dependent principal curvatures of the surface [2].

This potential is purely a result of particle confinement, and is independent of the electric charge of the particle; it is therefore the same for electrons and holes. It appears in the Schrödinger equation in curvilinear surface coordinates

This result is applicable in the limit $x_0 H \to 0$ where x_0 the thickness of the "two-dimensional" surface is and is the Mean curvature. Note x_0 corresponds to

the width of the normal to the surface quantum well in 2DES where particles are confined.

Now we reproduce the constrained quantum problem for the carriers confined in two dimensions [1]: separating the dependence of the wave function on surface and normal variables $\chi = \chi_t(q_1,q_2,t)\chi_n(q_3,t)$ we have a set of two equations determining the quantum evolution of the surface part χ_t and off-surface $\chi_n(q_3,t)$ part

$$-\frac{\hbar^2}{2m^*}\left[\Delta_S + \left(H^2 - K\right)\right]\chi_t = i\hbar\frac{\partial\chi_t}{\partial t}, \tag{1}$$

$$\Delta_S = \sum_{i,j=1}^{2}\frac{1}{\sqrt{g}}\frac{\partial}{\partial q_i}\left(\sqrt{g}\,g^{ij}\frac{\partial}{\partial q_j}\right), \tag{2}$$

$$\left[-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial q_3^2} + V_\lambda(q_3)\right]\chi_n = i\hbar\frac{\partial\chi_n}{\partial t}.$$

Please, keep these equations in mind in order to see the emerging equivalence between quantum and elastic properties.

Now we turn to the elastic energy of the membrane. The shape of membranes is due to the curvature of the membrane considered as a regular two-dimensional surface embedded in the Euclidean three-dimensional space. The elastic free energy of a piece of membrane is expressed in terms of the curvature invariant: the Gaussian curvature. The shape equation for the equilibrium conformation of membranes arises from a minimization technique.

The functional for the shape energy due to Ou-Yang and Helfrich is [3]

$$F = \frac{1}{2}k_c\oiint\left(2H - c_0\right)^2 dS + \lambda\oiint dS + \Delta p\int dV$$

where c_0 is the spontaneous curvature of the membrane's surface, k_c is the bending rigidity of the membrane, λ is the membrane's tensile strength or surface tension, Δp is the pressure difference between the upper and lower sides of the membrane.

Standard variational calculus computation $\delta F = 0$ yields the shape equation [3–5]:

$$2\lambda H - \Delta p = 2k_c\Delta_S H + k_c\left(2H^2 - 2K - c_0 H\right)\left(2H + c_0\right).$$

Here Δ_S is the Laplace-Beltrami operator. The shape equation is for the Mean curvature H.

Suppose the membrane is open and immersed in homogeneous medium, then the pressure difference vanishes $\Delta p = 0$. In case of vanishing spontaneous curvature $c_0 = 0$, which is only natural for symmetric membranes [3], the shape equation reduces to

$$\left[\Delta_S + 2\left(H^2 - K\right)\right] H(q_1, q_2) = \frac{\lambda}{k_c} H = \varepsilon^2 H. \tag{3}$$

Next, inserting $\chi_t = \psi(q_1, q_2) e^{i\frac{Et}{\hbar}}$ into (1) the stationary Schrödinger equation on the surface

$$\left[\Delta_S + \left(H^2 - K\right)\right] \psi(q_1, q_2) = \frac{2m^* E}{\hbar^2} \psi = \zeta^2 \psi. \tag{4}$$

The similarity between (3) and (4) is obvious for the stationary states of the Schrödinger equation. However, a factor of 2 stands in front of the geometric potential in the elastic shape equation.

This equivalence between these two equations is an example of the "*remarkable coincidence: The equations for many different physical situations have exactly the same appearance...this means that having studied one subject, we immediately have a great deal of direct and precise knowledge about the solutions of the equations of another.*" as Richard Feynman states in his famous course (V 2, ch. 12, p. 12–1).

Here see the profound meaning for the physics of membranes of the differential operator

$$\Delta = \Delta_S + \alpha\left(H^2 - K\right). \tag{5}$$

Here α is a parameter. Whenever we have a combined stationary elastic and quantum eigen-problem on a two dimensional open surface the following hold

$$\Delta_{\alpha=2} H = \varepsilon^2 H \Leftrightarrow \Delta_{\alpha=1} \psi = \zeta^2 \psi.$$

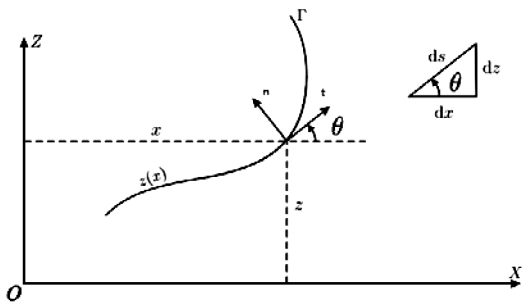

Fig. 1. The profile curve Γ

Here the correspondence goes in the following direction

$$\psi \infty H(q_1, q_2)$$

therefore we can assume that having a solution to the shape equation, we also have a solution to the Schrödinger equation on the surface. However, it is easier said than done. The shape equation is a fourth order (in terms of the position vector spanning the surface) nonlinear partial differential equation. The path to its solutions is far more complicated that to the solutions of the Schrödinger equation on the surface. We can reduce the complexity of the problem using the symmetries of the shape equation [6]. The symmetry group of the membrane shape equation (3) is restricted to the group of motions in R^3 whose basic generators v_j (j = 1, ..., 6) and their characteristics Q_j are listed in the Table 1 due to [6].

Table 1. The generators and their characteristics of the group of motions in R^3 which is the symmetry group of the membrane shape equation. The surface profile is given in Monge representation $\vec{R}(x, y) = [x, y, z(x, y)]$

GENERATORS	CHARACTERISTICS
Translations	
$v_1 = \partial_x$	$Q_1 = -z_1 = -\dfrac{\partial z}{\partial x}$
$v_2 = \partial_y$	$Q_2 = -z_2 = -\dfrac{\partial z}{\partial y}$
$v_3 = \partial_z$	$Q_3 = 1$
Rotations	
$v_4 = x\partial_y - y\partial_x$	$Q_4 = yz_1 - xz_2$
$v_5 = x\partial_z - z\partial_x$	$Q_5 = x - zz_1$
$v_6 = y\partial_z - z\partial_y$	$Q_6 = y - zz_2$

Since we know the symmetry group of the shape equation, it is possible to look for the so-called group-invariant solutions of the equation, that is, the solutions, which are invariant under the transformations of the symmetry group [7]. Each group-invariant solution is determined by a reduced equation obtained by a symmetry reduction of the original one. Essentially, different group-invariant solutions correspond to the groups generated by the vector fields v_1 and av_3+v_4 (the optimal system of one-dimensional subalgebras of the symmetry algebra of the shape equation), that is translationally-invariant and rotationally-invariant solutions.

Nevertheless, only a few analytic solutions to the shape equation are presently known. These are: spheres and circular cylinders, Clifford tori, Delaunay surfaces, circular biconcave discoids, nodoid-like and unduloid-like shapes, some types of Willmore and constant squared mean curvature surfaces as well as cylindrical surfaces. Besides for the spheres and circular cylinders, explicit parameterizations are available for the surfaces of Delaunay and the generalized cylindrical surfaces [8].

The axisymmetric membranes are surfaces of revolution obtained by revolving around the *Z*-axis its profile curve Γ laying in the *XOZ*-plane. If *s* denotes the arclength along the curve and θ(*s*) denotes the slope of the tangent to the curve with respect to the *OX*-axis measured counterclockwise, the following hold:

$$\frac{dz}{dx} = \tan(\theta).$$

One can represent the profile curve Γ also by the graph $(x,z(x))$ of the function $z = z(x)$ (see Fig. 1). Employing the calculation technique of [9], the shape-Schrödinger equation (3-5) reduces to the following nonlinear third-order ordinary differential equation:

$$\cos^3\theta\frac{d^3\theta}{dx^3} = 4\sin\theta\cos^2\theta\frac{d^2\theta}{dx^2}\frac{d\theta}{dx} - \cos\theta\left[\sin^2\theta - \left(1-\frac{\alpha}{4}\right)\cos^2\theta\right]\left(\frac{d\theta}{dx}\right)^3$$
$$-\frac{2\cos^3\theta}{x}\frac{d^2\theta}{dx^2} + \left(3+\frac{\alpha}{4}\right)\frac{\sin\theta\cos^2\theta}{x}\left(\frac{d\theta}{dx}\right)^2 + \left(\varepsilon^2 - \frac{\left(1-\frac{\alpha}{4}\right)\sin^2\theta - \cos^2\theta}{x^2}\right)\cos\theta\frac{d\theta}{dx}$$
$$+\left(\varepsilon^2 - \frac{\frac{\alpha}{4}\sin^2\theta + \cos^2\theta}{x^2}\right)\frac{\sin\theta}{x}.$$

The solution to the shape-Schrödinger equation for a rotational surface is

$$\psi_{\alpha=1} \infty H_{\alpha=2}(x) = -\frac{1}{2}\left[\cos\theta\frac{d\theta}{dx} + \frac{\sin\theta}{x}\right].$$

The solutions to θ having the property of non-constant mean curvature $H(x)$ is an open problem and will be discussed elsewhere.

In conclusion, we state the main observation in the paper: the shape equation for an elastic open membrane is equivalent to the Schrödinger equation on the surface. The main consequence is the concentration of the probability density for a (quasi-) particle on the surface where its curvature has a maximum (the elastic energy has a local maximum). Similar mechanism in one dimension is reported in [10].

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