Some considerations on thermodynamics of quantum mechanics on a circle and Kałuża–Klein models

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Abstract:

Introduction/purpose: Quantum mechanics on a circle has been investigated and applied to a Kałuża–Klein model with a compactified dimension.

Methods: Methods of quantum mechanics and statistical mechanics were employed. Additionally, a Kałuża–Klein toy model with compactified dimension was considered.

Results: The resulting partition function can be evaluated in a closed form, giving a special function. It presents a phase transition depending on the geometry. When used in a Kałuża–Klein model, it showed a phase transition regulated by the radius of the circle, and the transition disappears when the radius is infinite, that is in the flat space.

Conclusion: Quantum mechanics on a circle exhibits many peculiar characteristics. Energy levels are discrete because of the geometry, in contrast to the configuration space of the real line. It presents a phase transition depending on the circle radius, also when embedded in a Kałuża–Klein model. This characteristic disappears when the radius becomes infinite, in the flat space.

Keywords: quantum mechanics, statistical mechanics, phase transition, Jacobi theta function, Kałuża–Klein model.

Quantum mechanics on a circle

Consider the problem of one dimensional quantum mechanics on a circle of radius R with Hamiltonian

$$\mathcal{H}\psi = -\frac{\hbar^2}{2m}\left(\frac{d}{dx}\right)^2\psi = E\psi \ . \tag{1}$$

Therefore, the Schrödinger equation (1) has the periodic boundary condition

$$\psi(x) = \psi(x + 2\pi R) \ . \tag{2}$$

It leads to the wavefunctions of the form

$$\psi_{\pm}(x) = \exp(\pm ikx) \tag{3}$$

where $+$ and $-$ represent the solutions for particles moving clockwise and anticlockwise respectively, while k is given by

$$k = \frac{\sqrt{2mE}}{\hbar} \ . \tag{4}$$

Imposing the periodic boundary conditions (2) for the motion on the circle, the following relation is obtained:

$$\exp(\pm ikx) = \exp[\pm ik(x + 2\pi R)] = \exp[\pm i(kx + 2\pi n)] \tag{5}$$

Therefore,

$$k = \frac{1}{R}n \ , \tag{6}$$

that leads to the following expression for the energy eigenvalues

$$E_n = \frac{\hbar}{2mR^2}n^2 = a^2n^2 \ , \tag{7}$$

where $n \in \mathbb{Z}$. Those eigenvalues have a double degeneracy, as the clockwise and anticlockwise motions have the same energy. The momentum is given by the expression $p = \hbar k$.

This problem is related to the model of Kałuża–Klein (Kaluza, 1921; Klein, 1926), which introduced an extra spatial dimension to extend general relativity in order to unify gravity and electromagnetism. This extra dimension is compactified on a circle with a radius so small that it is not directly observable. Various extensions and variations of the model exist, starting from the ADD (Arkani-Hamed, Dimopoulos, Dvali) (Arkani-Hamed et al., 1998) model and the bulk scenario, where only gravity propagates to the extra dimension (Rizzo, 2010), to the UED (Universal extra dimensions) (Appelquist et al., 2001), in which all interactions of the Standard Model propagate into the extra dimension, among others (Kerner, 1968; Appelquist et al.; Randall & Sundrum, 1999; Zee, 2013). In (Fabiano & Panella, 2005, 2010) there are discussions and references to some of them.

To briefly illustrate this mechanism, consider what happens to gravitational interaction in a spatial dimension other than $D = 3$. Start with the Poisson's equation for the gravitational potential V generated by a single object of mass M located at the origin

$$\nabla^2 V = 4\pi G M \delta(r) \; . \tag{8}$$

From dimensional considerations, the delta has a dimension that is the inverse of length, because $\int \delta(x) \mathrm{d}x = 1$, therefore, $\delta \sim 1/r$, and $\delta \sim 1/r^D$ in D dimensions. Consequently, in D dimensions one obtains for the gravitational potential, integrating (8), the scaling relation

$$\nabla^2 V \sim \frac{V}{r^2} = 4\pi G M \delta(r) \sim \frac{1}{r^D} \; , \tag{9}$$

that provides the gravitational potential in D dimensions

$$V(r) \propto \frac{1}{r^{D-2}} \; . \tag{10}$$

Thanks to a theorem due to Bertrand (Bertrand, 1873), it is known that the only possible stable orbits (i.e., closed orbits) arising from a central potential are given by the Coulombic potential and the harmonic oscillator. This implies from (10) that Newtonian orbits are only stable in three dimensions, $D = 3$. Therefore, if further spatial dimensions exist beyond the usual three, they cannot be extended, but must instead be compactified on a circle of small radius, essentially a string, making it unobservable at low energies.

Thermodynamics

From the standard formula for the partition function (Landau & Lifshitz, 2013b; Huang, 2009)

$$Z = \text{tr}\ e^{-\beta\mathcal{H}} = \sum_{n=0}^{+\infty} \langle n|e^{-\beta\mathcal{H}}|n\rangle \tag{11}$$

where $\beta = \frac{1}{k_B T}$, and using the expression for the energy eigenvalues found in (7), one obtains the explicit form of the partition function

$$Z(a,\beta) = \sum_{n=-\infty}^{+\infty} e^{-\beta a^2 n^2} = \vartheta_3(0, e^{a^2\beta})\ . \tag{12}$$

The function $\vartheta_3(z,q)$ is the elliptic theta function, also known as the Jacobi theta function (Whittaker & Watson). It is interesting to observe that the infinite series of this discrete Gaussian provides a known function, while its corresponding finite sum does not have a closed form.

The expected value of the energy, $\langle E\rangle$, also known as the internal energy U could be calculated using the expression

$$U(a,\beta) = -\frac{\partial}{\partial\beta}\log[Z(a,\beta)]\ , \tag{13}$$

and by means of (12) it is possible to write it in the following form

$$U(a,\beta) = \frac{a^2 e^{-a^2\beta}\cdot\vartheta_3^{(0,1)}(0,e^{a^2\beta})}{\vartheta_3(0,e^{a^2\beta})}\ , \tag{14}$$

where $\vartheta_3^{(0,1)}(z,q)$ is the derivative of ϑ_3 with respect to the second variable.

Other thermodynamics functions readily obtained from the partition function are the free energy

$$F(a,\beta) = -\frac{1}{\beta}\log[Z(a,\beta)] \tag{15}$$

and the entropy

$$S(a,T) = -\frac{\partial F(a,T)}{\partial T}\ . \tag{16}$$

Figures (1) and (2) represent the internal energy obtained as a function of the inverse radius circle a and the inverse of temperature β in two and

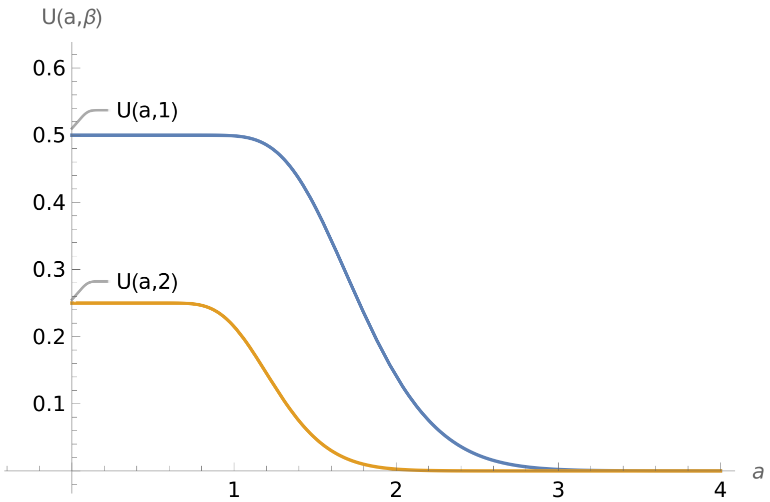


Figure 1 – Internal energy $U(a, \beta)$ as a function of energy parameter a for different values of β

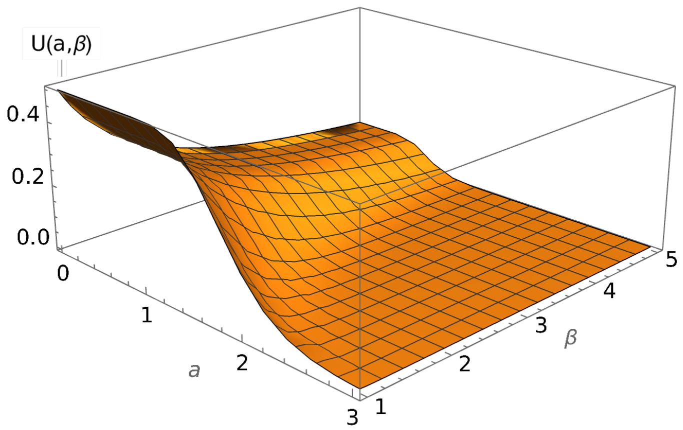


Figure 2 – Internal energy $U(a, \beta)$ as a function of a and β

three dimensions, respectively. From there, it is readily apparent that there is a phase transition driven by the variation of a at a fixed β, as it presents a sharp change. For example, Figure (1) for $\beta = 1$ indicates a critical value of a, that is, a_c, between 1.5 and 2, while for $\beta = 2$ it is found between 1 and 1.5.

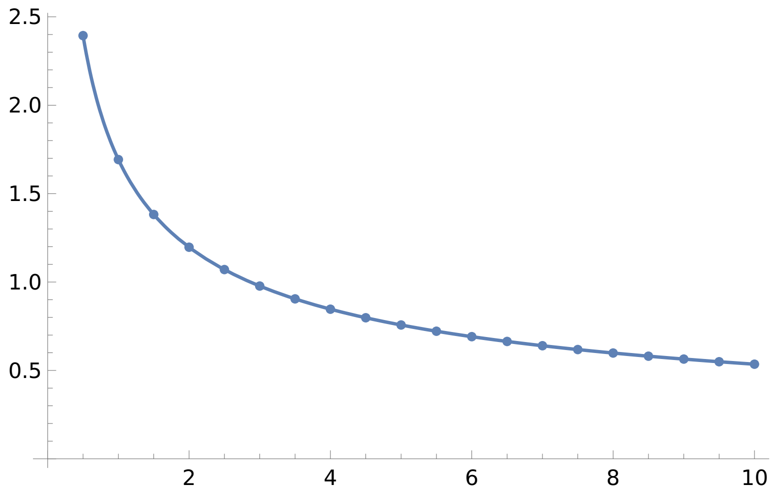


Figure 3 – Fit for critical values of a as function of β

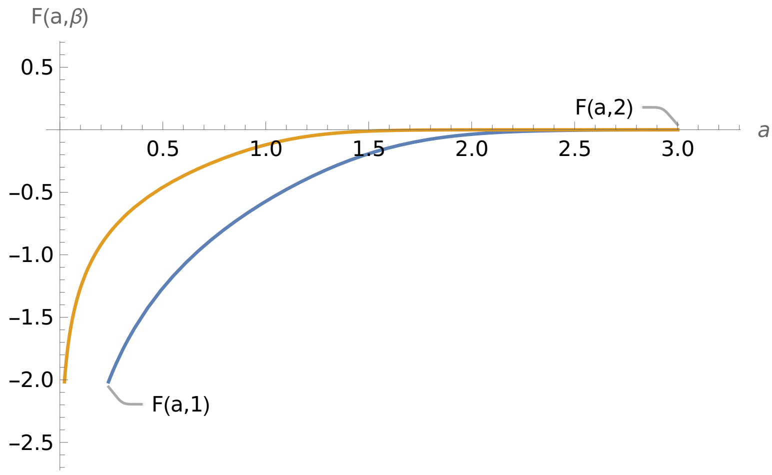


Figure 4 – Free energy $F(a,\beta)$ as a function of energy parameter a for different values of β

A careful numerical evaluation of those critical values as a function of β provides the following fit

$$a_c = \frac{1}{0.590782\sqrt{\beta} - 1.98913 \times 10^{-9}}\ , \tag{17}$$

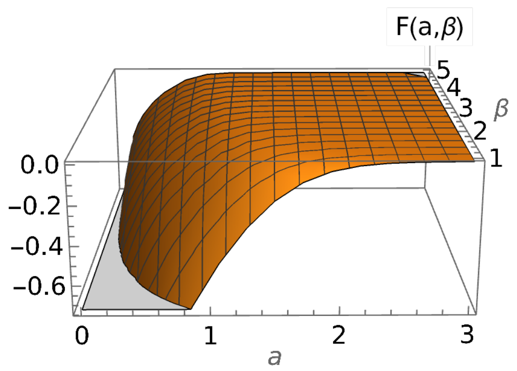
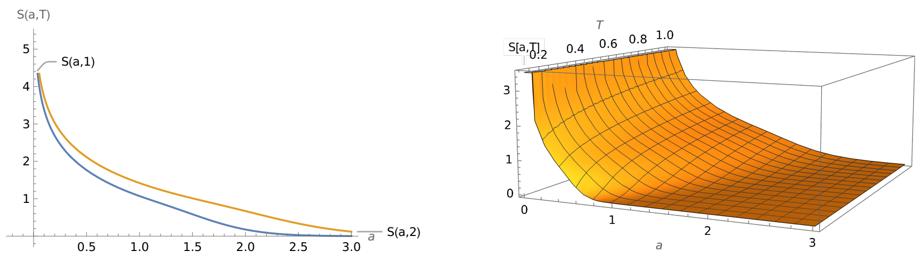


Figure 5 – Free energy $F(a, \beta)$ as a function of a and β



(a) Entropy 2d *(b) Entropy 3d*

Figure 6 – Entropy as a function of a and T

where both parameters at the denominator have a standard deviation error smaller than 10^{-9}.

The results are shown in Figure (3), and exhibit excellent agreement with the critical points, even at low temperatures. The formula (17) could be simplified in practice as $a_c \simeq 1.69267 \times \beta^{-1/2}$, that is the corresponding critical radius of the circle R_c from (7) behaves like

$$R_c \propto T^{-1/2} \; . \tag{18}$$

An observation is in order here. In (7), the energy increases with increasing a, whereas the results above show the opposite behavior for $U = \langle E \rangle$. This apparent paradox is resolved because U is calculated from the weighted average of energy E_n, and its weight, $\exp(-\beta E_n)$ decreases abruptly with E_n, that is a, so that only a few terms of the sum of the partition function actually contribute to $\langle E \rangle$.

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Further evidence of the phase transition is seen in the free energy $F(a, \beta)$, which exhibits a pronounced variation for the neighborhood of a critical value of a, as shown in Figures (4) and (5). Less apparent, but still present, is the same critical behaviour of entropy $S(a, T)$ (16), presented in Figures (6a) and (6b). Numerical evaluation confirms that the critical values of a_c for F and S coincide with the ones found from U in formula (17) and shown in Figure (3).

This particular phase transition does not depend on temperature, unlike, for instance, melting - the transition from ice to water. There are many examples of hase transitions driven by parameters other than temperature, such as the circle radius in our example. To name a few:

- The Ising model, a lattice of spins, could have transitions driven by the coupling constant strength J. At a fixed temperature, when $J \gg kT$, the spins align to a ferromagnetic order, while when J decreases, the spins lose their alignment and undergo a phase transition to a paramagnetic state.
- A XY model with spin–orbit coupling has a phase transition when the α spin–orbit coupling strength changes.
- Ferromagnetic materials such as iron can have phase transitions when exposed to changing magnetic fields, which alter the material's magnetization.
- At low temperatures close to absolute zero, some materials can undergo phase transitions driven by quantum fluctuations, which become relevant at these energies: they can shift between distinct magnetic states, like antiferromagnetic and paramagnetic phases. High–temperature superconductors, cuprates such as $YBa_2Cu_3O_7$ or Bose–Einstein condensates such as Rubidium–87 Rb^{87} belong to this class of materials.

A Kałuża–Klein toy model

Consider the Hamiltonian of a one dimensional quantum harmonic oscillator

$$\mathcal{H}^{\text{ho}} = \frac{p^2}{2m} + \frac{m\omega^2}{2} x^2 \,, \tag{19}$$

the wavefunctions are given by a combination of a Gaussian and Hermite polynomials (Landau & Lifshitz, 2013a; Whittaker & Watson)

$$\psi_n^{\mathsf{ho}}(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar}\right) \exp\left(-\frac{m\omega}{2\hbar}x^2\right) H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \ , \tag{20}$$

where

$$H_n(\xi) = (-1)^n \exp(\xi^2) \frac{d^n}{d\xi^n} \exp(-\xi^2) \ , \tag{21}$$

and the corresponding energy levels are given by the well–known formula

$$E_n^{\mathsf{ho}} = \hbar\omega \left(n + \frac{1}{2}\right) \ . \tag{22}$$

Proceeding in the same manner as in the section ”Thermodynamics”, one obtains

$$Z^{\mathsf{ho}}(a,\beta) = \sum_{n=0}^{+\infty} e^{-\beta a^2 \left(n+\frac{1}{2}\right)} = \frac{\exp\left(\frac{a^2\beta}{2}\right)}{\exp(a^2\beta) - 1} \ , \tag{23}$$

having defined $a^2 = \hbar\omega$. Its internal energy is given by

$$U^{\mathsf{ho}}(a,\beta) = \frac{a^2}{2} \frac{\exp(a^2\beta) + 1}{\exp(a^2\beta) - 1} \ , \tag{24}$$

and is shown in Figures (7) and (8) in two and three dimensions respectively.

In contrast to the case of (1), there are no critical values for the energy parameter a that could be found, that is, there are not any phase transitions for the harmonic oscillator.

Introduce now a two dimensional system with coordinates x and y, where the x coordinate lives on a circle with radius R, while $y \in \mathbb{R}$. The Hamiltonian of this toy model is given by

$$\mathcal{H}^{\mathsf{KK}} = \mathcal{H}_x + \mathcal{H}_y^{\mathsf{ho}} \ , \tag{25}$$

where the Hamiltonian acting on the compactified coordinate x is described by (1) and its wavefunction obeys the boundary condition (2), while the Hamiltonian of the harmonic oscillator described in (19) acts on the coordinate y.

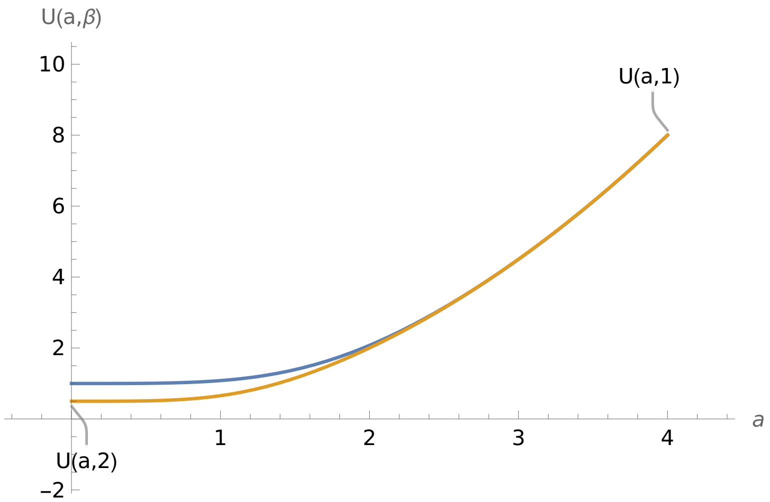

Figure 7 – Internal energy $U^{ho}(a, \beta)$ of harmonic oscillator as a function of energy parameter a for different values of β

The two components of the Hamiltonian do not interact with each other, and proceeding in the same fashion as before, one obtains

$$E^{\mathsf{KK}} = E_{n_x} + E^{\mathsf{ho}}_{n_y} = \frac{\hbar}{2mR^2} n_x^2 + \hbar\omega \left(n_y + \frac{1}{2} \right) \tag{26}$$

for the energy levels, and

$$\begin{aligned} Z^{\mathsf{KK}} &= \sum_{n_x, n_y} \langle n_x, n_y | e^{-\beta \mathcal{H}^{\mathsf{KK}}} | n_x, n_y \rangle = \\ &\sum_{n_x, n_y} \langle n_x, n_y | e^{-\beta \mathcal{H}_x} \otimes e^{-\beta \mathcal{H}^{\mathsf{ho}}_y} | n_x, n_y \rangle = \\ &\sum_{n_x} \langle n_x | e^{-\beta \mathcal{H}_x} | n_x \rangle \times \sum_{n_y} \langle n_y | e^{-\beta \mathcal{H}^{\mathsf{ho}}_y} | n_y \rangle \end{aligned} \tag{27}$$

for the partition function. This result is due to the fact that $\mathcal{H}_x$ acts on x and $\mathcal{H}^{\mathsf{ho}}_y$ on y, and they are independent. This implies that the eigenstates $|n_x, n_y\rangle$ of $\mathcal{H}^{\mathsf{KK}}$ can be written as tensor products $|n_x\rangle \otimes |n_y\rangle$, where $|n_x\rangle$ and $|n_y\rangle$ are eigenstates of $\mathcal{H}_x$ and $\mathcal{H}^{\mathsf{ho}}_y$, respectively. Using the explicit formulæ found in (12) and (23), with a slight change in notation to avoid

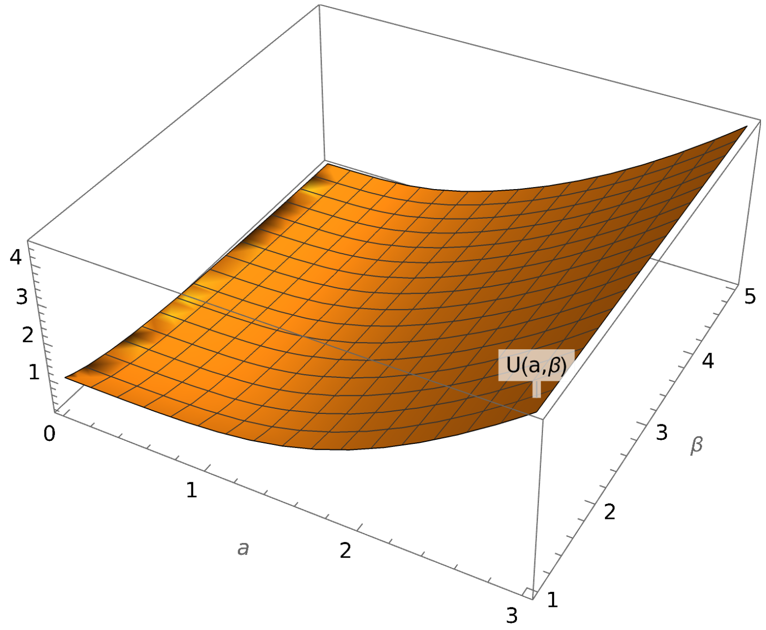

Figure 8 – Internal energy $U^{ho}(a,\beta)$ of harmonic oscillator as a function of energy parameter a and β

confusion between the two energies, one obtains the final result

$$Z^{\mathrm{KK}} = Z_x \times Z_y^{\mathrm{ho}} = \sum_{n_x=-\infty}^{+\infty} e^{-\beta E_{n_x}} \times \sum_{n_y=0}^{+\infty} e^{-\beta E^{\mathrm{ho}}_{n_y}} =$$

$$\sum_{n_x=-\infty}^{+\infty} e^{-\beta a_1^2 n_x^2} \times \sum_{n_y=0}^{+\infty} e^{-\beta a_2^2 \left(n_y+\frac{1}{2}\right)} = \vartheta_3(0, e^{a_1^2\beta}) \times \frac{\exp\left(\frac{a_2^2\beta}{2}\right)}{\exp(a_2^2\beta)-1} \,. \tag{28}$$

Using (13) and the explicit expressions of internal energies from (14) and (24) one arrives at the result

$$U^{\mathrm{KK}} = U + U^{\mathrm{ho}} = \frac{a_1^2 e^{-a_1^2\beta} \cdot \vartheta_3^{(0,1)}(0, e^{a_1^2\beta})}{\vartheta_3(0, e^{a_1^2\beta})} + \frac{a_2^2}{2}\frac{\exp(a_2^2\beta)+1}{\exp(a_2^2\beta)-1} \,, \tag{29}$$

because the two Hamiltonians are independent from each other.

Therefore, this Kałuża–Klein model exhibits the same phase transition as observed previously with the Hamiltonian (1), with the only difference being higher values of internal energy. The a_2 parameter, which corresponds

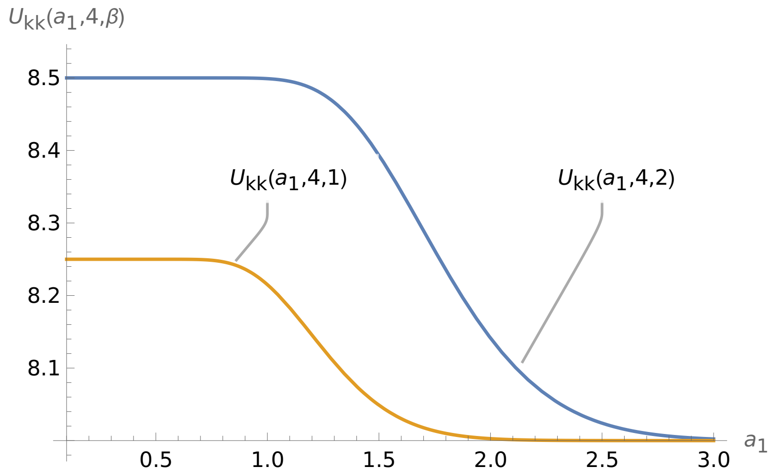

Figure 9 – Internal energy $U^{KK}(a_1, a_2, \beta)$ of toy KK model as a function of energy parameter a_1 and fixed a_2 for different values of β

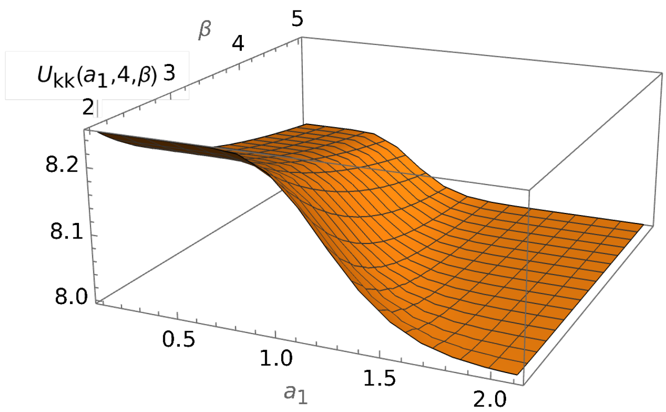

Figure 10 – Internal energy $U^{KK}(a_1, a_2, \beta)$ of toy KK model as a function of energy parameter a_1 and fixed a_2 for different values of β

to the harmonic oscillator component, is irrelevant for the existence of the phase transition. Figures (9) and (10) show the behaviour of the internal energy U^{KK} (29) as a function of the inverse radius circle a_1 for different values of the inverse temperature β, at a fixed harmonic oscillator frequency a_2, in two and three dimensions respectively. The critical value of the inverse radius circle is clearly the same as in (1), as seen in Figures (1) and (2). Therefore, the fit for its critical value found in formula (17) and shown in Figure (3) is the same. As expected, when the radius R of the circle is infinite, that is $a_1 = 0$, so that $x \in \mathbb{R}$, the internal energy U^{KK} does not present any kind of steep change with the variation of other parameters a_2 and β, therefore, there is not a phase transition anymore when the Kałuża–Klein model transforms to a model in the usual two dimensional space.

Conclusion

Quantum mechanics on a circle exhibits some surprising behaviour. Contrary to the case of the configuration space of the real line, its energy levels are discrete. The partition function can be expressed in closed form as a Jacobi theta function. It presents a phase transition, controlled by the geometry of the configuration space, specifically the radius of the circle. When considered in a simple two dimensional Kałuża–Klein model, it exhibits again a phase transition, that disappears in the limit of a flat space, for an infinite radius of the circle.

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Neka razmatranja o termodinamici kvantne mehanike na krug i Kaluza-Klajn modeli

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OBLAST: matematika
KATEGORIJA (TIP) ČLANKA: originalni naučni rad

Sažetak:

Uvod/cilj: Kvantna mehanika na krugu je istražena i primenjena na Kaluza-Klajn model sa kompaktifikovanom dimenzijom.

Metode: Korišćene su metode kvantne mehanike i statističke mehanike. Takođe, razmatran je Kaluza-Klajn model igračke kompaktne dimenzije.

Rezultati: Rezultujuća particiona funkcija se može proceniti u zatvorenom obliku, dajući posebnu funkciju. Predstavlja fazni prelaz u zavisnosti od geometrije. Kada se koristi u modelu Kaluza-Klajn, pokazuje fazni prelaz regulisan poluprečnikom kruga, a prelaz nestaje kada je poluprečnik beskonačan, odnosno u ravnom prostoru.

Zaključak: Kvantna mehanika na krugu pokazuje mnoge neobične karakteristike. Nivoi energije su odvojeni usled geometrije, nasuprot konfiguracionom prostoru prave linije. Predstavlja fazni prelaz u zavisnosti od radijusa kruga, takođe kada je isti ugrađen u Kaluza-Klajn model. Ova karakteristika nestaje kada poluprečnik postane beskonačan, u ravnom prostoru.

Ključne reči: kvantna mehanika, statistička mehanika, fazni prelaz, Jakobijeva teta funkcija, Kaluza-Klajn model.

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