Quantum Particle Constrained to a Curved Surface

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We certify that we have read this thesis and that in our opinion it is fully adequate in scope and quality as a thesis for the degree of Master of Science in Physics.

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ABSTRACT

This thesis begins with an introduction of discussing the motion of P non interacting particles constrained in a curved surface of N dimensions. First the particles are described in the flat space R and Cartesian coordinates, an external potential, V_ρ is considered to maintain the system constrained in a curved subspace D_N. Assuming normal forces to keep particles on the curved surface, the part of Schrödinger equation which is independent of the potential V_ρ and contains the curve space variables will be separated to internal and external parts, therefore a new Schrödinger equation is raised that depends on curved surface geometrical properties.

In continuation, to explain this problem clearly, we study the motion of one quantum particle that is bounded at an arbitrary point p on a curved surface S in three dimensions. In order to get the true result, a potential V_λ is assumed for the constrained particle so the wave function will be uniformly compressed. Since classical mechanics principal guides us to avoid tangential forces, only normal constraint forces are acceptable to keep particle on the surface. Choosing point Q as an immediate neighborhood for point p and considering differential geometry relations for these points, Schrödinger equation can be obtained. Hence it will be demonstrated that, the internal potential for bounded particle is a function of surface curvatures which cannot be found from metric tensors or its derivatives and so on classical Lagrangian. Therefore there is a strike contrast with classical mechanics where Lagrangian and Newtonian approach give same results.

In addition, inconsequence, Schrödinger equation for a particle constrained on a Spherical shell, Cylindrical shell and a Toroid is determined. Finally we obtained Schrödinger equation for a particle constrained on a pseudosphere surface.

Keywords: Schrödinger equation, constrain, space curve, quantum particle, differential geometry, curvature

ÖZ

Bu tez, N boyutlu bir eğri uzayında sınırlandırılan P etkileşimsiz parçacıkların hareketinin tartışılmasıyla başlamaktadır. İlk olarak parçacıklar düz uzay R ve Kartezyen koordinatlarında tanımlanır, bir dış potansiyel olan V_ρ, eğri bir alt uzayda D_N sınırlandırılmış sistemi korumak için kabul edilir. Parçacıkları eğri uzayında tutmak için normal kuvvetler varsayarsak, Schrödinger denkleminin V_ρ potansiyelinden bağımsız olan ve eğri uzayı değişkenlerini içeren kısmı iç ve dış parçalara ayrılacaktır, bu nedenle eğri uzayına bağlı yeni bir Schrödinger denklemi ortaya çıkar. geometrik özellikler.

Devamında, bu sorunu açık bir şekilde açıklamak için, bir eğri yüzeyi S üzerinde keyfi bir p noktasında sınırlanan bir kuantum parçacığının hareketini üç boyutlu olarak inceliyoruz. Doğru sonucu elde etmek için, kısıtlı parçacık için bir potansiyel V_λ varsayılır, böylece dalga fonksiyonu düzgün bir şekilde sıkıştırılır. Klasik mekanik ilkesi teğetsel kuvvetlerden kaçınmamıza rehberlik ettiğinden, parçacığı yüzeyde tutmak için yalnızca normal kısıtlama kuvvetleri kabul edilebilir. Q noktası p noktası için yakın komşuluk olarak seçilerek ve bu noktalar için diferansiyel geometri ilişkileri dikkate alınarak Schrödinger denklemi elde edilebilir. Dolayısıyla, sınırlı parçacık için iç potansiyelin, metrik tensörlerden veya türevlerinden ve klasik Lagrange'dan bulunamayan yüzey eğriliklerinin bir fonksiyonu olduğu gösterilecektir. Bu nedenle, Lagrange ve Newton yaklaşımının aynı sonuçları verdiği klasik mekanik ile bir vuruş karşıtlığı vardır.

Ayrıca Küresel kabuk, Silindirik kabuk ve Toroid üzerinde kısıtlanmış bir parçacık için tutarsızlık, Schrödinger denklemi belirlenir. Sonunda, bir psödoküre yüzeyi üzerinde kısıtlanmış bir parçacık için Schrödinger denklemini elde ettik.

Anahtar Kelimeler: Schrödinger denklemi, kısıtlama, uzay eğrisi, kuantum parçacığı, diferansiyel geometri, eğrilik

DEDICATION

- My dear grandmother and precious parents, who hold my back at every second of my life. I am indebted them more than they know.
- My lovely husband, Hossein, who always encourages me in my career.
- My sweetheart son Adrian and my beloved niece Tania who are all I have.
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Chapter 1

INTRODUCTION

One of the most famous problems in classical mechanic is particle's motion analysis, which can be solved utilizing two different methods, Lagrangian equation and Newtonian approach. The first one deals with generalizing coordinates in which constraint is defined independent of the curve properties. It means that Lagrangian only depends on space metric properties. The second way is considering a particle free fall based on Newtonian equations where an external force is applied to bind the particles to the space curve. These two different ways give same result.

However, in quantum mechanics the problem solving is completely different [1]. When a quantum particle is constrained on a curve or surface, Lagrangian equation cannot lead us to an appropriate Schrödinger equation as this equation depends only on the curve metric properties which are not affected by the path geometry. On the other hand, Newtonian approach leads us to a Schrödinger equation which is under an unfamiliar condition. To constrain particles on a curved surface, we assume external forces which are orthogonal based on uncertainty relations. Therefore wave function sees a sharp potential that is infinite for constrained particles and compresses wave packet in transverse direction.

In this thesis we have to use the Newtonian approach which leads us to an appropriate Schrödinger equation that is dependent of curved surface geometry [1-8].

At first we consider the Cartesian space R as a classic system with p constrains and N coordinates $(q^1 .....q^N)$ which are generalized, so we assumed a system of independent particles with $p + N$ dimensions, in which $x^\alpha = x^\alpha (q^1, q^2, ..., q^N)$ are coordinates where $\alpha = 1,2,...,N + p$. Then D_N is introduced as a curved subspace of R_{N+p} that we assumed that any configuration of the constraint system as a subtended to a point in D_N .Since q's are internal coordinates the external coordinates are introduced as $u^1 ,...,u^p$ then a set of coordinates $(q^1 ,q^2 ,..., q^N ,u^1, ...,u^p)$ is imputed to all points of a neighborhood of $S \subset R_{N+p}$ of D_N (where $u^1 = u^2 = ... = u^p$ then it would be a point of D_N) [1]. It's time that we enter the potential $V_\rho (u^1,...,u^p)$, where ρ is compressing parameter to squeeze the system from R_{N+p} to the S. In a small neighborhood, at a limit of u's variation around $\alpha = 0$, we can write

$$\lim_{\rho\to\infty} V_\rho(u^1, u^2, ..., u^p) = \begin{cases} 0 & (u^1)^2 + \cdots + (u^p)^2 = 0 \\ \infty & (u^1)^2 + \cdots + (u^p)^2 \neq 0. \end{cases} \tag{1.1}$$

It should be noted that we cannot choose potential and external coordinates quite arbitrary, so based on classical mechanics the constrained motion can be found only when for all points of D_N constrained forces are normal. As the position of quantum particle is not clear, it is reasonable to choose normal constrained forces in all points of our system in R_{N+p}. So the gradient of potential should be selected $\nabla[V_\rho(u^1,..., u^p)]$, that intersects the subset D_N for all the points of neighborhood S orthogonally, it would be confirmed where internal and external coordinates are orthogonal, in this case for an optional position vector $\boldsymbol{R}(q^1,...,q^N, u^1,..., u^p)$ in subset S is given as

$$\frac{\partial \overrightarrow{\boldsymbol{R}}}{\partial u^\alpha} \cdot \frac{\partial \overrightarrow{\boldsymbol{R}}}{\partial q^j} = 0, \tag{1.2}$$

where $\alpha = 1,2,...,p$ and $j = 1,2,...,N$ and bold letters, in this study, are used for vectors.

Based on the expressed situation, we will find an unfamiliar condition for constrained particles, where subspace potential $U\ (q^1,\ldots,q^N)$ will be determined as a function of mean and total curvatures that obviously couldn't be found from subspace's metric properties. Finally the Schrödinger equation which depends on curvatures will be obtained. Since Lagrangian could not be used, this result is in contrary with the result of classical mechanics where Lagrangian equation and Newtonian approach give same result [2].

1.1 Geometrical analysis in *N* dimensions

Let us continue by considering $\boldsymbol{r} = \boldsymbol{r}\ (q^1,\ldots, q^N)$, with internal coordinates *(q's)*, as parameterization of D_N, where q's and external coordinates *(u's)* have to be chosen orthogonal for making a coordinate system in R_{N+p}. Therefore for all points of neighborhood S:

$$\boldsymbol{R}(q^1,\ldots,q^N,u^1,\ldots,u^p) =$$

$$\boldsymbol{r}(q^1,\ldots,q^N) + \sum_{\beta=1}^{p} f^\beta(q^1,\ldots,q^N,u^1,\ldots,u^p)\widehat{\boldsymbol{n}_\beta}\,(q^1,\ldots,q^N), \tag{1.3}$$

with

$$det\left[\frac{\partial f^\beta}{\partial u^\alpha}\right] \neq 0. \tag{1.4}$$

Then, $u^1,\ldots,u^p$ are spanned by normal system $\widehat{\boldsymbol{n}_\beta}$ $((\widehat{\boldsymbol{n}_\beta}.\widehat{\boldsymbol{n}_\alpha}) = \delta_{\alpha\beta})$ for all the points of subspace D_N , so for $\boldsymbol{R}$

$$\frac{\partial \boldsymbol{R}}{\partial u^\alpha} = \sum_{\gamma=1}^{p} \frac{\partial f^\gamma}{\partial u^\alpha}\widehat{\boldsymbol{n}_\gamma}, \tag{1.5}$$

and

$$\frac{\partial \boldsymbol{R}}{\partial q^j} = \frac{\partial \boldsymbol{r}}{\partial q^j} + \sum_{\beta=1}^{p}\left[\frac{\partial f^\beta}{\partial q^j}\widehat{\boldsymbol{n}_\beta} + f^\beta\frac{\partial \widehat{\boldsymbol{n}_\beta}}{\partial q^j}\right]. \tag{1.6}$$

Since constraint force F, were introduced from classical mechanics as ∇V_ρ, imagine a moment that u^{α}'s and q^{j}'s are orthogonal, F can be written in terms of variables Q^{j} where $Q^j = q^j$, $j=1,...,N$, $Q^{N+\alpha} = u^{\alpha}$ and $\alpha = 1,...,p$, we can write

$$F = \boldsymbol{\nabla V}_\rho = \sum_{i,l=1}^{N+p} G^{il} \frac{\partial \boldsymbol{V}_\rho}{\partial Q^i} \frac{\partial \boldsymbol{R}}{\partial Q^l} = \sum_{\alpha,\beta=1}^{p} G^{N+\alpha,N+\beta} \frac{\partial \boldsymbol{V}_\rho}{\partial u^\alpha} \frac{\partial \boldsymbol{R}}{\partial u^\beta}, \tag{1.7}$$

where

$$G_{il} = \frac{\partial \boldsymbol{R}}{\partial Q^i} \cdot \frac{\partial \boldsymbol{R}}{\partial Q^l} \qquad , \qquad G^{il} = (G^{-1})_{il}. \tag{1.8}$$

Now the orthogonally condition for internal and external varieties can be rewritten as

$$\sum_{\gamma=1}^{p} \frac{\partial f^\gamma}{\partial u^\alpha} \left[\frac{\partial f^\gamma}{\partial q^j} + \sum_{\beta=1}^{p} \mu_{j;\gamma\beta} f^\beta \right] = 0. \tag{1.9}$$

We can assume inside the parentheses equal to zero as there is no α (it doesn't contain the external variables $u^1,...,u^p$) where

$$\mu_{j;\gamma\beta} = \widehat{\boldsymbol{n}_\gamma} \cdot \frac{\partial \widehat{\boldsymbol{n}_\beta}}{\partial q^j} = -\mu_{j;\beta\gamma}, \tag{1.10}$$

that is antisymmetric in indexes γ and β. Using partial differential theory [9], the integrability condition for considering inside the parenthesis zero can be written as a symmetric tensor

$$\Omega_{\sigma,ij} = -\frac{\partial \boldsymbol{r}}{\partial q^i} \cdot \frac{\partial \widehat{\boldsymbol{n}}_\sigma}{\partial q^j} = \Omega_{\sigma;ji}. \tag{1.11}$$

From differential geometry result, we know the components of $\mu_{j;\gamma\beta}$ must satisfy the condition [1],

$$A_{\gamma\beta;jk} = g^{lm}\left(\Omega_{\gamma;lk}\Omega_{\beta;mj} - \Omega_{\gamma;lj}\Omega_{\beta;mk}\right) = 0. \tag{1.12}$$

This condition enables us to get a particular solution $f^{\gamma}(\ q^1, \ldots, q^N, u^1, \ldots, u^p\ )$ that $\gamma = 1,2, \ldots, p$ therefore by taking derivative of f^{γ} with respect to each of u^{α}'s, we have p independent solutions. Reminding $det\left[\frac{\partial f^{\beta}}{\partial u^{\alpha}}\right] \neq 0$ and introducing, $\frac{\partial f^{\gamma}}{\partial u^{\alpha}} = h_{\alpha}^{\gamma}$,

$$\frac{\partial}{\partial q^j}\left[\sum_{\gamma=1}^{p} h_{\alpha}^{\gamma} h_{\alpha'}^{\gamma}\right] = -\sum_{\gamma,\beta=1}^{p} \mu_{j;\gamma\beta}\left(h_{\alpha}^{\gamma} h_{\alpha'}^{\beta} + h_{\alpha'}^{\gamma} h_{\alpha}^{\beta}\right) = 0. \tag{1.13}$$

Since the values of f^{γ} can be arbitrarily selected at a fixed point $(q_0^1, \ldots, q_0^N)$ of the subspace D_N , we can write

$$f^{\gamma}(q_0^1, \ldots, q_0^N) = u^{\gamma} \quad , \quad \gamma = 1,2, \ldots, p. \tag{1.14}$$

Here we selected a Cartesian coordinate system at points $(q_0^1, \ldots, q_0^N)$ for normal subspace. By considering Jacobian matrix h_{α}^{γ} we start with matrix $h_{\alpha}^{\gamma} = \delta_{\alpha}^{\gamma}$ at $(q_0^1, \ldots, q_0^N)$ that will be always an orthogonal matrix. Change of normal $\widehat{\boldsymbol{n}_{\nu}}'$ is introducing as

$$\widehat{\boldsymbol{n}_{\nu}}' = \sum_{\sigma=1}^{p} h_{\nu}^{\sigma}\, \widehat{\boldsymbol{n}_{\sigma}}\,, \tag{1.15}$$

where h_{ν}^{σ} is orthogonal character, so new normals in every normal subspace form an orthogonal basis. Choosing new normals leads us to write $\mu_{j;\nu\rho}$ as

$$\mu'_{j;\nu\rho} = \widehat{\boldsymbol{n}'}_{\nu} \frac{\partial \widehat{\boldsymbol{n}'}_{\rho}}{\partial q^j} = \sum_{\sigma=1}^{p} h_{\nu}^{\sigma}\left[\frac{\partial h_{\rho}^{\sigma}}{\partial q^j} + \sum_{z=1}^{p} \mu_{j;\sigma z}\, h_{\rho}^{z}\right] = 0. \tag{1.16}$$

Based on orthogonally condition, derivative of every $\widehat{\boldsymbol{n}_{\nu}}'$ for all points of D_N have to be contained in the tangent subspace. So for all points in D_N there are same f^{β}'s as

$$f^{\beta} = f^{\beta}(u^1, \ldots, u^p) \quad , \quad \det\left[\frac{\partial f^{\beta}}{\partial u^{\alpha}}\right] \neq 0. \tag{1.17}$$

In this case, we can write the position vector and its derivatives as

$$\boldsymbol{R}(q^1, \ldots, q^N, u^1, \ldots, u^p)$$
$$= \boldsymbol{r}(q^1, \ldots, q^N) + \sum_{\beta=1}^{p} f^\beta(u^1, \ldots, u^p)\widehat{n'_\beta}(q^1, \ldots, q^N), \tag{1.18}$$

and

$$\frac{\partial \boldsymbol{R}}{\partial q^j} = \frac{\partial \boldsymbol{r}}{\partial q^j} + \sum_{\beta=1}^{p} f^\beta \frac{\partial \widehat{n'_\beta}}{\partial q^j}. \tag{1.19}$$

Also we can see $A_{\gamma\beta;jk} = 0$ is always true when D_N is a curve or hypersurface of R_{N+p}.

1.2 Schrödinger equation for the constrained system

Now we should write the Schrödinger equation regard to the constrain, so R_{N+p} is

$$\boldsymbol{R}(q^1, \ldots, q^N, u^1, \ldots u^p) = \boldsymbol{r}(q^1, \ldots, q^N) + \sum_{\beta=1}^{p} u^\beta \widehat{n'_\beta}(q^1, \ldots, q^N). \tag{1.20}$$

Since the Cartesian coordinate is easier to interpret, it is chosen for normal subspaces of D_N, so

$$\frac{\partial \boldsymbol{R}}{\partial u^\alpha} = \widehat{\boldsymbol{n}}'_\alpha \quad , \quad \alpha = 1,2, \ldots, p. \tag{1.21}$$

Then,

$$\frac{\partial \boldsymbol{R}}{\partial q^j} = \frac{\partial \boldsymbol{r}}{\partial q^j} - \sum_{\beta=1}^{p} u^\beta \Omega_{\beta;ij} g^{ik} \frac{\partial \boldsymbol{r}}{\partial q^k} \quad , \quad j = 1,2, \ldots, N, \tag{1.22}$$

where

$$g^{ik} = (g^{-1})_{ik}, \quad g_{lm} = \frac{\partial \boldsymbol{r}}{\partial q^l} \cdot \frac{\partial \boldsymbol{r}}{\partial q^m}. \tag{1.23}$$

Equations (1.21) and (1.22) for metric tensor G_{lm} we have

$$G_{jk} = g_{jk} - 2\sum_{\beta=1}^{p} u^{\beta}\Omega_{\beta;jk} + \sum_{\beta,\gamma=1}^{p} u^{\beta}u^{\gamma}\Omega_{\beta;ij}\Omega_{\gamma;mk}g^{im}, \tag{1.24}$$

where

$$G_{j,N+\alpha} = G_{N+\alpha,j} = 0, \quad G_{N+\alpha,N+\beta=}\delta_{\alpha\beta} , \tag{1.25}$$

where $j, k = 1,2, \dots, N;\ \alpha, \beta = 1,2, \dots p$. Now it's the time to write Schrödinger equation in R_{N+p}

$$-\frac{\hbar^2}{2\mathrm{m}}\frac{1}{\sqrt{G}}\frac{\partial}{\partial Q^i}\left\{\sqrt{G}G^{ij}\frac{\partial\psi}{\partial Q^j}\right\} + V_{\rho}(u^1, \dots, u^p)\psi = i\hbar\frac{\partial\psi}{\partial t}. \tag{1.26}$$

As it is known m is the particle mass and $G^{ij} = (G^{-1})_{ij}, G = det(G_{ij})$. The only quantities that can affect constraining potential are external variables, thus to obtain the values of V_ρ for all points of the neighborhood S they should be known in a normal subspace selected at one point in D_N ,which is chosen arbitrary [1]. It means since the values of V_ρ can be selected as we like and the only condition is normality in D_N, other subspaces would be explained by change in $\widehat{\boldsymbol{n}'}_{\beta}(q^1, \dots, q^N)$.

In order to solve Schrödinger equation, we divide equation (26) into two equations regard to orthogonal coordinate. Where for $\alpha \neq \beta$, $G^{N+\alpha,N+\beta} = 0$, we have

$$-\frac{\hbar^2}{2\mathrm{m}}\sum_{\mathrm{i,j=1}}^{\mathrm{N}}\frac{1}{\sqrt{G}}\frac{\partial}{\partial q^i}\left\{\sqrt{G}G^{ij}\frac{\partial\psi}{\partial q^j}\right\} - \frac{\hbar^2}{2\mathrm{m}}\sum_{\alpha=1}^{\mathrm{p}}\left\{\frac{\partial^2\psi}{\partial(u^\alpha)^2} + \frac{\partial}{\partial u^\alpha}(ln\sqrt{G})\psi\right\} + V_\rho\psi$$
$$= i\hbar\frac{\partial\psi}{\partial t}, \tag{1.27}$$

where one of them includes derivatives of internal variables and another one consists external ones.

To solve Schrödinger equation, we are interested in write this equation to find the possibility of obtain the internal coordinates in a specific volume element of D_N that shouldn't be dependent of external variables values. Also this possibility can be written as $|\chi_i|^2\sqrt{g}dq^1,\dots,dq^N$ where $\chi_i=\chi_i(q^j,t)$, (i stands for internal) is defined as internal wave function, thus

$$dP=|\psi|^2dD=|\psi|^2\sqrt{G}dq^1,\dots,dq^Ndu^1,\dots,du^p, \tag{1.28}$$

and

$$\left|\psi\left[\frac{G}{g}\right]^{\frac{1}{4}}\right|^2\sqrt{g}\,dq^1,\dots,dq^Ndu^1,\dots,du^p=|\chi|^2\sqrt{g}dq^1,\dots,dq^Ndu^1,\dots,du^p, \tag{1.29}$$

where dP is the probability for volume element dD in R_{N+P}. $\chi_e(u^\alpha,t)$, is introduced that e means external. Therefore Schrödinger equation can be rewritten based on new wave function, $X=X_i(q^j,t)X_e(u^\alpha,t)$, as

$$-\frac{\hbar^2}{2m}\sum_{i,j=1}^{N}\frac{1}{\sqrt{G}}\frac{\partial}{\partial q^i}\left[\sqrt{G}G^{ij}\frac{\partial}{\partial q^i}\left[\frac{\chi}{\sqrt{h}}\right]\right]$$

$$-\frac{\hbar^2}{2m}\frac{1}{\sqrt{h}}\sum_{\beta=1}^{p}\left[\frac{\partial^2\chi}{\partial(u^\beta)^2}+\frac{1}{4h^2}\left[\left[\frac{\partial h}{\partial u^\beta}\right]^2-2h\frac{\partial^2 h}{\partial(u^\beta)^2}\right]\chi\right]$$

$$+\frac{1}{\sqrt{h}}V_\rho(u^1,\dots,u^p)\chi=i\hbar\frac{\partial\chi/\partial t}{\sqrt{h}}, \tag{1.30}$$

that, $h=(\frac{G}{g})^{\frac{1}{2}}$. When it's studied at limit ρ goes to infinity, the potential barrier is normal to D_N in all directions, which is completely far from zero except at small values of external coordinates around $u^\alpha=0$, $\alpha=1,2,\dots,p$ .In last equation, we cancel all the coefficients by taking $u^\alpha\rightarrow 0$, only we keep it in the last term .It is obvious from (1.24) , (1.25) , (1.30) and $h=1$, in all points of the subspace that

$$-\frac{\hbar^2}{2m}\sum_{i,j=1}^{N}\frac{1}{\sqrt{g}}\frac{\partial}{\partial q^i}\left[\sqrt{g}g^{ij}\frac{\partial\chi}{\partial q^j}\right]-\frac{\hbar^2}{8m}\sum_{\beta=1}^{p}\left[\left[\frac{\partial h}{\partial u^\beta}\right]^2-2\frac{\partial^2 h}{\partial(u^\beta)^2}\right]_{u^\alpha=0}\chi$$

$$-\frac{\hbar^2}{2m}\sum_{\beta=1}^{p}\frac{\partial^2\chi}{\partial(u^\beta)^2}+V_\rho(u^1,\dots,u^p)\chi=i\hbar\frac{\partial\chi}{\partial t}. \quad (1.31)$$

This equation can be broken into two parts regard to internal and external terms, as

$$-\frac{\hbar^2}{2m}\sum_{\beta=1}^{p}\frac{\partial^2\chi_e}{\partial(u^\beta)^2}+V_\rho(u^1,\dots,u^p)\chi_e=i\hbar\frac{\partial\chi_e}{\partial t}, \quad (1.32)$$

and

$$-\frac{\hbar^2}{2m}\sum_{j,k=1}^{N}\frac{\partial}{\partial q^j}\left[\sqrt{g}g^{jk}\frac{\partial\chi_i}{\partial q^k}\right]$$

$$-\frac{\hbar^2}{8m}\sum_{\beta=1}^{p}\left[\left[\frac{\partial h}{\partial u^\beta}\right]^2-2\frac{\partial^2 h}{\partial(u^\beta)^2}\right]_{u^\alpha=0}\chi_i=i\hbar\frac{\partial\chi_i}{\partial t}\ . \quad (1.33)$$

The external term that is a Schrödinger equation in p dimensional Cartesian system in the presence of potential V_ρ, can be neglected in our study [1], [2] but the internal term is the important part that consists internal potential which depends on D_N geometry and appears as

$$U_i(q^1,\dots,q^N)=-\frac{\hbar^2}{8m}\sum_{\beta=1}^{p}\left[\left[\frac{\partial h}{\partial u^\beta}\right]^2-2\frac{\partial^2 h}{\partial(u^\beta)^2}\right]_{u^\alpha=0}. \quad (1.34)$$

Since the first and second derivatives of h are appeared, we need a series expansion of h until second order in u^α*'s.* Thus using (1.24), (1.25) we can write

$$h=\left[\frac{G}{g}\right]^{1/2}=1-\sum_{\beta=1}^{p}\Omega_{\beta;j}^{j}\,u^\beta+\frac{1}{2}\sum_{\beta,\gamma=1}^{p}\left(\Omega_{\beta;i}^{i}\Omega_{\gamma;k}^{k}-\Omega_{\beta;i}^{k}\Omega_{\gamma;k}^{i}\right)u^\beta u^\gamma+\dots, \quad (1.35)$$

where we wrote a mixed tensor of $g^{jl}\Omega_{\beta;il}$ as $\Omega_{\beta;i}^{j}$. From the expansion of h

$$\left[\frac{\partial h}{\partial u^{\beta}}\right]_{u^{\alpha}=0}=-\Omega^{j}_{\beta;j} \qquad , \qquad \left[\frac{\partial^2 h}{\partial (u^{\beta})^2}\right]_{u^{\alpha}=0}=\Omega^{i}_{\beta;i}\Omega^{k}_{\beta;k}-\Omega^{k}_{\beta;i}\Omega^{i}_{\beta;k}, \tag{1.36}$$

add these two in (1.34)

$$U_i(q^1,\dots,q^N)=-\frac{\hbar^2}{8m}\left(\sum_{\sigma=1}^{p}\left(\Omega^{j}_{\sigma;j}\right)^2+2\sum_{\sigma=1}^{p}\Omega^{l}_{\sigma;k}\Omega^{k}_{\sigma;l}-\Omega^{l}_{\sigma;l}\Omega^{k}_{\sigma;k}\right). \tag{1.37}$$

Introducing R as total curvature and M as mean curvature of the subspace D_N imbedded in R_{N+P},

$$M=\left[\sum_{\sigma=1}^{p}(\Omega^{j}_{\sigma;j})^2\right]^{1/2} \qquad , \qquad R=\sum_{\sigma=1}^{p}\left(\Omega^{l}_{\sigma;k}\Omega^{k}_{\sigma;l}-\Omega^{l}_{\sigma;l}\Omega^{k}_{\sigma;k}\right), \tag{1.38}$$

where total curvature, R, is only dependent of intrinsic properties of subspace D_N , that is not same for mean curvature [1]. Finally the potential is given by

$$U_i(q^1,\dots,q^N)=-\frac{\hbar^2}{8m}(M^2+2R) \tag{1.39}$$

Where Gaussian curvature, $K_G=2R$. This result is in a complete contrast with the Lagrangian method used in classical scales.

Chapter 2

CURVE DIFFERENTIAL GEOMETRY AND QUANTUM MECHANICS OF A CONSTRAINED PARTICLE IN 3 DIMENSIONAL CURVED SURFACE

In previous chapters Schrödinger equation was determined for *P* constrained particles in *N* dimensions. Now for better understanding of the case, we investigate the motion of one particle bounded on a surface in three dimensions. Before direct heading to geometry analysis, Gauss-Weingarten equation (GWE) is explained [9].

2.1 Gauss-Weingarten equation

Regarding Figure.2.1 for an arbitrary point *P* on surface *S*, $\boldsymbol{X}_u = \frac{\partial \boldsymbol{X}}{\partial u}, \boldsymbol{X}_v = \frac{\partial \boldsymbol{X}}{\partial v}$ and $\boldsymbol{n}$ are the basis vectors since they are linearly independent (where, bold letters are used for vectors). So $\boldsymbol{X}_u = \boldsymbol{e}_u, \boldsymbol{X}_v = \boldsymbol{e}_v$ which, are not unit vectors however $\boldsymbol{n} = \frac{\boldsymbol{e}_u \times \boldsymbol{e}_v}{|\boldsymbol{e}_u \times \boldsymbol{e}_v|}$ is unit normal.

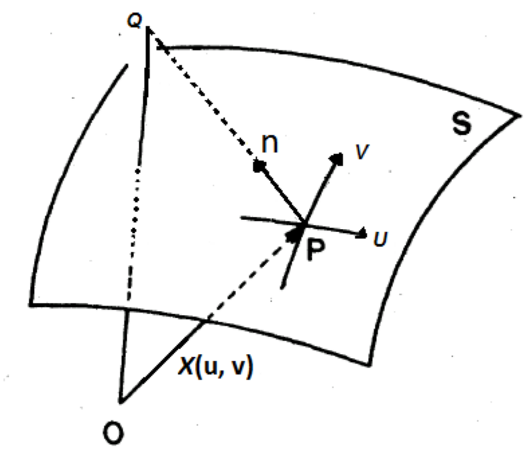

Figure 2.1: Illustration of the surface parametrization for arbitrary point *p*.

GWE connects the partial derivatives of $\boldsymbol{e}_u$, $\boldsymbol{e}_v$ and $\boldsymbol{n}$ in terms of their linear combination. Let us define the surface metric tensor to be

$$g_{ij} = \begin{pmatrix} E & F \\ F & G \end{pmatrix}, \tag{2.1}$$

such that $E = \boldsymbol{e}_u.\boldsymbol{e}_u$, $G = \boldsymbol{e}_v.\boldsymbol{e}_v$ and $F = \boldsymbol{e}_u.\boldsymbol{e}_v$. Since $\boldsymbol{n}.\boldsymbol{n} = 1$ then

$$\frac{\partial}{\partial u}(\boldsymbol{n}.\boldsymbol{n}) = 2\boldsymbol{n}.\frac{\partial \boldsymbol{n}}{\partial u} = 2\boldsymbol{n}.\boldsymbol{n}_u = 0, \tag{2.2}$$

and

$$\frac{\partial}{\partial v}(\boldsymbol{n}.\boldsymbol{n}) = 2\boldsymbol{n}.\frac{\partial \boldsymbol{n}}{\partial v} = 2\boldsymbol{n}.\boldsymbol{n}_v = 0. \tag{2.3}$$

Therefore $\boldsymbol{n} \perp \boldsymbol{n}_u$ also $\boldsymbol{n} \perp \boldsymbol{n}_v$ which, mean $\boldsymbol{n}_u$ and $\boldsymbol{n}_v$ lie on the surface, where they can be written as a linear combination of $\boldsymbol{e}_u$ and $\boldsymbol{e}_v$ as

$$\boldsymbol{n}_u = a\boldsymbol{e}_u + b\boldsymbol{e}_v, \tag{2.4}$$

$$\boldsymbol{n}_v = c\boldsymbol{e}_u + d\boldsymbol{e}_v. \tag{2.5}$$

Also we know $\boldsymbol{e}_u.\boldsymbol{n} = \boldsymbol{e}_v.\boldsymbol{n} = 0$, then

$$\partial_u(\boldsymbol{e}_u.\boldsymbol{n}) = 0 \implies \boldsymbol{e}_{uu}.\boldsymbol{n} + \boldsymbol{e}_u.\boldsymbol{n}_u = 0, \tag{2.6}$$

$$\partial_v(\boldsymbol{e}_u.\boldsymbol{n}) = 0 \implies \boldsymbol{e}_{uv}.\boldsymbol{n} + \boldsymbol{e}_u.\boldsymbol{n}_v = 0, \tag{2.7}$$

$$\partial_u(\boldsymbol{e}_v.\boldsymbol{n}) = 0 \implies \boldsymbol{e}_{vu}.\boldsymbol{n} + \boldsymbol{e}_v.\boldsymbol{n}_u = 0, \tag{2.8}$$

$$\partial_v(\boldsymbol{e}_v.\boldsymbol{n}) = 0 \implies \boldsymbol{e}_{vv}.\boldsymbol{n} + \boldsymbol{e}_v.\boldsymbol{n}_v = 0. \tag{2.9}$$

From (2.4) and (2.5)

$$\boldsymbol{n}.\boldsymbol{n}_u = 0 \Rightarrow a\boldsymbol{n}.\boldsymbol{e}_u + b\boldsymbol{n}.\boldsymbol{e}_v = 0, \tag{2.10}$$

$$\boldsymbol{n}.\boldsymbol{n}_v = 0 \Rightarrow c\boldsymbol{n}.\boldsymbol{e}_u + d\boldsymbol{n}.\boldsymbol{e}_v = 0, \tag{2.11}$$

from (2.6)

$$\boldsymbol{e}_{uu}.\boldsymbol{n} = -\boldsymbol{e}_u.\boldsymbol{n}_u = h_{uu}, \tag{2.12}$$

and from (2.7) and (2.8)

$$\boldsymbol{e}_{uv}.\boldsymbol{n} = -\boldsymbol{e}_u.\boldsymbol{n}_v = \boldsymbol{e}_{vu}.\boldsymbol{n} = -\boldsymbol{e}_v.\boldsymbol{n}_u = h_{uv} = h_{vu}. \tag{2.13}$$

Also from (2.9)

$$\boldsymbol{e}_{vv}.\boldsymbol{n} = -\boldsymbol{e}_v.\boldsymbol{n}_v = h_{vv}, \tag{2.14}$$

in which

$$h_{ab} = \begin{pmatrix} h_{uu} & h_{uv} \\ h_{vu} & h_{vv} \end{pmatrix} = \begin{pmatrix} e & f \\ f & g \end{pmatrix}. \tag{2.15}$$

Where, h is called the second fundamental form of the surface S, which plays an important role in geometry analysis in the next section.

Next, from (2.1)

$$\frac{\partial E}{\partial u} = 2\boldsymbol{e}_{uu}.\boldsymbol{e}_u \Longrightarrow \boldsymbol{e}_{uu}.\boldsymbol{e}_u = \frac{1}{2}E_u, \tag{2.16}$$

$$\frac{\partial E}{\partial v} = 2\boldsymbol{e}_{uv}.\boldsymbol{e}_u \Longrightarrow \boldsymbol{e}_{uv}.\boldsymbol{e}_u = \frac{1}{2}E_v. \tag{2.17}$$

Same calculation for G gives

$$\boldsymbol{e}_{vv}.\boldsymbol{e}_v = \frac{1}{2}G_v, \tag{2.18}$$

$$\boldsymbol{e}_{vu}.\boldsymbol{e}_v = \frac{1}{2}G_u. \tag{2.19}$$

For F

$$F = \boldsymbol{e}_u.\boldsymbol{e}_v \Longrightarrow F_u = \boldsymbol{e}_{uu}.\boldsymbol{e}_v + \boldsymbol{e}_u.\boldsymbol{e}_{vu} = \boldsymbol{e}_{uu}.\boldsymbol{e}_v + \frac{1}{2}E_v \Longrightarrow$$

$$\boldsymbol{e}_{uu}.\boldsymbol{e}_v = F_u - \frac{1}{2}E_v\ . \tag{2.20}$$

And same calculations for F_v gives

$$\boldsymbol{e}_{vv}.\boldsymbol{e}_u = F_v - \tfrac{1}{2}G_u. \tag{2.21}$$

Regarding (2.15), (2.16) and (2.20)

$$\boldsymbol{e}_{uu} = \Gamma_{uu}^u\boldsymbol{e}_u + \Gamma_{uu}^v\boldsymbol{e}_v + e\boldsymbol{n}, \tag{2.22}$$

where, Γ_{bc}^a's are the Christoffel symbols and same for $\boldsymbol{e}_{vv}$ and $\boldsymbol{e}_{uv} = \boldsymbol{e}_{vu}$ we have,

$$\boldsymbol{e}_{vv} = \Gamma_{vv}^u\boldsymbol{e}_u + \Gamma_{vv}^v\boldsymbol{e}_v + g\boldsymbol{n}, \tag{2.23}$$

$$\boldsymbol{e}_{uv} = \Gamma_{uv}^u\boldsymbol{e}_u + \Gamma_{uv}^v\boldsymbol{e}_v + f\boldsymbol{n}, \tag{2.24}$$

Equation (2.4) and (2.5) are modified as

$$\boldsymbol{n}_u = \alpha_u^u\boldsymbol{e}_u + \alpha_u^v\boldsymbol{e}_v, \tag{2.25}$$

$$\boldsymbol{n}_v = \alpha_v^u\boldsymbol{e}_u + \alpha_v^v\boldsymbol{e}_v, \tag{2.26}$$

considering, $a = \alpha_u^u$, $b = \alpha_u^v$, $c = \alpha_v^u$ and $d = \alpha_v^v$ when α_j^i's are surface curvature tensor elements. From (2.16) to (2.24) we can write

$$\boldsymbol{e}_u.\boldsymbol{e}_{uu} = \frac{1}{2}E_u = \Gamma_{uu}^u\boldsymbol{e}_u.\boldsymbol{e}_u + \Gamma_{uu}^v\boldsymbol{e}_u.\boldsymbol{e}_v + 0, \tag{2.27}$$

$$\boldsymbol{e}_v.\boldsymbol{e}_{uu} = F_u - \frac{1}{2}E_v = \Gamma_{uu}^u\boldsymbol{e}_v.\boldsymbol{e}_u + \Gamma_{uu}^v\boldsymbol{e}_v.\boldsymbol{e}_v + 0, \tag{2.28}$$

$$\boldsymbol{e}_u.\boldsymbol{e}_{uv} = \frac{1}{2}E_v = \Gamma_{uv}^u\boldsymbol{e}_u.\boldsymbol{e}_u + \Gamma_{uv}^v\boldsymbol{e}_u.\boldsymbol{e}_v + 0, \tag{2.29}$$

$$\boldsymbol{e}_v.\boldsymbol{e}_{uv} = \frac{1}{2}G_u = \Gamma_{uv}^u\boldsymbol{e}_v.\boldsymbol{e}_u + \Gamma_{uv}^v\boldsymbol{e}_v.\boldsymbol{e}_v + 0, \tag{2.30}$$

$$\boldsymbol{e}_v.\boldsymbol{e}_{vv} = \frac{1}{2}G_v = \Gamma_{vv}^u\boldsymbol{e}_v.\boldsymbol{e}_u + \Gamma_{vv}^v\boldsymbol{e}_v.\boldsymbol{e}_v + 0, \tag{2.31}$$

$$\boldsymbol{e}_u.\boldsymbol{e}_{vv} = F_v - \frac{1}{2}G_u = \Gamma_{vv}^u\boldsymbol{e}_u.\boldsymbol{e}_u + \Gamma_{vv}^v\boldsymbol{e}_u.\boldsymbol{e}_v + 0. \tag{2.32}$$

In addition from (2.12) to (2.14) and (2.25) and (2.26), we have

$$\boldsymbol{e}_u.\boldsymbol{n}_u = \alpha_u^u\boldsymbol{e}_u.\boldsymbol{e}_u + \alpha_u^v\boldsymbol{e}_u.\boldsymbol{e}_v = -e, \tag{2.33}$$

also

$$\boldsymbol{e}_v.\boldsymbol{n}_u = \alpha_u^u \boldsymbol{e}_v.\boldsymbol{e}_u + \alpha_u^v \boldsymbol{e}_v.\boldsymbol{e}_v = -f, \tag{2.34}$$

$$\boldsymbol{e}_v.\boldsymbol{n}_v = \alpha_v^u \boldsymbol{e}_v.\boldsymbol{e}_u + \alpha_v^v \boldsymbol{e}_v.\boldsymbol{e}_v = -g. \tag{2.35}$$

From (27) to (32)

$$\frac{1}{2}E_u = \Gamma_{uu}^u E + \Gamma_{uu}^v F, \tag{2.36}$$

$$F_u - \frac{1}{2}E_v = \Gamma_{uu}^u F + \Gamma_{uu}^v G, \tag{2.37}$$

$$\frac{1}{2}E_v = \Gamma_{uv}^u E + \Gamma_{uv}^v F, \tag{2.38}$$

$$\frac{1}{2}G_u = \Gamma_{uv}^u F + \Gamma_{uv}^v G, \tag{2.39}$$

$$F_v - \frac{1}{2}G_u = \Gamma_{vv}^u E + \Gamma_{vv}^v F, \tag{2.40}$$

$$\frac{1}{2}G_v = \Gamma_{vv}^u F + \Gamma_{vv}^v G, \tag{2.41}$$

they can be written as

$$\begin{pmatrix} \frac{1}{2}E_u & \frac{1}{2}E_v & F_v - \frac{1}{2}G_u \\ F_u - \frac{1}{2}E_v & \frac{1}{2}G_u & \frac{1}{2}G_v \end{pmatrix} = \begin{pmatrix} E & F \\ F & G \end{pmatrix} \begin{pmatrix} \Gamma_{uu}^u & \Gamma_{uv}^u & \Gamma_{vv}^u \\ \Gamma_{uu}^v & \Gamma_{uv}^v & \Gamma_{vv}^v \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} \Gamma_{uu}^u & \Gamma_{uv}^u & \Gamma_{vv}^u \\ \Gamma_{uu}^v & \Gamma_{uv}^v & \Gamma_{vv}^v \end{pmatrix} = \begin{pmatrix} E & F \\ F & G \end{pmatrix}^{-1} \begin{pmatrix} \frac{1}{2}E_u & \frac{1}{2}E_v & F_v - \frac{1}{2}G_u \\ F_u - \frac{1}{2}E_v & \frac{1}{2}G_u & \frac{1}{2}G_v \end{pmatrix}. \tag{2.42}$$

In addition, same calculations for (2.33) to (2.35)

$$\alpha_u^u E + \alpha_u^v F = -e, \tag{2.43}$$

$$\alpha_u^u F + \alpha_u^v G = -f, \tag{2.44}$$

$$\alpha_v^u F + \alpha_v^v G = -g. \tag{2.45}$$

Then

$$\begin{pmatrix} \alpha_u^u & \alpha_v^u \\ \alpha_u^v & \alpha_v^v \end{pmatrix} \begin{pmatrix} E & F \\ F & G \end{pmatrix} = -\begin{pmatrix} e & f \\ f & g \end{pmatrix}, \tag{2.46}$$

finally, Gauss-Weingaten equation is defined as

$$\begin{pmatrix} \alpha_u^u & \alpha_v^u \\ \alpha_u^v & \alpha_v^v \end{pmatrix} = -\begin{pmatrix} E & F \\ F & G \end{pmatrix}^{-1} \begin{pmatrix} e & f \\ f & g \end{pmatrix}. \tag{2.47}$$

2.2 Mean and principal curvatures

As it was explained before, potential of the constrained particle depends on mean and principal curvatures which should be calculated using curvilinear geometry [9]. Hence, let us consider point *P* on a two-dimensional curved surface embedded in a three-dimensional space, where, $\{q^1, q^2\}$ are described as surface coordinates $(q^1, q^2 \in R)$, a mapping that dedicate $\{q^1, q^2\}$ to some point in *3D* space can be introduced as

$$\boldsymbol{r}(q^1, q^2) = \begin{pmatrix} X(q^1, q^2) \\ Y(q^1, q^2) \\ Z(q^1, q^2) \end{pmatrix}, \tag{2.48}$$

where, *r* is the surface parametrization in three dimensions described using Cartesian coordinates. In order to construct a coordinate system, two considered vectors on the surface are given by

$$\boldsymbol{e}_i = \frac{\partial \boldsymbol{r}}{\partial q^i}, \quad i = 1,2, \tag{2.49}$$

where, it is tangent to the surface and some points that are in a direction where q^i increases. It is time to utilize these tangent vectors to introduce the affiliated normal vector

$$\boldsymbol{n} = \frac{\boldsymbol{e}_1 \times \boldsymbol{e}_2}{|\boldsymbol{e}_1 \times \boldsymbol{e}_2|}. \tag{2.50}$$

It is common to choose $\boldsymbol{n}$ as a unit vector, which is not correct for $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$, also they are not introduced to be perpendicular, hence the lack of orthogonality will be fixed by using the first fundamental form (metric) as $g_{ij} = \boldsymbol{e}_i.\boldsymbol{e}_j$ where $i, j = 1, 2$. Next step for calculating the surface curvature is assuming second fundamental form. Therefore

$$K_{ij} = \boldsymbol{e}_i.\frac{\partial \boldsymbol{n}}{\partial q_j} = -\boldsymbol{n}.\frac{\partial \boldsymbol{e}_i}{\partial q_j} = -\boldsymbol{n}.\frac{\partial^2 \boldsymbol{r}}{\partial q_i \partial q_j}, \tag{2.51}$$

where, K_{ij} is called extrinsic curvature tensor. Considering a plane that contains normal $\boldsymbol{n}$ and unit tangent vector $\boldsymbol{t}$ at point P, which cuts the surface and constructs a cross sectional curve whose normal curvature at the considered point is $K = K_{ij}t^i t^j$. Regarding to quadratic form of normal curvature, there are two directions for external curvature as $\boldsymbol{P}_a = P_a^i \boldsymbol{e}_i$, called principal directions, which are the eigenvectors of K_{ij} and they are orthogonal ($\boldsymbol{P}_1.\boldsymbol{P}_2 = 0$), so we have

$$K_{ij}P_a^j = K_a g_{ij} P_a^j \Longrightarrow K_j^i P_a^j = K_a P_a^i. \tag{2.52}$$

Then, the total curvature, $k = g^{ij}K_{ij} = K_i^i$, gives the mean curvature as

$$M = \frac{1}{2}k = \frac{1}{2}(K_1^1 + K_2^2) = \frac{1}{2}(K_1 + K_2). \tag{2.53}$$

In order to obtain Gaussian curvature, determinant of K_i^j should be taken, therefore it can be written as

$$K_G = \det K_i^j = K_1 K_2\,. \tag{2.54}$$

Knowing mean and principal curvature, M and K_G, we can easily compute the Schrödinger equation for constrained particle on curved surfaces.

2.3 Quantum mechanics of a constrained particle on a surface

In order to keep a particle constrained to a surface *S*, particle feels forces normal to *S* in all of its points that compress the wave function in transverse direction. It causes a constant potential on *S* which is infinity in orthogonal direction. As it was studied, an immediate neighborhood for particle position should be introduced in which particle can be released from constraining. Therefore, let us consider a particle at point *P* on the surface S with parametric position equation $\boldsymbol{r} = \boldsymbol{r}(q^1, q^2)$ and neighborhood $Q(q^1, q^2, q^3)$ with position equation as

$$\boldsymbol{R}(q^1, q^2, q^3) = \boldsymbol{r}(q^1, q^2) + q^3\boldsymbol{n}(q^1, q^2). \tag{2.55}$$

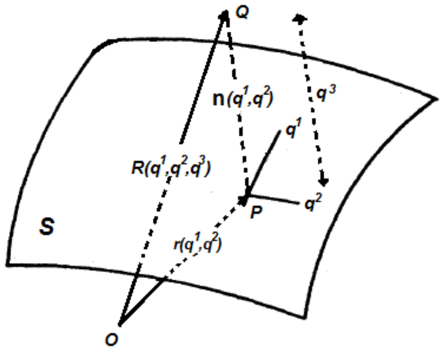

Figure 2.2: Curvilinear system for a particle at arbitrary point *p* on the surface *S*.

Where, as it's shown in figure.2.2, $\boldsymbol{n}$ is the normal at point *p*. Since to write Schrödinger equation, we need Laplacian of neighborhood metric tensor [1-8], the first step is finding components of the metric tensor G_{ij}

$$G_{ij} = \frac{\partial \boldsymbol{R}}{\partial q^i} \cdot \frac{\partial \boldsymbol{R}}{\partial q^j} = \left(\frac{\partial \boldsymbol{r}}{\partial q^i} + q^3 \frac{\partial \boldsymbol{n}(q^1, q^2)}{\partial q^i}\right) \cdot \left(\frac{\partial \boldsymbol{r}}{\partial q^j} + q^3 \frac{\partial \boldsymbol{n}(q^1, q^2)}{\partial q^j}\right), \tag{2.56}$$

with *i, j = 1, 2, 3* and

$$\frac{\partial \boldsymbol{R}}{\partial q^3} = \boldsymbol{n}(q^1, q^2). \tag{2.57}$$

And for the surface *S*, the metric tensor components that are the coefficients of first fundamental form are defined as $g_{ij} = \frac{\partial \boldsymbol{r}}{\partial q^i} . \frac{\partial \boldsymbol{r}}{\partial q^j}$. To obtain G_{ij} as functions of q's, $\frac{\partial \boldsymbol{n}}{\partial q^i}$ that embedded in the tangent plain can be written as

$$\frac{\partial \boldsymbol{n}}{\partial q^i} = \alpha_i^j \frac{\partial \boldsymbol{r}}{\partial q^j}, \tag{2.58}$$

when

$$\alpha_1^1 = \frac{1}{g}(g_{12}h_{21} - g_{22}h_{11}), \qquad \alpha_1^2 = \frac{1}{g}(h_{11}g_{21} - h_{21}g_{11}), \tag{2.59}$$

$$\alpha_2^1 = \frac{1}{g}(h_{22}g_{12} - h_{12}g_{22}), \qquad \alpha_2^2 = \frac{1}{g}(h_{21}g_{12} - h_{22}g_{11}), \tag{2.60}$$

where g is determinant of g_{ij} and h_{ij}'s are the coefficients of the second fundamental form defined the extrinsic curvature of the surface. For more clarification of geometry analysis refer to section 2.1(Gauss-Weingarten equation). From equation (2.56)

$$G_{ij} = \frac{\partial \boldsymbol{r}}{\partial q^i} . \frac{\partial \boldsymbol{r}}{\partial q^j} + q^3 \left(\frac{\partial \boldsymbol{n}}{\partial q^i} . \frac{\partial \boldsymbol{r}}{\partial q^j} + \frac{\partial \boldsymbol{r}}{\partial q^i} . \frac{\partial \boldsymbol{n}}{\partial q^j} \right) + (q^3)^2 \frac{\partial \boldsymbol{n}}{\partial q^i} . \frac{\partial \boldsymbol{n}}{\partial q^j} . \tag{2.61}$$

Using $g_{ij} = \frac{\partial \boldsymbol{r}}{\partial q^i} . \frac{\partial \boldsymbol{r}}{\partial q^j}$ and (2.58), G_{ij} can be written as

$$\begin{aligned} G_{ij} &= g_{ij} + q^3(\alpha_i^k g_{kj} + \alpha_j^k g_{ik}) + \left(\alpha_i^k g_{kl} \alpha_j^l\right)(q^3)^2 \\ &= g_{ij} + (\alpha g + (\alpha g)^T)_{ij} q^3 + (\alpha g \alpha^T)_{ij} (q^3)^2, \end{aligned} \tag{2.62}$$

where, *T* stands for transposed matrix. $G_{i3} = G_{3i} = 0$,with $i, j = 1, 2$, $G_{33=}1$.

Therefore

$$G_{ij=}\begin{pmatrix} G_{11} & G_{12} & 0 \\ G_{21} & G_{22} & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{2.63}$$

Since for an arbitrary metric tensor *f* in a curvilinear coordinates, for a general scalar function ψ Laplacian is define as

$$\nabla^2\psi = \frac{1}{\sqrt{f}}\frac{\partial}{\partial q^i}\left(\sqrt{f}f^{ij}\frac{\partial}{\partial q^j}\right)\psi, \tag{2.64}$$

where $f = \det f_{ij}$ [10]. Now Schrödinger equation can be written as

$$-\frac{\hbar^2}{2m}\frac{1}{\sqrt{G}}\frac{\partial}{\partial q^i}\left[\sqrt{G}G^{ij}\frac{\partial\psi}{\partial q^j}\right] + V_\lambda(q^3)\psi = i\hbar\frac{\partial\psi}{\partial t}, \tag{2.65}$$

where V_λ is the potential that keeps the particle constrained on the surface, which is obviously equal to zero when $q^3 = 0$. Therefore the Schrödinger equation is given as

$$-\frac{\hbar^2}{2m}H(q^1,q^2,q^3)\psi - \frac{\hbar^2}{2m}\left[\frac{\partial^2\psi}{(\partial q^3)^2} + \frac{\partial}{\partial q^3}\left(\ln\sqrt{G}\right)\frac{\partial\psi}{\partial q^3}\right] + V_\lambda(q^3)\psi = i\hbar\frac{\partial\psi}{\partial t}, \tag{2.66}$$

where $H(q^1,q^2,q^3)$ is defined as surface part, with $i,j = 1,2$. Now this equation is divided to two exterior and interior parts while in internal part G_{ij} that represents exterior metric tensor should be eliminated in a way that g_{ij} appears. Therefore probability of finding internal coordinate in dV as a volume element of the curve space that is independent of outer variables should be found, which can be written as

$$dp = |\psi|^2 dV = |\psi|^2\sqrt{G}dq^1dq^2dq^3. \tag{2.67}$$

To obtain $\sqrt{G}$ from (2.62) for matrix G_{ij}

$$G_{ij} = \begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix} + \left(\begin{bmatrix} \alpha_1^1 & \alpha_1^2 \\ \alpha_2^1 & \alpha_2^2 \end{bmatrix}\begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix} + \begin{bmatrix} g_{11} & g_{21} \\ g_{12} & g_{22} \end{bmatrix}\begin{bmatrix} \alpha_1^1 & \alpha_2^1 \\ \alpha_1^2 & \alpha_2^2 \end{bmatrix}\right)q_3 + \begin{bmatrix} \alpha_1^1 & \alpha_1^2 \\ \alpha_2^1 & \alpha_2^2 \end{bmatrix}\begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix}\begin{bmatrix} \alpha_1^1 & \alpha_2^1 \\ \alpha_1^2 & \alpha_2^2 \end{bmatrix}(q^3)^2, \tag{2.68}$$

after simplifying and determining elements of this matrix, determinant of G_{ij}can be calculated as

$$\det G_{ij} = \frac{1}{g}\left\{\left(h_{11}h_{22} - {h_{21}}^2\right)(q^3)^2 + q^3(-h_{22}g_{11} - g_{22}h_{11} + 2g_{12}h_{21} + g\right\}^2. \tag{2.69}$$

For the first part in parentheses, using (2.59), (2.60) we can write

$$\det\alpha = \alpha_1^1\alpha_2^2 - \alpha_1^2\alpha_2^1 = \frac{1}{g^2}\left(h_{11}h_{22} - {h_{21}}^2\right)(g_{11}g_{22} - {g_{21}}^2)$$
$$= \frac{1}{g}\left(h_{11}h_{22} - {h_{21}}^2\right) \Longrightarrow g\det\alpha = h_{11}h_{22} - {h_{21}}^2, \tag{2.70}$$

and for second part where $Tr\alpha = \alpha_1^1 + \alpha_2^2$

$$gTr\alpha = (-h_{22}g_{11} - g_{22}h_{11} + 2g_{12}h_{21})\,. \tag{2.71}$$

Using (2.69), (2.70) and (2.71)

$$\det G_{ij} = \frac{1}{g}\{(g\det\alpha)(q^3)^2 + q^3 g(Tr\alpha) + g\}^2,$$
$$\Longrightarrow \sqrt{G} = \sqrt{g}(1 + q^3 Tr\alpha + (q^3)^2\det\alpha). \tag{2.72}$$

It is time to write the volume element as

$$dV = f(q^1, q^2, q^3)dSdq^3, \tag{2.73}$$

where, $f = 1 + q^3 Tr\alpha + (q^3)^2\det\alpha$ and the element of surface dS can be obtained as

$$dS = |\boldsymbol{q}^1 dq^1 \times \boldsymbol{q}^2 dq^2|, \tag{2.74}$$

where, $\boldsymbol{q}^i dq^i$'s are immeasurably small element of surface. From determinant of surface metric, we have

$$g = g_{11}g_{22} - g_{12}g_{21} = g_{11}g_{22} - (\boldsymbol{q}^1 . \boldsymbol{q}^2)^2 = g_{11}g_{22}(1 - \cos^2\theta)$$

$$= |\boldsymbol{q}^1|^2|\boldsymbol{q}^2|^2 \sin^2\theta = |\boldsymbol{q}^1 \times \boldsymbol{q}^2|^2 \Rightarrow |\boldsymbol{q}^1 \times \boldsymbol{q}^2| = \sqrt{g}\ ,$$

$$\Rightarrow dS = \sqrt{g} dq^1 dq^2\ . \tag{2.75}$$

Referring (2.67)

$$dp = |\psi|^2 f\sqrt{g} dq^1 dq^2 dq^3 = \left|\psi\sqrt{f}\right|^2 \sqrt{g} dq^1 dq^2 dq^3$$

$$= |X|^2 \sqrt{g} dq^1 dq^2 dq^3, \tag{2.76}$$

since the wave function can be modified as $X(q^1, q^2, q^3) = \sqrt{f}\psi(q^1, q^2, q^3)$, Schrödinger equation (2.66) is expressed as

$$-\frac{\hbar^2}{2m}\frac{1}{\sqrt{G}}\frac{\partial}{\partial q^i}\left[\sqrt{G}G^{ij}\frac{\partial}{\partial q^j}\frac{X}{\sqrt{f}}\right] - \frac{\hbar^2}{2m}\frac{1}{\sqrt{f}}\frac{\partial^2 X}{(\partial q^3)^2}$$

$$+\frac{1}{4f^2}\left[\left(\frac{\partial f}{\partial q^3}\right)^2 - 2f\frac{\partial^2 f}{(\partial q^3)^2}\right]X + \frac{1}{\sqrt{f}}V_\lambda X = i\hbar\frac{1}{\sqrt{f}}\frac{\partial X}{\partial t}. \tag{2.77}$$

The wave function value is clearly far from zero at limit around $q^3 = 0$ where the squeezing parameter λ goes to infinity and the wave function feels sharp potential from two sides of the S in the normal directions. At this time Schrödinger equation can be written as

$$-\frac{\hbar^2}{2m}\frac{1}{\sqrt{g}}\frac{\partial}{\partial q^i}\left[\sqrt{g}g^{ij}\frac{\partial X}{\partial q^j}\right] - \frac{\hbar^2}{8m}\left[\left(\frac{\partial f}{\partial q^3}\right)^2 - 2\frac{\partial^2 f}{(\partial q^3)^2}\right]X - \frac{\hbar^2}{2m}\frac{\partial^2 X}{(\partial q^3)^2}$$

$$+V_\lambda X = i\hbar\frac{\partial X}{\partial t}. \tag{2.78}$$

Now obviously wave function can be separated into internal (X_{in}) and external (X_e) parts

$$-\frac{\hbar^2}{2m}\frac{1}{\sqrt{g}}\frac{\partial}{\partial q^i}\left[\sqrt{g}g^{ij}\frac{\partial X_{in}}{\partial q^j}\right] - \frac{\hbar^2}{8m}\left[\left(\frac{\partial f}{\partial q^3}\right)^2 - 2\frac{\partial^2 f}{(\partial q^3)^2}\right]X_{in} = i\hbar\frac{\partial X_{in}}{\partial t}, \tag{2.79}$$

and

$$-\frac{\hbar^2}{2m}\frac{\partial^2 X_e}{(\partial q^3)^2}+V_\lambda(q^3)X_e=i\hbar\frac{\partial X_e}{\partial t}\,. \tag{2.80}$$

Where, exterior part as one-dimensional Schrödinger equation is ignorable in this study, on the other hand interior part is the important one as serves Schrödinger equation for the wave function of constrained particle on the surface under an internal potential which depends on surface geometrical properties and is given as

$$U(q^1,q^2)=-\frac{\hbar^2}{2m}\left[\left(\frac{1}{2}\frac{\partial f}{\partial q^3}\right)^2-\frac{\partial^2 f}{(\partial q^3)^2}\right]. \tag{2.81}$$

By calculating first and second derivatives of f with respect to q_3

$$\frac{\partial f}{\partial q^3}=\left(\frac{1}{g}(g_{11}h_{22}+g_{22}h_{11}-2g_{12}h_{12})\right)^{\frac{1}{2}} \quad , \quad \frac{\partial^2 f}{(\partial q^3)^2}=\frac{1}{g}\det h_{ij}\,. \tag{2.82}$$

Introducing mean and Gaussian curvatures as M and K_G respectively [9], internal potential can be written as

$$U(q^1,q^2)=-\frac{\hbar^2}{2m}[M^2-K_G], \tag{2.83}$$

where k_1 and k_2 are principle curvatures of surface

$$K_G=k_1k_2\,, \tag{2.84}$$

$$M=\frac{1}{2}(k_1+k_2). \tag{2.85}$$

Presence of internal potential as a function of mean and Gaussian curvatures significantly demonstrates dependent of constraint particle motion to surface geometry which can be different for various surfaces with different g_{ij}'s. Since Lagrangian ($L=\frac{1}{2}m\sum_{i,j=1}^{2}g_{ij}(q^1,q^2)\dot{q}^1\dot{q}^2$) is independent of surface geometry and clearly depends only on surface metric variables, it is not an appropriate method to solve this problem.

Chapter 3

EXAMPLES OF CONSTRAINING A QUANTUM PARTICLE TO A SURFACE

3.1 Constrained particle on a spherical shell

Computing the mean and principal curvature was explained thoroughly in previous chapter. Defining local coordinates as, $q^1 = \theta\ , q^2 = \varphi$, a parametrization for a sphere with radius a is given by

$$\boldsymbol{r} = \begin{pmatrix} a \sin\theta \cos\varphi \\ a \sin\theta \sin\varphi \\ a \cos\theta \end{pmatrix}. \tag{3.1}$$

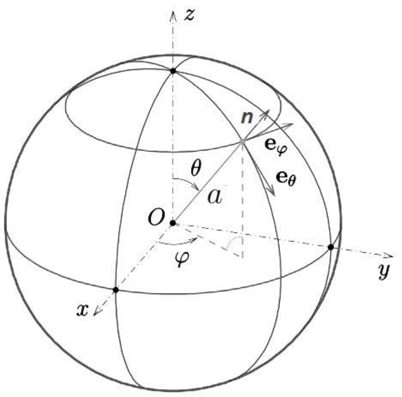

Figure 3.1: A spherical surface of radius a.

The tangent vectors on the sphere surface are defined as

$$\boldsymbol{e}_\theta = \frac{\partial \boldsymbol{r}}{\partial \theta} = \begin{pmatrix} a \cos\theta \cos\varphi \\ a \cos\theta \sin\varphi \\ -\, a \sin\theta \end{pmatrix}, \tag{3.2}$$

and

$$\boldsymbol{e}_\varphi = \frac{\partial \boldsymbol{r}}{\partial \varphi} = \begin{pmatrix} -a\sin\theta\sin\varphi \\ a\sin\theta\cos\varphi \\ 0 \end{pmatrix}, \tag{3.3}$$

therefore, the unit normal is described as

$$\boldsymbol{n} = \frac{\boldsymbol{e}_\theta \times \boldsymbol{e}_\varphi}{\left|\boldsymbol{e}_\theta \times \boldsymbol{e}_\varphi\right|} = \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix}. \tag{3.4}$$

In addition, the for the first fundamental form on the sphere we get

$$g_{ij} = \boldsymbol{e}_i.\boldsymbol{e}_j = \begin{pmatrix} \boldsymbol{e}_\theta.\boldsymbol{e}_\theta & \boldsymbol{e}_\theta.\boldsymbol{e}_\varphi \\ \boldsymbol{e}_\varphi.\boldsymbol{e}_\theta & \boldsymbol{e}_\varphi.\boldsymbol{e}_\varphi \end{pmatrix} = \begin{pmatrix} a^2 & 0 \\ 0 & a^2\sin^2\theta \end{pmatrix}, \tag{3.5}$$

$$\Rightarrow g^{ij} = \begin{pmatrix} \frac{1}{a^2} & 0 \\ 0 & \frac{1}{a^2\sin^2\theta} \end{pmatrix}. \tag{3.6}$$

Now the second fundamental form coefficients on the sphere are described as

$$K_{\theta\varphi} = K_{\varphi\theta} = -\boldsymbol{n}.\frac{\partial^2 \boldsymbol{r}}{\partial\theta\partial\varphi} = 0, \tag{3.7}$$

$$\begin{aligned} K_{\theta\theta} = -\boldsymbol{n}.\frac{\partial^2 \boldsymbol{r}}{\partial^2\theta} &= -\begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix}.\begin{pmatrix} -a\sin\theta\cos\varphi \\ -a\sin\theta\sin\varphi \\ -a\cos\theta \end{pmatrix} \\ &= a(\sin^2\theta\cos^2\varphi + \sin^2\theta\sin^2\varphi + \cos^2\theta) = a, \end{aligned} \tag{3.8}$$

$$\begin{aligned} K_{\varphi\varphi} = -\boldsymbol{n}.\frac{\partial^2 \boldsymbol{r}}{\partial^2\varphi} &= -\begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix}.\begin{pmatrix} -a\sin\theta\cos\varphi \\ -a\sin\theta\sin\varphi \\ 0 \end{pmatrix} \\ &= a(\sin^2\theta\cos^2\varphi + \sin^2\theta\sin^2\varphi) = a\sin^2\theta. \end{aligned} \tag{3.9}$$

Where extrinsic curvature tensor is determined as $K_{ij} = \begin{pmatrix} a & 0 \\ 0 & a\sin^2\theta \end{pmatrix}$ which leads us to obtain matrix K_i^j where diagonal components are surface principal curvatures so we compute K_i^i's as

$$K_1 = K_\theta^\theta = K_{\theta i} g^{\theta i} = K_{\theta\theta} g^{\theta\theta} + K_{\theta\varphi} g^{\theta\varphi} = a \frac{1}{a^2} + 0 = \frac{1}{a}, \tag{3.10}$$

$$K_2 = K_\varphi^\varphi = K_{\varphi i} g^{\varphi i} = K_{\varphi\varphi} g^{\varphi\varphi} + K_{\varphi\theta} g^{\varphi\theta} = a \sin^2\theta \frac{1}{a^2 \sin^2\theta} + 0 = \frac{1}{a}. \tag{3.11}$$

Knowing $K_1$and K_2 are principle curvatures, the mean and Gaussian curvatures are given by

$$M = \frac{1}{2}(K_1 + K_2) = \frac{1}{a}, \tag{3.12}$$

and

$$K_G = (K_1 . K_2) = \frac{1}{a^2}. \tag{3.13}$$

As it was argued, internal potential for a spherical shell can be written as

$$U(q_1, q_2) = -\frac{\hbar^2}{2m}[M^2 - K_G] = -\frac{\hbar^2}{2m}\left[\left(\frac{1}{a}\right)^2 - \frac{1}{a^2}\right] = 0. \tag{3.14}$$

Therefore, the Schrödinger equation for a constrained particle on a spherical shell can be written as

$$-\frac{\hbar^2}{2m}\frac{1}{\sqrt{g}}\frac{\partial}{\partial q^i}\left[\sqrt{g} g^{ij} \frac{\partial X_{in}}{\partial q^j}\right] = i\hbar \frac{\partial X_{in}}{\partial t}. \tag{3.15}$$

Regarding (3.5) and (3.6), time independent Schrödinger equation can be written as

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta \frac{\partial X_{in}}{\partial\theta}\right] + \frac{1}{\sin^2\theta}\frac{\partial}{\partial\varphi}\left[\frac{\partial X_{in}}{\partial\varphi}\right] = -\frac{2mEa^2}{\hbar^2} X_{in}, \tag{3.16}$$

considering $X_{in} = R(a) Y_{l,m_l}(\theta, \varphi)$ where on the surface *R(a)* is constant and $Y_{l,m_l}(\theta, \varphi) = \Theta(\theta)\Phi(\varphi)$ is spherical harmonics with $l = 0,1,2, \ldots$ and $m_l = 0, \pm 1, \pm 2, \ldots$ are orbital and magnetic quantum numbers respectively, for Laplacian L^2 we can write

$$L^2 Y_{l,m_l} = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial Y_{l,m_l}}{\partial\theta}\right] + \frac{1}{\sin^2\theta}\frac{\partial^2 Y_{l,m_l}}{\partial\varphi^2} = l(l+1)Y_{l,m_l}, \tag{3.17}$$

that can be separated as

$$\begin{gathered}\frac{\partial^2 \Phi}{\partial\varphi^2} = -{m_l}^2\varphi\ , \\ \sin\theta\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial\Theta}{\partial\theta}\right] + [l(l+1)\sin^2\theta - {m_l}^2]\Theta = 0.\end{gathered} \tag{3.18}$$

Therefore, general solution for this Schrödinger equation is given as

$$X_{in}(\theta,\varphi) = Re^{im_l\varphi}p_l^{m_l}(\cos\theta), \tag{3.19}$$

where $p_l^{m_l}$ is associated Legendre function [11].

3.2 Constrained particle on a cylindrical shell

Defining local coordinates as, $q^1 = \theta\ , q^2 = z$, a parametrization for a cylinder with radius ρ is given by

$$\boldsymbol{r} = \begin{pmatrix}\rho\cos\varphi \\ \rho\sin\varphi \\ z\end{pmatrix}. \tag{3.20}$$

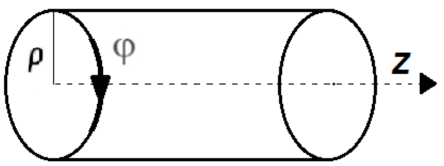

Figure 3.2: A cylindrical surface of coordinates (ρ, φ, z).

The tangent vectors on the sphere surface are defined as

$$\boldsymbol{e}_z = \frac{\partial\boldsymbol{r}}{\partial z} = \begin{pmatrix}0\\0\\1\end{pmatrix}, \tag{3.21}$$

$$\boldsymbol{e}_\varphi = \frac{\partial\boldsymbol{r}}{\partial\varphi} = \begin{pmatrix}-\rho\sin\varphi \\ \rho\cos\varphi \\ 0\end{pmatrix}, \tag{3.22}$$

in this case the unit normal is described as

$$\boldsymbol{n} = \frac{\boldsymbol{e}_\varphi \times \boldsymbol{e}_z}{|\boldsymbol{e}_\varphi \times \boldsymbol{e}_z|} = \begin{pmatrix} \cos\varphi \\ \sin\varphi \\ 0 \end{pmatrix}. \tag{3.23}$$

In addition for metric on the cylindrical surface we get

$$g_{ij} = \boldsymbol{e}_i . \boldsymbol{e}_j = \begin{pmatrix} \boldsymbol{e}_\varphi . \boldsymbol{e}_\varphi & \boldsymbol{e}_\varphi . \boldsymbol{e}_z \\ \boldsymbol{e}_z . \boldsymbol{e}_\varphi & \boldsymbol{e}_z . \boldsymbol{e}_z \end{pmatrix} = \begin{pmatrix} \rho^2 & 0 \\ 0 & 1 \end{pmatrix},$$

$$\Rightarrow g^{ij} = \begin{pmatrix} \frac{1}{\rho^2} & 0 \\ 0 & 1 \end{pmatrix}. \tag{3.24}$$

The second fundamental form coefficients are given by

$$K_{\varphi z} = K_{z\varphi} = -\boldsymbol{n}. \frac{\partial^2 \boldsymbol{r}}{\partial\varphi\partial z} = 0, \tag{3.25}$$

$$K_{\varphi\varphi} = -\boldsymbol{n}. \frac{\partial^2 \boldsymbol{r}}{\partial^2 \varphi} = -\begin{pmatrix} \cos\varphi \\ \sin\varphi \\ 0 \end{pmatrix} . \begin{pmatrix} -\rho\cos\varphi \\ -\rho\sin\varphi \\ 0 \end{pmatrix} = \rho(\cos^2\varphi + \sin^2\varphi) = \rho, \tag{3.26}$$

$$K_{zz} = -\boldsymbol{n}. \frac{\partial^2 \boldsymbol{r}}{\partial^2 z} = -\begin{pmatrix} \cos\varphi \\ \sin\varphi \\ 0 \end{pmatrix} . \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} = 0. \tag{3.27}$$

Then extrinsic curvature tensor is computed as $K_{ij} = \begin{pmatrix} \rho & 0 \\ 0 & 0 \end{pmatrix}$ which leads us to find principal curvatures so

$$K_1 = K_\varphi^\varphi = K_{\varphi i} g^{\varphi i} = K_{\varphi\varphi} g^{\varphi\varphi} + K_{\varphi z} g^{\varphi z} = \rho \frac{1}{\rho^2} + 0 = \frac{1}{\rho},$$
$$K_2 = K_z^z = K_{zi} g^{zi} = K_{zz} g^{zz} + K_{\varphi z} g^{\varphi z} = 0. \tag{3.28}$$

Determining $K_2 = 0$, Gaussian curvature is clearly zero and mean curvature obviously is equal to $M = \frac{1}{2} K_1 = \frac{1}{2\rho}$. Therefore, internal potential for a cylindrical shell can be written as

$$U(q_1, q_2) = -\frac{\hbar^2}{2m}[M^2 - K_G] = -\frac{\hbar^2}{8m}\frac{1}{\rho^2}. \tag{3.29}$$

Finally the Schrödinger equation for a constrained particle on a cylindrical shell is given by

$$-\frac{\hbar^2}{2m}\frac{1}{\sqrt{g}}\frac{\partial}{\partial q^i}\left[\sqrt{g}g^{ij}\frac{\partial X_{in}}{\partial q^j}\right]-\frac{\hbar^2}{8m}\frac{1}{\rho^2}X_{in}=i\hbar\frac{\partial X_{in}}{\partial t}, \tag{3.30}$$

using this equation and (3.23) and assuming $X_{in}=\Phi(\varphi)Z(z)$, independent Schrödinger is modified as

$$\frac{1}{\Phi(\varphi)}\frac{\partial^2\Phi(\varphi)}{\partial\varphi^2}=-\frac{2mE\rho^2}{\hbar^2}-\frac{1}{4}-\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}\rho^2=-\alpha^2. \tag{3.31}$$

Hence applying separation method [12], it can be written as

$$\frac{\partial^2\Phi(\varphi)}{\partial\varphi^2}=-\alpha^2\Phi(\varphi), \tag{3.32}$$

and

$$\frac{\partial^2 Z}{\partial z^2}=-\beta^2 Z. \tag{3.33}$$

Where $\beta^2=\frac{1}{4\rho^2}+\frac{2mE}{\hbar^2}-\frac{\alpha^2}{\rho^2}$ and α are constants. Considering L, the length of cylinder, using boundary conditions, $Z(0)=Z(L)=0$, so (3.33) can be written as

$$Z(z)=\sin(\beta z)=\sin\left(\frac{n\pi}{L}z\right)\ , \qquad n=1,2,3,\dots. \tag{3.34}$$

Therefore, the general solution can be written as

$$X_{in}(\varphi,z)=\sin\left(\frac{n\pi}{L}z\right)e^{i\alpha\varphi}, \tag{3.35}$$

where using (3.34) and β definition, it is clear that, $\alpha=\sqrt{\frac{1}{4}+\frac{2mE\rho^2}{\hbar^2}-\frac{n^2\pi^2\rho^2}{L^2}}$.

3.3 Constrained particle on a Toroid

The same computing structure leads us to Schrodinger equation for a constrained particle on a toroid where local coordinates are $q^1 = \theta$, $q^2 = \varphi$, the parametrization is given by

$$\boldsymbol{r} = \begin{pmatrix} (R + r\cos\theta)\cos\varphi \\ (R + r\cos\theta)\sin\varphi \\ r\sin\theta \end{pmatrix}. \tag{3.36}$$

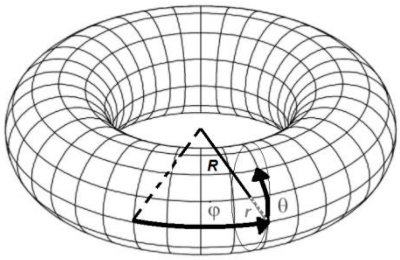

Figure 3.3: A Toroid surface major radius R and minus radius r.

Where R is the distance between toroid center and center of the tube also r is tube radius, which are called major and minus radiuses respectively. The tangent vectors on the toroid surface are defined as

$$\boldsymbol{e}_\theta = \frac{\partial \boldsymbol{r}}{\partial \theta} = \begin{pmatrix} -r\sin\theta\cos\varphi \\ -r\sin\theta\sin\varphi \\ r\cos\theta \end{pmatrix}, \tag{3.37}$$

$$\boldsymbol{e}_\varphi = \frac{\partial \boldsymbol{r}}{\partial \varphi} = \begin{pmatrix} -(R + r\cos\theta)\sin\varphi \\ (R + r\cos\theta)\cos\varphi \\ 0 \end{pmatrix}, \tag{3.38}$$

therefore, the unit normal is described as

$$\boldsymbol{n} = \frac{\boldsymbol{e}_\theta \times \boldsymbol{e}_\varphi}{|\boldsymbol{e}_\theta \times \boldsymbol{e}_\varphi|} = \frac{-1}{r(R + r\cos\theta)} \begin{pmatrix} r(R + r\cos\theta)\cos\theta\cos\varphi \\ r(R + r\cos\theta)\cos\theta\sin\varphi \\ r(R + r\cos\theta)\sin\theta \end{pmatrix}$$

$$= \begin{pmatrix} -\cos\theta\cos\varphi \\ -\cos\theta\sin\varphi \\ -\sin\theta \end{pmatrix}. \tag{3.39}$$

In addition the for the first fundamental form on the toroid we get

$$g_{ij} = \boldsymbol{e}_i.\boldsymbol{e}_j = \begin{pmatrix} e_\theta.e_\theta & e_\theta.e_\varphi \\ e_\varphi.e_\theta & e_\varphi.e_\varphi \end{pmatrix} = \begin{pmatrix} r^2 & 0 \\ 0 & (R + r\cos\theta)^2 \end{pmatrix},$$

$$\Longrightarrow g^{ij} = \begin{pmatrix} \dfrac{1}{r^2} & 0 \\ 0 & \dfrac{1}{(R + r\cos\theta)^2} \end{pmatrix}. \tag{3.40}$$

Now the second fundamental form coefficients on the toroid are described as

$$K_{\theta\varphi} = K_{\varphi\theta} = -\boldsymbol{n}.\frac{\partial^2 \boldsymbol{r}}{\partial\theta\partial\varphi} = 0, \tag{3.41}$$

$$K_{\theta\theta} = -\boldsymbol{n}.\frac{\partial^2 \boldsymbol{r}}{\partial^2\theta} = \begin{pmatrix} \cos\theta\cos\varphi \\ \cos\theta\sin\varphi \\ \sin\theta \end{pmatrix}.\begin{pmatrix} -r\cos\theta\cos\varphi \\ -r\cos\theta\sin\varphi \\ -r\sin\theta \end{pmatrix} = -r, \tag{3.42}$$

$$K_{\varphi\varphi} = -\boldsymbol{n}.\frac{\partial^2 \boldsymbol{r}}{\partial^2\varphi} = \begin{pmatrix} \cos\theta\cos\varphi \\ \cos\theta\sin\varphi \\ \sin\theta \end{pmatrix}.\begin{pmatrix} -(R + r\cos\theta)\cos\varphi \\ -(R + r\cos\theta)\sin\varphi \\ 0 \end{pmatrix}$$
$$= -(R + r\cos\theta)\cos\theta. \tag{3.43}$$

Therefore $K_{ij} = \begin{pmatrix} -r & 0 \\ 0 & -(R + r\cos\theta)\cos\theta \end{pmatrix}$ and K_i^i's are given by

$$K_1 = K_\theta^\theta = K_{\theta i} g^{\theta i} = K_{\theta\theta} g^{\theta\theta} + K_{\theta\varphi} g^{\theta\varphi} = -r\frac{1}{r^2} + 0 = \frac{-1}{r}, \tag{3.44}$$

$$K_2 = K_\varphi^\varphi = K_{\varphi i} g^{\varphi i} = K_{\varphi\varphi} g^{\varphi\varphi} + K_{\varphi\theta} g^{\varphi\theta}$$

$$= -(R + r\cos\theta)\cos\theta \frac{1}{(R + r\cos\theta)^2} + 0 = \frac{-\cos\theta}{R + r\cos\theta}. \tag{3.45}$$

Knowing K_1 and K_2 as principle curvatures, the mean and Gaussian curvatures are given by

$$M = \frac{1}{2}\left(\frac{-1}{r} + \frac{-\cos\theta}{R + r\cos\theta}\right) = \frac{-(R + 2r\cos\theta)}{2r(R + r\cos\theta)}, \tag{3.46}$$

and

$$K_G = \frac{\cos\theta}{r(R + r\cos\theta)}. \tag{3.47}$$

As it was argued, internal potential for a toroid can be written as

$$U(q_1, q_2) = -\frac{\hbar^2}{2m}[M^2 - K_G] = -\frac{\hbar^2}{8m}\frac{R^2}{r^2(R + r\cos\theta)^2}. \tag{3.48}$$

Finally the independent Schrödinger equation for a constrained particle on a toroid [13] is defined as

$$-\frac{\hbar^2}{2m}\frac{1}{\sqrt{g}}\frac{\partial}{\partial q^i}\left[\sqrt{g}g^{ij}\frac{\partial X_{in}}{\partial q^j}\right] - \frac{\hbar^2}{8m}\left[\frac{R^2}{r^2(R + r\cos\theta)^2}\right]X_{in} = EX_{in}, \tag{3.49}$$

which can be separated where $X_{in} = \Theta(\theta)\Phi(\varphi)$ as

$$\frac{(R + r\cos\theta)}{r^2}\frac{1}{\Theta(\theta)}\frac{\partial}{\partial\theta}\left[(R + r\cos\theta)\frac{\partial\Theta(\theta)}{\partial\theta}\right] + \frac{R^2}{4r^2}$$
$$+ \frac{2mE}{\hbar^2}(R + r\cos\theta)^2 = -\frac{1}{\Phi(\varphi)}\left[\frac{\partial^2\Phi(\varphi)}{\partial\varphi^2}\right]. \tag{3.50}$$

Therefore

$$X_{in} = \Theta(\theta)\mathrm{e}^{\mathrm{i}\alpha\varphi}, \tag{3.51}$$

where $\Theta(\theta)$ satifies

$$\frac{(R + r\cos\theta)^2}{r^2}\frac{\partial^2\Theta(\theta)}{\partial\theta^2} - \frac{(R + r\cos\theta)}{r}\sin\theta\frac{\partial\Theta(\theta)}{\partial\theta} \tag{3.52}$$
$$+ \left[\frac{R^2}{4r^2} + \frac{2mE}{\hbar^2}(R + r\cos\theta)^2 - \alpha^2\right]\Theta(\theta) = 0.$$

3.4 Constrained particle on a pseudosphere

In this section we find the Schrodinger equation for a constrained particle on a pseudosphere surface which is called antisphere or tractrisoid too [14-16]. For local coordinates $q^1 = \mathrm{u}$ and $q^2 = \mathrm{v}$, the pseudosphere parametrization is

$$\boldsymbol{r} = \begin{pmatrix} \operatorname{sech} u \cos v \\ \operatorname{sech} u \sin v \\ u - \tanh u \end{pmatrix}. \tag{3.53}$$

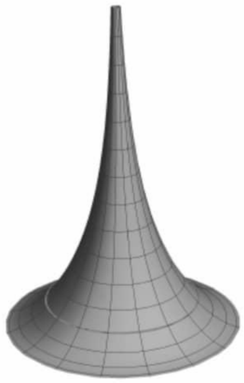

Figure 3.4: Illustration of pseudosphere upper half. [14]

Then tangent vectors on this surface are computed as

$$\boldsymbol{e}_u = \frac{\partial \boldsymbol{r}}{\partial u} = \begin{pmatrix} -\operatorname{sech} u \tanh u \cos v \\ -\operatorname{sech} u \tanh u \sin v \\ 1 - \operatorname{sech}^2 u \end{pmatrix}, \tag{3.54}$$

$$\boldsymbol{e}_v = \frac{\partial \boldsymbol{r}}{\partial v} = \begin{pmatrix} -\operatorname{sech} u \sin v \\ \operatorname{sech} u \cos v \\ 0 \end{pmatrix}, \tag{3.55}$$

thus the unit normal is defined as

$$\boldsymbol{n} = \frac{\boldsymbol{e}_u \times \boldsymbol{e}_v}{|\boldsymbol{e}_u \times \boldsymbol{e}_v|} = \frac{1}{\operatorname{sech} u \tanh u} \begin{pmatrix} -\operatorname{sech} u \cos v + \operatorname{sech}^3 u \cos v \\ -\operatorname{sech} u \sin v + \operatorname{sech}^3 u \sin v \\ -\operatorname{sech}^2 u \tanh u \end{pmatrix}$$

$$= \begin{pmatrix} -\tanh u \cos v \\ -\tanh u \sin v \\ -\operatorname{sech} u \end{pmatrix}. \tag{3.56}$$

Also, for the first fundamental form on this surface we can write

$$g_{ij} = \boldsymbol{e}_i.\boldsymbol{e}_j = \begin{pmatrix} \boldsymbol{e}_u.\boldsymbol{e}_u & \boldsymbol{e}_u.\boldsymbol{e}_v \\ \boldsymbol{e}_v.\boldsymbol{e}_u & \boldsymbol{e}_v.\boldsymbol{e}_v \end{pmatrix} = \begin{pmatrix} \tanh^2 u & 0 \\ 0 & \operatorname{sech}^2 u \end{pmatrix},$$

$$\Rightarrow g^{ij} = \begin{pmatrix} \dfrac{1}{\tanh^2 u} & 0 \\ 0 & \dfrac{1}{\operatorname{sech}^2 u} \end{pmatrix}. \tag{3.57}$$

Now the second fundamental form coefficients in this case are described as

$$K_{uv} = K_{vu} = -\boldsymbol{n}.\frac{\partial^2 \boldsymbol{r}}{\partial u \partial v} = 0, \tag{3.58}$$

$$\begin{aligned} K_{uu} &= -\boldsymbol{n}.\frac{\partial^2 \boldsymbol{r}}{\partial^2 u} \\ &= \begin{pmatrix} \tanh u \cos v \\ \tanh u \sin v \\ \operatorname{sech} u \end{pmatrix}.\begin{pmatrix} \operatorname{sech} u \tanh^2 \mathrm{u} \cos v - \operatorname{sech}^3 u \cos v \\ \operatorname{sech} u \tanh^2 \mathrm{u} \sin v - \operatorname{sech}^3 u \sin v \\ 2 \operatorname{sech}^2 u \tanh u \end{pmatrix} \\ &= \operatorname{sech} u \tanh u, \end{aligned} \tag{3.59}$$

$$K_{vv} = -\boldsymbol{n}.\frac{\partial^2 \boldsymbol{r}}{\partial^2 v} = \begin{pmatrix} \tanh u \cos v \\ \tanh u \sin v \\ \operatorname{sech} u \end{pmatrix}.\begin{pmatrix} -\operatorname{sech} u \cos v \\ -\operatorname{sech} u \sin v \\ 0 \end{pmatrix} = -\operatorname{sech} u \tanh u\,. \tag{3.60}$$

And K_i^i's are given by

$$K_1 = K_u^u = K_{ui}g^{ui} = K_{uu}g^{uu} + K_{uv}g^{uv} = \frac{1}{\sinh \mathrm{u}}, \tag{3.61}$$

$$K_2 = K_v^v = K_{vi}g^{vi} = K_{vv}g^{vv} + K_{vu}g^{vu} = -\sinh u. \tag{3.62}$$

Using $K_1$and K_2that are principle curvatures, the mean and Gaussian curvatures are written as

$$M = \frac{1}{2}(K_1 + K_2) = \frac{1}{2}(\sinh u - \operatorname{csch} u), \tag{3.63}$$

$$K_G = -1\,. \tag{3.64}$$

Therefore, pseudosphere has constant negative Gaussian curvature. Hence internal potential for the surface is obtained as

$$U(q_1, q_2) = -\frac{\hbar^2}{2m}[M^2 - K_G] = -\frac{\hbar^2}{8m}[(\sinh u - \operatorname{csch} u)^2 + 4]$$

$$= -\frac{\hbar^2}{8m}(\cosh^2 u + \coth^2 u), \tag{3.65}$$

finally, the Schrödinger equation can be written as

$$-\frac{\hbar^2}{2m}\frac{1}{\sqrt{g}}\frac{\partial}{\partial q^i}\left[\sqrt{g}g^{ij}\frac{\partial X_{in}(u,v)}{\partial q^j}\right] - \frac{\hbar^2}{8m}(\cosh^2 u + \coth^2 u)X_{in}(u,v)$$

$$= EX_{in}(u,v). \tag{3.66}$$

That shows Schrödinger equation for a bounded particle on a pseudosphere. Using separation method

$$X_{in}(u,v) = U(u)V(v), \tag{3.67}$$

and Schrödinger equation can be modified as

$$\frac{1}{U}\frac{1}{\operatorname{sech} u \tanh u}\frac{\partial}{\partial u}\left[\frac{1}{\sinh u}\frac{\partial U}{\partial u}\right] + \frac{2mE}{\hbar^2} + \frac{1}{4}(\cosh^2 u + \coth^2 u) \tag{3.68}$$

$$= -\frac{1}{sech^2 u}\frac{1}{V}\frac{\partial^2 V}{\partial v^2}.$$

So

$$\frac{1}{U}\frac{1}{\sinh u}\frac{\partial}{\partial u}\left[\frac{1}{\sinh u}\frac{\partial U}{\partial u}\right] + \frac{2mE}{\hbar^2}\operatorname{sech}^2 \mathrm{u} + \frac{1}{4} + \frac{1}{4\sinh^2 u} = -\frac{1}{V}\frac{\partial^2 V}{\partial v^2}, \tag{3.69}$$

which, should be equal to α^2 where, α is a constant. Therefore

$$X_{in} = U(u)e^{i\alpha v}, \tag{3.70}$$

and $U(u)$ satisfies

$$\frac{1}{\sinh u}\frac{\partial}{\partial u}\left[\frac{1}{\sinh u}\frac{\partial U}{\partial u}\right] + \left(\frac{1}{4} + \frac{1}{4\sinh^2 u} + \frac{2mE}{\hbar^2}\operatorname{sech}^2 u - \alpha^2\right)U(u) = 0\,. \tag{3.70}$$

Chapter 4

CONCLUSION

In classical mechanics, Lagrangian equation and Newton approach give same results, also for two isometric surfaces the equation of motion is identical, in contrast, in quantum scales, on a curve space, Schrödinger equation depends on the mean and Gaussian curvatures. This dependency is more important where in internal potential equation, M as mean curvature appears, which cannot be found just using metric tensor components of surface and its derivatives (unlike Gaussian curvature K_G). It shows disability of Lagrangian in motion of quantum particles on curve spaces.

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