Curvature and symmetry breaking in wave mechanics

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Abstract. We calculate the spectrum of the wave equation on an intrinsically curved disk for negative curvature up to second order perturbation theory. Adding the Gaussian curvature to the Laplacian leads to spontaneous symmetry breaking at certain values of curvature resembling the emergence of mass.

1. Introduction
The wave equation on a nonflat space exhibits the effect of curvature in two ways: the kinetic term, i.e. the Laplacian, is modified by the appearance of curvature dependent terms, cf. sec. 2; in addition a ‘quantum geometry potential’ $U_{QG}$ may be introduced which expresses the confinement to the curved space in an unambiguous way. For the Schrödinger equation on a curved surface in flat $\mathbb{R}^3$ it has the shape $U_{QG} = -\frac{1}{2m} K^2 (M^2 - K)$ [1], where $M$ denotes the extrinsic and $K$ the intrinsic or Gaussian curvature. When the coupling to the ambient space represented by $M$ is neglected, $M = 0$; with $\frac{1}{2m} K^2$ set equal to one, $U_{QG}$ consists in simply adding the Gaussian curvature

$$U_{QG} = K.$$  

The influence of curvature on the spectrum may be investigated mathematically by methods of perturbation theory as presented in [2] or [3]. The idea to tackle curvature in wave equations has conceptually similar but technically varying been applied to curved quantum waveguides [4] and to hydrogen in a gravitational field [5]. In the following, perturbation theory is used to study the spectrum of the Schrödinger operator on an intrinsically curved disk. The focus lies on the effect of the quantum geometry potential (1).

In sec. 2 we settle the necessary differential geometry. Sec. 3 gives formulas and notation of the flat disk which are used in sec. 4 to determine the matrix elements of the perturbation expansion in intrinsic curvature. We present a numerical calculation of a section of the spectrum up to second order for negative curvature. It displays spontaneous symmetry breaking further described in sec. 5. Sec. 6 discusses conceptual issues of the calculation and relates the result to Hund’s paradox concerning the existence of stable chiral molecules.

2. Intrinsically curved disk
Let a quantum object be confined to a unit disk by an infinite potential well surrounding the disk. Let the disk be *intrinsically* curved, that is, let it be equipped with a metric with non-vanishing Gaussian curvature. The metric of this isotropically curved surface may be written as

$$g_{mn} = \begin{pmatrix} 1 & 0 \\ 0 & \rho^2 (1 - \frac{1}{2} K \rho^2)^2 \end{pmatrix},$$  

where $\rho$ is the radial coordinate and $K$ is the Gaussian curvature. The Laplace-Beltrami operator in this metric is then

$$\Delta_{QG} = \frac{1}{\sqrt{\det(g_{mn})}} \frac{\partial}{\partial \rho} \left( \sqrt{\det(g_{mn})} g^{mn} \frac{\partial}{\partial \rho} \right).$$

The spectrum of this operator is calculated up to second order perturbation theory. The results are displayed in Table 1, which shows the energy levels for different values of curvature. The spectrum displays spontaneous symmetry breaking, which is further described in sec. 5.
which for small values of $\rho$ and $K$ is the metric tensor of geodesic polars. When $K$ tends to zero it reduces to the flat metric of the plane in polar coordinates.

Employing the formula $K = \frac{1}{2 \sqrt{g_{11}} \sqrt{g_{22}}} \left( \frac{\partial}{\partial \rho} \left( \sqrt{g_{11}} \frac{\partial}{\partial \rho} \right) + \frac{\partial}{\partial \phi} \left( \sqrt{g_{22}} \frac{\partial}{\partial \phi} \right) \right)$ [6][7] for the Gaussian curvature we get for the metric (2)

$$K(\rho) = \frac{K}{1 - \frac{K}{6} \rho^2},$$

which has $\lim_{\rho \to 0} K(\rho) = K$ for small $\rho$.

With the metric (2), calculation of the Laplacian $\Delta = \frac{1}{\sqrt{g}} \frac{\partial}{\partial \rho} \left( \sqrt{g} g^{\rho \rho} \frac{\partial}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial}{\partial \phi} \left( \sqrt{g} \rho^2 \frac{\partial}{\partial \phi} \right)$ yields

$$\Delta(\rho, \phi, K) = \frac{\partial^2}{\partial \rho^2} + \frac{1 - \frac{1}{6} K \rho^2}{\rho (1 - \frac{1}{6} K \rho^2)} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2 (1 - \frac{1}{6} K \rho^2)^2} \frac{\partial^2}{\partial \phi^2},$$

using $g = \det(g_{mn})$ and $\sqrt{g} = \rho (1 - \frac{1}{6} K \rho^2)$. Now, splitting the coefficients of $\frac{\partial}{\partial \rho}$ and $\frac{\partial^2}{\partial \phi^2}$, (4) can be decomposed into

$$\Delta = \Delta^{flat} + \Delta^1,$$

where

$$\Delta^{flat}(\rho, \phi) = \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2}$$

is the familiar Laplacian of the plane in polar coordinates, and

$$\Delta^1(\rho, \phi, K) = -\frac{K}{3(1 - \frac{1}{6} K \rho^2)} \left( \frac{\partial}{\partial \rho} - \frac{\partial^2}{\partial \phi^2} \right) + \frac{K^2}{36(1 - \frac{1}{6} K \rho^2)^2} \rho^2 \frac{\partial^2}{\partial \phi^2},$$

is the curvature part whose matrix elements will be evaluated in sec. 4. However, no term is neglected or approximated in the full Laplacian (4).

3. The unperturbed system

The stationary Schrödinger equation on the flat disk is

$$\hat{H}^0 \psi^0(\rho, \phi) = E^0 \psi^0(\rho, \phi),$$

with the Hamiltonian

$$\hat{H}^0 = -\frac{\hbar^2}{2 m} \Delta^{flat}(\rho, \phi).$$

Here $\Delta^{flat}(\rho, \phi)$ is given by (6). Again we set $\frac{\hbar^2}{2 m} \equiv 1$.

Requiring the wavefunctions to be zero outside the disk and finite at $\rho = 0$, the eigenfunctions to $\hat{H}^0$ are

$$\psi_{MN}(\rho, \phi) = \frac{J_M(k_{MN} \rho) e^{\pm \lambda \phi}}{\sqrt{2\pi} \sqrt{\int_0^1 dp \rho J_M(k_{MN} \rho)^2}}$$

(10)

Here $J_M$ denotes the Bessel function of the first kind of order $M$ [8] with $M$ an integer and $k_{MN}$ the $N$-th zero of $J_M$.

The energies $E_n^0$ of the unperturbed system are simply $k_{MN}^2$. Table 1 shows their values for the ground state with energy $E_0^0$ and the first nine excited states.

The corresponding wavefunctions $\psi_n^0(\rho, \phi)$, $n = 0 ... 9$, are given by (10), labeled in the sequence of increasing unperturbed energies as listed in table 1, $\psi_n^0(\rho, \phi) = \psi_{MN}(\rho, \phi)$. Due to the factor $e^{\pm \lambda \phi}$ in (10), any energy with $M \neq 0$ has multiplicity two. The $\psi_{MN}(\rho, \phi)$ build a system of mutually orthonormal eigenfunctions, $\int_0^1 \int_0^{2\pi} dp \rho \phi \psi_{MN}^*(\rho, \phi) \psi_{M'N'}(\rho, \phi) = \delta_{M'M} \delta_{NN'}$. 

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Table 1. The first ten energies $E_n^0 = k_{MN}^2$, $n = 0 \ldots 9$, of the flat disk. M denotes the quantum number of angular momentum, N the number of radial zeros.

| Energy | n | M N | $k_{MN}^2$ | Energy | n | M N | $k_{MN}^2$ |
|--------|---|-----|------------|--------|---|-----|------------|
| $E_0^0$ | 0 | 0 1 | 5.76 | $E_5^0$ | 5 | 1 2 | 49.3 |
| $E_1^0$ | 1 | 1 1 | 14.7 | $E_6^0$ | 6 | 1 4 | 57.6 |
| $E_2^0$ | 2 | 2 1 | 26.4 | $E_7^0$ | 7 | 2 2 | 70.9 |
| $E_3^0$ | 3 | 0 2 | 30.5 | $E_8^0$ | 8 | 0 3 | 74.8 |
| $E_4^0$ | 4 | 3 1 | 40.7 | $E_9^0$ | 9 | 5 1 | 76.9 |

4. Matrix elements and energies

With $\hat{H} = -\nabla^2$, the Hamiltonian $\hat{H}^1$ representing the curvature induced perturbation is the negative of the curvature part (7) of the Laplacian (4),

$$\hat{H}^1(\rho, \phi, K) = \frac{K}{3(1 - \frac{1}{6} K \rho^2)} (\rho \frac{\partial}{\partial \rho} - \frac{\partial^2}{\partial \phi^2}) - \frac{K^2}{36(1 - \frac{1}{6} K \rho^2)^2} \rho^2 \frac{\partial^2}{\partial \phi^2}. \tag{11}$$

The matrix elements $V_{nm'}$ of $\hat{H}^1(\rho, \phi, K)$ are to be constructed with respect to the unperturbed wavefunctions of the flat system. Nevertheless, as integration measure we take the volume element of the curved metric (2), cf. sec. 6 below:

$$dV^{\text{curved}} = \sqrt{g} d\rho d\phi = \rho(1 - \frac{1}{6} K \rho^2) d\rho d\phi. \tag{12}$$

Thus, the matrix elements $V_{nm'}(K)$ are

$$V_{nm'}(K) = \int_0^1 d\rho d\phi \rho (1 - \frac{1}{6} K \rho^2)^{\frac{3}{2}} \psi_{mn}(\rho, \phi) \hat{H}^1(\rho, \phi, K) \psi_{mn'}(\rho, \phi). \tag{13}$$

Since $\frac{1}{\rho^2} \int_0^{2\pi} d\phi e^{i[\alpha M - \beta N] \phi} = \delta_{MN}$, the perturbation $\hat{H}^1$ of (11) only depends on $\rho$,

$$\hat{H}^1(\rho, K) = \frac{K}{3(1 - \frac{1}{6} K \rho^2)} (\rho \frac{\partial}{\partial \rho} + M^2) + \frac{K^2 M^2 \rho^2}{36(1 - \frac{1}{6} K \rho^2)^2}. \tag{14}$$

To $\hat{H}^1(\rho, K)$ of (14) we add the Gaussian curvature (3) as the quantum geometry potential $U_{\text{QG}}$ of (1),

$$U_{\text{QG}}(\rho, K) = K(\rho) = \frac{K}{1 - \frac{1}{6} K \rho^2}. \tag{15}$$

Thus, the curvature induced perturbation $\hat{H}^{1\text{QG}}$ is

$$\hat{H}^{1\text{QG}}(\rho, K) = \hat{H}^1(\rho, K) + \frac{K}{1 - \frac{1}{6} K \rho^2}, \tag{16}$$

with $\hat{H}^1$ of (14).

Using the radial part of (10) we get for the matrix elements

$$V_{nm'}^{\text{QG}}(K) = \frac{\int_0^1 d\rho \rho (1 - \frac{1}{6} K \rho^2) J_M(k_{MN} \rho) \hat{H}^{1\text{QG}}(\rho, K) J_M(k_{MN'} \rho)}{\sqrt{\int_0^1 d\rho \rho J_M(k_{MN} \rho)^2} \sqrt{\int_0^1 d\rho \rho J_M(k_{MN'} \rho)^2}}. \tag{17}$$
with the Hamiltonian (16). The perturbation (17) does not change the angular part of the wavefunctions. According to standard perturbation theory the expansion of the energy up to second order is [3]

\[ E_n^{QG}(K) = E_n^0 + V_{nn}^{QG}(K) + \sum_{n' \neq n} \frac{V_{nn'}^{QG}(K) V_{n'n}^{QG}(K)}{E_n^0 - E_{n'}^0}, \]  

(18)

with the matrix elements of (17). The energies given in (18) can be calculated numerically. Fig. 1 shows a section of the spectrum for \( K = -14 \cdots -10 \). Remarkably, perturbation theory turns out to be still convergent at these high values of \( |K| \).

**Figure 1.** A section of the spectrum of the intrinsically curved disk in dependence on the intrinsic curvature \( K \): Laplacian plus quantum geometry potential \( U_{QG} \). Energy levels whose states have opposite parity cross below the energy \( E_0^0 \) of the flat ground state.

5. **Curvature induced spontaneous symmetry breaking**

Generally, spontaneous symmetry breaking means that the ground state of a system does not have the full symmetry of the system’s Hamiltonian, i.e. it is not an eigenstate of one of the symmetry operators that commute with the Hamiltonian. Induced by the quantum geometry potential, this happens with respect to parity in the case of the intrinsically curved disk. The parity operator \( \hat{P} \) is

\[ \hat{P} : \rho \to \rho, \phi \to \phi + \pi. \]  

(19)
The eigenvalues \( p_{\pm} \) of \( \hat{P} \) are \( p_{\pm} = \pm 1 \). Since the curvature modifies the radial dependence only, cf. sec. 4, the perturbed states have the angular dependence \( e^{\pm i M \phi} \) of (10). Therefore, they are symmetric under (19) when \( M \) is even, and they are antisymmetric when \( M \) is odd.

The unperturbed Hamiltonian \( \hat{H}^0 \), (9), and the perturbation \( \hat{H}^{1 \text{QG}} \), (16), are invariant under the parity transformation \( \hat{P} \), (19), and hence also the full Hamiltonian \( \hat{H}^{\text{QG}} = \hat{H}^0 + \hat{H}^{1 \text{QG}} \):

\[
[\hat{H}^{\text{QG}}, \hat{P}] = \hat{H}^{\text{QG}} \hat{P} - \hat{P} \hat{H}^{\text{QG}} = 0. \quad (20)
\]

Therefore parity should be conserved.

However, as shown in Fig. 1, energy levels whose corresponding states have opposite parity cross below the energy \( E_0^0 \) of the flat ground state

\[
\begin{align*}
n = 0, \, p = +1 \quad &\text{with} \quad n = 9, \, p = -1, \\
n = 1, \, p = -1 \quad &\text{with} \quad n = 6, \, p = +1.
\end{align*}
\]

Graphically and numerically the curvatures and energies of these crossings can be determined to be

\[
K = -11.528, \quad E = -1.12 \quad \text{for } (21) \quad \text{and} \quad K = -11.468, \quad E = 5.14 \quad \text{for } (22).
\]

Thus, at these particular values of curvature, new ground states which have no definite parity can be constructed by superposition.

6. Discussion

To evaluate the matrix elements, sec. 4, we choose the volume element \( dV_{\text{curved}} = \rho(1 - \frac{1}{2}K \rho^2)dpd\rho d\phi \) of the curved disk. This choice is a conceptual issue, not a necessity from rigorous mathematics. It is motivated by the physical situation to be modeled. As soon as the curvature perturbation is switched on, curvature is to be taken into account whenever it affects an evaluation. If we interpret our model as scattering of the wavefunctions \( \phi \) by the curved metric then the situation conceptually parallels calculations using the distorted wave Born approximation [9][10][11].

In our calculation, the curved metric and the quantum geometry potential induced by it produce spontaneous symmetry breaking in a system which is spatially finite. This is to be contrasted to the usual procedure of the so called thermodynamic limit where, in order to obtain for example the spontaneous magnetization of ferromagnetism, the volume has to become infinitely large [12]. Thus, the curved metric locally opens a system and evokes an effect which in statistical mechanics is related to infinitely many degrees of freedom.

Violation of parity conservation, as observed in case of the intrinsically curved disk, is connected to Hund’s paradox concerning stable chiral molecules which should not exist according to quantum theory in closed systems. As has been pointed out by F. Hund [13] standard quantum mechanics admits chiral states described by wavefunctions which are not eigenstates of \( \hat{P} \) only at the price that they cannot be stable under unitary time evolution. Because these states are constructed as a superposition of states separated from each other by a finite amount of energy, the enantiomers are driven to oscillate between each other.

The paradox consists in the fact that there exist chiral molecules in nature which are stable. They do not oscillate and their wavefunctions should be ground states of some Hamiltonian. Last but not least the mass of our bodies consists to a large extent of - obviously stable - chiral molecules.

In case of the calculation presented above the new ground states without definite parity would not oscillate because they are built by a superposition of states lying all at the same energy. It is remarkable that the effect of spontaneous symmetry breaking can be assigned to the presence of the quantum geometry potential \( U_{\text{QG}} \) since in the case of the Schrödinger operator without \( U_{\text{QG}} \) none of the crossings of states with opposite parity would occur below \( E_0^0 \) [14].

This allows an interpretation of \( U_{\text{QG}} \) as a mass term.

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