

Constraints in quantum mechanics

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We discuss the introduction of constraints in a system of n noninteracting particles which obey the laws of nonrelativistic quantum mechanics. In this paper the particles are first thought of as being unconstrained (described by the $3n$ Cartesian coordinates of a flat space R), but subject to an external potential V which, in a certain suitable limit, forces the system to remain in a curved subspace V of R . This idea was already employed in a previous work where we have discussed the motion of one constrained particle. It was then shown that in order to obtain a meaningful result the particle wave function should be "uniformly compressed" into a surface (or curve), avoiding, in this way, the tangential forces which correspond to the dissipative constraints of classical mechanics. The resulting Schrödinger equation could then be separated in such a way that the part which contained the surface (or curve) variables was independent of the potential V employed in the constraining process. In the present paper we show that this procedure cannot be carried out for all subspaces V of R in the case of a many-particle system, unless V satisfies a certain geometrical condition. The many-particle Schrödinger equation (as was already the case of the one-particle systems) contains, besides the kinetic energy term, potentials which are not bending invariants, that is, cannot be obtained from the metric tensor g_{ij} of V or its derivatives. This gives rise to different Schrödinger equations for isometric subspaces, in striking contrast with the usual quantization procedures which start from the classical Lagrangian of the constrained system.

I. INTRODUCTION

In a previous paper¹ we have discussed the description provided by quantum mechanics for the motion of a particle subject to one or two independent constraints (motion over a surface or curve). The basic idea was to first consider the particle as freely moving in our ordinary three-dimensional space, but subject to external forces, of increasing intensity, in order to effectively bind the particle to the desired surface or curve. It was then shown that this procedure gives a perfectly well-defined result, provided that some precautions (discussed below) are taken in the definition of the potentials and wave functions. The more interesting feature of the results obtained in this way is the presence, in the resulting Schrödinger equation, of a potential (of geometrical origin) that is not a *bending invariant*, since it cannot be derived from the intrinsic properties of the surface or curve to which the particles are supposed to be attached. This situation can be illustrated by the following example¹: Let us consider a particle moving on a plane surface which is continuously folded (without stretching) around a straight line. Ac-

ording to our results, there will appear during the folding process an attractive potential, of increasing intensity, around the edge of the folded plane which will be responsible, when the plane is completely folded over itself, for the boundary condition associated to the motion of a particle over a half plane. This potential will never be obtained in a usual quantization procedure² starting from the classical Lagrangian of the (already) constrained particle, $L = \frac{1}{2}mg_{ij}\dot{q}^i\dot{q}^j$, because L only depends on the metric properties of the plane surface, which are not affected by the folding process. We can easily see from this example that the treatment of the constraint discussed in Ref. 1 is the most adequate to describe a real-world situation, in which every attempt to reduce the dimension of the system is strongly opposed by the uncertainty relations. This effect, of course, has no counterpart in the classical description of the same problem.

The aim of this paper is to investigate how far we can extend the formalism developed in Ref. 1 for a system containing an arbitrary number of particles. In order to better develop our reasoning let us consider a classical system described by the N generalized coordinates q^1, \dots, q^N obtained from

a system of independent particles, of $N+p$ dimensions, through the use of p -independent spatial constraints. If we call R_{N+p} the Cartesian space of $N+p$ dimensions, described by the coordinates x^α , $\alpha=1,2,\dots,N+p$, we can imagine any configuration of the constrained system as corresponding to a point in a curved subspace V_N of R_{N+p} , defined by the parametric equations:

$$x^\alpha = x^\alpha(q^1, q^2, \dots, q^N) \quad \alpha=1,2, \dots, N+p. \quad (1)$$

Let us assume, for the time being, that we can ascribe to all points of a suitable neighborhood

$\mathcal{N} \subset R_{N+p}$ of V_N the set of coordinates $(q^1, \dots, q^N, u^1, \dots, u^p)$, where $u^1 = u^2, \dots, u^p = 0$ gives the equation for an arbitrary point of V_N (from now on the q 's and u 's will be, respectively, referred to as internal and external coordinates). In order to compress the system from R_{N+p} into an increasingly smaller neighborhood \mathcal{N} (i.e., limiting the range of variation of the u 's around $u^\alpha = 0$, $\alpha=1,2, \dots, p$) we can imagine a family of potentials $V_\lambda(u^1, u^2, \dots, u^p)$, where λ is an appropriate "squeezing parameter" which determines the strength of the constraint:

$$\lim_{\lambda \rightarrow \infty} V_\lambda(u^1, u^2, \dots, u^p) = \begin{cases} 0, & (u^1)^2 + \dots + (u^p)^2 = 0 \\ \infty, & (u^1)^2 + \dots + (u^p)^2 \neq 0. \end{cases} \quad (2)$$

We cannot, however, choose the external coordinates and consequently the potentials V_λ in a completely arbitrary way, since otherwise we could obtain a constrained motion depending on the choice of V_λ , which, naturally, is an unacceptable result. In order to select an appropriate family of potentials V_λ we shall use, as a guiding principle, a property derived from classical mechanics which says that the constrained motion can be uniquely determined only when the constraint forces have a normal direction for all points of V_N (frictionless constraint). Well, since in quantum mechanics we can no longer predict the position of the particles with pointlike accuracy, it is perfectly natural to select only constraint forces which have normal directions in all points of the space R_{N+p} where the system can possibly be found.³ This idea can be put into practice by selecting V_λ such that $\vec{\nabla}[V_\lambda(u^1, \dots, u^p)]$ intersects orthogonally the subspace V_N for all points of the neighborhood \mathcal{N} . This condition can be satisfied (as we shall see in Sec. II) by requiring the orthogonality between internal and external coordinates, that is,

$$\frac{\partial \vec{R}}{\partial u^\alpha} \cdot \frac{\partial \vec{R}}{\partial q^j} = 0, \quad \alpha=1,2, \dots, p, \quad j=1,2, \dots, N \quad (3)$$

where $\vec{R}(q^1, \dots, q^N, u^1, \dots, u^p)$ is the position vector of an arbitrary point in \mathcal{N} . The problem of

representing the constraint by means of the potential $V_\lambda(u^1, \dots, u^p)$, taken in the limit (2), will then be reduced to the question of knowing whether, given a subspace V_N , such a system of coordinates can actually be constructed. This question will be discussed in Sec. II of this paper where we obtain a necessary and sufficient condition for the construction of a coordinate system satisfying the orthogonality condition (3). We note that this condition is identically satisfied for $p=1$ (one constraint: V_N is a *hypersurface* of R_{N+p}) or $N=1$ ($N+p-1$ constraints: V_N is a *curve* of R_{N+p}), which explains why our problem can always be solved for a one-particle system (the case considered in Ref. 1), since in this case we have $N+p=3$, which implies in $N=1, p=2$ (curve) or $N=2, p=1$ (surface).

We obtain in Sec. III the Schrödinger equation for a subspace V_N where (3) can be satisfied. As already stressed in Ref. 1 this construction gives rise to "subspace potentials" $U(q^1, \dots, q^N)$ which depend on *both* mean and total curvatures and therefore cannot be obtained from the metric properties of V_N alone. The question of what happens to the V_N 's where condition (3) cannot be satisfied is also considered. The answer, within the framework of the present ideas, is that every attempt to reduce the system from R_{N+p} to V_N will give a result which depends on the type of external potential V_λ employed during the constraining process.

II. GEOMETRICAL CONSIDERATIONS

Let us consider the possibility of constructing a coordinate system in R_{N+p} such that the internal (q^1, \dots, q^N) and external (u^1, \dots, u^p) variables are mutually orthogonal. Since the internal coordinates are supposed to be a parametrization $\vec{r} = \vec{r}(q^1, \dots, q^N)$ of the curved subspace V_N , we can write for all points of the neighborhood \mathcal{N}

$$\vec{R}(q^1, \dots, q^N, u^1, \dots, u^p) = \vec{r}(q^1, \dots, q^N) + \sum_{\beta=1}^p f^\beta(q^1, \dots, q^N, u^1, \dots, u^p) \hat{n}_\beta(q^1, \dots, q^N), \quad (4)$$

with

$$\det \left[\frac{\partial f^\beta}{\partial u^\alpha} \right] \neq 0, \quad (5)$$

where we have introduced an arbitrary nonsingular coordinate system, u^1, \dots, u^p , in the subspace spanned by the system of normals \hat{n}_β ($\hat{n}_\beta \cdot \hat{n}_\alpha = \delta_{\alpha\beta}$) at every point of V_N . From (4) we have

$$\frac{\partial \vec{R}}{\partial u^\alpha} = \sum_{\gamma=1}^p \frac{\partial f^\gamma}{\partial u^\alpha} \hat{n}_\gamma \quad (6)$$

and

$$\frac{\partial \vec{R}}{\partial q^j} = \frac{\partial \vec{r}}{\partial q^j} + \sum_{\beta=1}^p \left[\frac{\partial f^\beta}{\partial q^j} \hat{n}_\beta + f^\beta \frac{\partial \hat{n}_\beta}{\partial q^j} \right]. \quad (7)$$

Assuming, for a moment, that the u^α 's and q^j 's are orthogonal we can write the classical force \vec{F} due to the potential $V_\lambda(u^1, \dots, u^p)$, in terms of the variables Q^j , $Q^j = q^j$, $j = 1, 2, \dots, N$, $Q^{N+\alpha} = u^\alpha$, $\alpha = 1, 2, \dots, p$, as

$$\begin{aligned} F = \vec{\nabla} V_\lambda &= \sum_{i,l=1}^{N+p} G^{il} \frac{\partial V_\lambda}{\partial Q^i} \frac{\partial \vec{R}}{\partial Q^l} \\ &= \sum_{\alpha,\beta=1}^p G^{N+\alpha, N+\beta} \frac{\partial V_\lambda}{\partial u^\alpha} \frac{\partial \vec{R}}{\partial u^\beta}, \end{aligned} \quad (8)$$

where

$$G_{il} = \frac{\partial \vec{R}}{\partial Q^i} \cdot \frac{\partial \vec{R}}{\partial Q^l}$$

and

$$G^{il} = (G^{-1})_{il}.$$

It is now easy to see from (8) and (6) that \vec{F} is everywhere contained in the normal hyperplanes of V_N as we intuitively anticipated.

Returning to the main object of our calculations we can, from (6) and (7), write condition (3) as

$$\sum_{\gamma=1}^p \frac{\partial f^\gamma}{\partial u^\alpha} \left[\frac{\partial f^\gamma}{\partial q^j} + \sum_{\beta=1}^p \mu_{j;\gamma\beta} f^\beta \right] = 0, \quad (9)$$

where

$$\mu_{j;\gamma\beta} = \hat{n}_\gamma \cdot \frac{\partial \hat{n}_\beta}{\partial q^j} = -\mu_{j;\beta\gamma}. \quad (10)$$

Since the quantity between parentheses in (9) does not contain the index α we can write from (5)

$$\frac{\partial f^\gamma}{\partial q^j} + \sum_{\beta=1}^p \mu_{j;\gamma\beta} f^\beta = 0, \quad (11)$$

for all values of γ and j . According to the well-known theory of partial differential equations,⁴ the integrability condition for the system (11) is given by

$$A_{\gamma\beta;jk} = 0 \quad (12)$$

where

$$\begin{aligned} A_{\gamma\beta;jk} &= \frac{\partial}{\partial q^k} \mu_{j;\gamma\beta} - \frac{\partial}{\partial q^j} \mu_{k;\gamma\beta} \\ &+ \sum_{\sigma=1}^p (\mu_{j;\sigma\gamma} \mu_{k;\sigma\beta} - \mu_{j;\sigma\beta} \mu_{k;\sigma\gamma}). \end{aligned} \quad (13)$$

Condition (12) can be written in a simpler form in terms of the components of the symmetric tensor

$$\Omega_{\sigma,ij} = -\frac{\partial \vec{r}}{\partial q^i} \cdot \frac{\partial \hat{n}_\sigma}{\partial q^j} = \Omega_{\sigma,ji}, \quad (14)$$

which appear in the coefficients of the second fundamental form of the subspace V_N embedded in R_{N+p} . In fact, we know from the results of differential geometry,⁵ that the components $\mu_{j;\gamma\beta}$ are not completely independent, but must satisfy the condition

$$A_{\gamma\beta;jk} = g^{lm} (\Omega_{\gamma;lk} \Omega_{\beta,mj} - \Omega_{\gamma;lj} \Omega_{\beta,mk}), \quad (15)$$

where summations were carried out over repeated coordinate indexes. The integrability condition for our system (11) can then also be obtained by setting the right-hand side of (15) equal to zero. The fact that this condition enables us to integrate the

system (11) leads to a simple geometrical interpretation. Really, since (11) do not contain explicitly the external variables u^1, u^2, \dots, u^p we can get, from a particular solution $f^\gamma(q^1, \dots, q^n, u^1, \dots, u^p)$,

$\gamma=1, 2, \dots, p$, p independent solutions by taking the derivative of f^γ with respect to each of the u^α 's [remember condition (5)]. Calling $\partial f^\gamma / \partial u^\alpha = h_\alpha^\gamma$ we have from (11)

$$\frac{\partial}{\partial q^j} \left[\sum_{\gamma=1}^p h_\alpha^\gamma h_\alpha^\gamma \right] = - \sum_{\gamma, \beta=1}^p \mu_{j; \gamma\beta} (h_\alpha^\gamma h_\alpha^\beta + h_\alpha^\beta h_\alpha^\gamma) = 0, \tag{16}$$

because $\mu_{j; \gamma\beta}$ is antisymmetric in the indexes γ and β [see (10)]. On the other hand, assuming the integrability of (11), we can arbitrarily choose the values taken by f^γ at a fixed point (q_0^1, \dots, q_0^N) of V_N . Let us then select

$$f^\gamma(q_0^1, \dots, q_0^N) = u^\gamma, \quad \gamma=1, 2, \dots, p. \tag{17}$$

[As a matter of fact, since $\mu_{j; \gamma\beta}$ contains only the variables q^j , the external variables will appear as constants of integration in the solution of (11). What we have done in (17) was to choose a Cartesian coordinate system for the normal subspace at the point (q_0^1, \dots, q_0^N) .] If we now consider the behavior of the Jacobian matrix h_α^γ , it is obvious from (16) and (17) that we begin with the identity matrix $h_\alpha^\gamma = \delta_\alpha^\gamma$ at (q_0^1, \dots, q_0^N) , and, although h_α^γ changes from one to another point of V_N , it will always remain an orthogonal matrix. We will profit from this circumstance by introducing the *change of normals*

$$\hat{n}'_\nu = \sum_{\sigma=1}^p h_\nu^\sigma \hat{n}_\sigma, \tag{18}$$

where, due to the orthogonal character of h_ν^σ , the new normals still form an orthogonal basis in every normal subspace of V_N . The tensors $\mu_{j; \nu\rho}$ relative to this new choice of normals are given by

$$\mu'_{j; \nu\rho} = \hat{n}'_\nu \frac{\partial \hat{n}'_\rho}{\partial q^j} = \sum_{\sigma=1}^p h_\nu^\sigma \left[\frac{\partial h_\rho^\sigma}{\partial q^j} + \sum_{z=1}^p \mu_{j; \sigma z} h_\rho^z \right] = 0, \tag{19}$$

since the h_ρ^γ 's satisfy the same system (11) for all values of ρ . In Eq. (19) we have a necessary condition for the orthogonality relation (3): We must have a choice of normals for which $\mu_{j; \sigma\tau}$ vanishes identically; or in other words, the derivative of every normal \hat{n}'_ν must be contained in the tangent subspace for all points of V_N . In this case, as (11) clearly shows, we have the same f^β 's for all points in V_N :

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

Equation (19) is also a sufficient condition, as can be seen by writing (4) in terms of the normals \hat{n}'_ν :

$$\vec{R}(q^1, \dots, q^N; u^1, \dots, u^p) = \vec{r}(q^1, \dots, q^N) + \sum_{\beta=1}^p f^\beta(u^1, \dots, u^p) \hat{n}'_\beta(q^1, \dots, q^N), \tag{20}$$

and obtaining

$$\frac{\partial \vec{R}}{\partial q^j} = \frac{\partial \vec{r}}{\partial q^j} + \sum_{\beta=1}^p f^\beta \frac{\partial \hat{n}'_\beta}{\partial q^j},$$

which, by hypothesis, is orthogonal to all normals \hat{n}'_α and, therefore, to the derivatives $\partial \vec{R} / \partial u^\alpha$ as given in (6).

As a last remark we observe that (12) is always satisfied when V_N is either a *curve* or a *hypersurface* of R_{N+p} . This can be seen from (15), where the first case corresponds to $j=k$ (one internal variable only) and the second to $\beta=\gamma$ (with only one normal, its derivatives must necessarily lie on the tangent subspace).

III. SCHRÖDINGER EQUATION FOR THE CONSTRAINED SYSTEM

In order to write the Schrödinger equation obeyed by our system during the constraining process we shall assume that we can find, in the subspace V_N (to which the coordinates of our system will ultimately belong),

a set of normals \hat{n}'_β satisfying condition (19).⁶ The parametrization of R_{N+p} which holds in a neighborhood \mathcal{N} of V_N will then be written in the form (20)

$$\vec{R}(q^1, \dots, q^N, u^1, \dots, u^p) = \vec{r}(q^1, \dots, q^N) + \sum_{\beta=1}^p u^\beta \hat{n}'_\beta(q^1, \dots, q^N), \quad (21)$$

where we have, for the sake of simplicity, selected Cartesian coordinates for all normal subspaces of V_N . From (21) we obtain⁷

$$\frac{\partial \vec{R}}{\partial u^\alpha} = \hat{n}'_\alpha, \quad \alpha = 1, 2, \dots, p \quad (22)$$

$$\frac{\partial \vec{R}}{\partial q^j} = \frac{\partial \vec{r}}{\partial q^j} - \sum_{\beta=1}^p u^\beta \Omega_{\beta;ij} g^{ik} \frac{\partial \vec{r}}{\partial q^k}, \quad j = 1, 2, \dots, N \quad (23)$$

with

$$g^{ik} = (g^{-1})_{ik}, \quad g_{lm} = \frac{\partial \vec{r}}{\partial q^l} \cdot \frac{\partial \vec{r}}{\partial q^m}. \quad (24)$$

From (22) and (23) the components of the metric tensor G_{lm} are

$$G_{jk} = g_{jk} - 2 \sum_{\beta=1}^p u^\beta \Omega_{\beta;jk} + \sum_{\beta,\gamma=1}^p u^\beta u^\gamma \Omega_{\beta;ij} \Omega_{\gamma;mk} g^{im}, \quad (25)$$

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

with $j, k = 1, 2, \dots, N$; $\alpha, \beta = 1, 2, \dots, p$. The Schrödinger equation in R_{N+p} will then be written as

$$-\frac{\hbar^2}{2m} \frac{1}{\sqrt{G}} \frac{\partial}{\partial Q^i} \left[\sqrt{G} G^{ij} \frac{\partial \psi}{\partial Q^j} \right] + V_\lambda(u^1, \dots, u^p) \psi = i \hbar \frac{\partial \psi}{\partial t}, \quad (26)$$

where $G^{ij} = (G^{-1})_{ij}$, $G = \det(G_{ij})$, and m is the mass of the particles.⁸ Notice that, since the constraining potential depends only on the external variables, the values of V_λ are determined for all points of the neighborhood \mathcal{N} once they are known in one normal subspace chosen at an arbitrary point of V_N . In other words, we have the liberty to choose arbitrarily [as far as (2) is satisfied] the values taken by V_λ in *but one* normal subspace of V_N , the value in the other subspaces being automatically defined by the change in the normals $\hat{n}'_\beta(q^1, \dots, q^N)$. As a matter of fact, this is not an unexpected result, since it agrees with the intuitive idea of tangential forces.

Now we can turn our attention to the solution of (26). Owing to the particular structure of (24) (orthogonal coordinates) we can break up the summation in (26) into two parts: one containing only derivatives with respect to internal variables, and other derivatives with respect to external variables:

$$-\frac{\hbar^2}{2m} \sum_{ij=1}^N \frac{1}{\sqrt{G}} \frac{\partial}{\partial q^i} \left[\sqrt{G} G^{ij} \frac{\partial \psi}{\partial q^j} \right] - \frac{\hbar^2}{2m} \sum_{\alpha=1}^p \left[\frac{\partial^2 \psi}{\partial (u^\alpha)^2} + \frac{\partial}{\partial u^\alpha} (\ln \sqrt{G}) \psi \right] + V_\lambda \psi = i \hbar \frac{\partial \psi}{\partial t}, \quad (27)$$

where we also have used the fact that $G^{N+\alpha, N+\beta} = 0$ for $\alpha \neq \beta$. The next step is to redefine the wave function ψ in a way that is more adequate to describe the physical meaning of the compression process. The first thing we must bear in mind is that we are interested in the probability of finding the internal coordinates of our system within a certain volume element of V_N , independent of the values taken by the external variables u^α . Moreover, we are especially interested in the possibility of writing this same probability as $|\chi_i|^2 \sqrt{g} dq^1 \cdots dq^N$, where χ_i is an internal wave function. This goal can be accomplished by writing the elementary probability dP for the volume element dV in R_{N+p} as

$$\begin{aligned} dP &= |\psi|^2 dV = |\psi|^2 \sqrt{G} dq^1 \cdots dq^N du^1 \cdots du^p \\ &= \left| \psi \left[\frac{G}{g} \right]^{1/4} \right|^2 \sqrt{g} dq \cdots dq^N du^1 \cdots du^p = |\chi|^2 \sqrt{g} dq^1 \cdots dq^N du^1 \cdots du^p, \end{aligned} \quad (28)$$

provided that χ can be separated as $\chi_i(q^j, t) \chi_e(u^\alpha, t)$ (the subscripts i and e stand, respectively, for internal

and external). The Schrödinger equation (27) can now be written in terms of the new wave function χ . After performing elementary calculations we have

$$-\frac{\hbar^2}{2m} \sum_{i,j=1}^N \frac{1}{\sqrt{G}} \frac{\partial}{\partial q^i} \left[\sqrt{G} G^{ij} \frac{\partial}{\partial q^j} \left[\frac{\chi}{\sqrt{h}} \right] \right] - \frac{\hbar^2}{2m} \frac{1}{\sqrt{h}} \sum_{\beta=1}^p \left\{ \frac{\partial^2 \chi}{\partial (u^\beta)^2} + \frac{1}{4h^2} \left[\left(\frac{\partial h}{\partial u^\beta} \right)^2 - 2h \frac{\partial^2 h}{\partial (u^\beta)^2} \right] \chi \right\} + \frac{1}{\sqrt{h}} V_\lambda(u^1, \dots, u^p) \chi = i\hbar \frac{\partial \chi}{\partial t}, \quad (29)$$

where $h = (G/g)^{1/2}$. We are now ready to take into account the effect of the constraining potential $V_\lambda(u^1, \dots, u^p)$. Since in the limit when $\lambda \rightarrow \infty$ [see (2)] the wave function “sees” steep potential barriers in all directions orthogonal to V_N , its value will be significantly different from zero only for a very small range of values of u^α around $u^\alpha = 0, \alpha = 1, 2, \dots, p$. In this case we can safely take $u^\alpha \rightarrow 0$ in all coefficients of Eq. (29), except, of course, in the term $V_\lambda(u^1, \dots, u^p)$. The result from (25) and (29) is

$$-\frac{\hbar^2}{2m} \sum_{i,j=1}^N \frac{1}{\sqrt{g}} \frac{\partial}{\partial q^i} \left[\sqrt{g} g^{ij} \frac{\partial \chi}{\partial q^j} \right] - \frac{\hbar^2}{8m} \sum_{\beta=1}^p \left[\left(\frac{\partial h}{\partial u^\beta} \right)^2 - 2 \frac{\partial^2 h}{\partial (u^\beta)^2} \right]_{u^\alpha=0} \chi - \frac{\hbar^2}{2m} \sum_{\beta=1}^p \frac{\partial^2 \chi}{\partial (u^\beta)^2} + V_\lambda(u^1, \dots, u^p) \chi = i\hbar \frac{\partial \chi}{\partial t}, \quad (30)$$

since, obviously, $h = 1$ in all points of V_N . Setting $\chi = \chi_i(q^j, t) \chi_e(u^\alpha, t)$ we get the separate equations

$$-\frac{\hbar^2}{2m} \sum_{\beta=1}^p \frac{\partial^2 \chi_e}{\partial (u^\beta)^2} + V_\lambda(u^1, \dots, u^p) \chi_e = i\hbar \frac{\partial \chi_e}{\partial t}, \quad (31)$$

$$-\frac{\hbar^2}{2m} \sum_{j,k=1}^N \frac{\partial}{\partial q^j} \left[\sqrt{g} g^{jk} \frac{\partial \chi_i}{\partial q^k} \right] - \frac{\hbar^2}{8m} \sum_{\beta=1}^p \left[\left(\frac{\partial h}{\partial u^\beta} \right)^2 - 2 \frac{\partial^2 h}{\partial (u^\beta)^2} \right]_{u^\alpha=0} \chi_i = i\hbar \frac{\partial \chi_i}{\partial t}. \quad (32)$$

Expression (31) is just the Schrödinger equation in a p -dimensional Cartesian space in the presence of the potential V_λ , and can be ignored in all future calculations. Expression (32), however, is much more interesting, due to the presence of the internal potential

$$U_i(q^1, \dots, q^N) = -\frac{\hbar^2}{8m} \sum_{\beta=1}^p \left[\left(\frac{\partial h}{\partial u^\beta} \right)^2 - 2 \frac{\partial^2 h}{\partial (u^\beta)^2} \right]_{u^\alpha=0}, \quad (33)$$

which depend on the geometrical properties (not necessarily intrinsic) of the subspace V_N embedded in R_{N+p} . The first thing we must take into account in the calculation of U_i is that since only first- and second-order derivatives appear in (33), we do not need an exact expression for h , but only a series expansion up to the second order in the u^α s. Using (25) we obtain, after some lengthy but not too difficult calculations,

$$h = \left(\frac{G}{g} \right)^{1/2} = 1 - \sum_{\beta=1}^p \Omega_{\beta,j}^j u^\beta + \frac{1}{2} \sum_{\beta,\gamma=1}^p (\Omega_{\beta,i}^i \Omega_{\gamma,k}^k - \Omega_{\beta,i}^k \Omega_{\gamma,k}^i) u^\beta u^\gamma + \dots, \quad (34)$$

where $\Omega_{\beta,i}^j$ is the mixed tensor $g^{jl} \Omega_{\beta,il}$. From (34) it follows that

$$\left(\frac{\partial h}{\partial u^\beta} \right)_{u^\alpha=0} = -\Omega_{\beta,j}^j, \quad (35)$$

$$\left(\frac{\partial^2 h}{\partial (u^\beta)^2} \right)_{u^\alpha=0} = \Omega_{\beta,i}^i \Omega_{\beta,k}^k - \Omega_{\beta,i}^k \Omega_{\beta,k}^i.$$

Substituting (35) into (33) we obtain at last

$$U_i(q^1, \dots, q^N) = -\frac{\hbar^2}{8m} (M^2 + 2R), \quad (36)$$

where

$$M = \left[\sum_{\sigma=1}^p (\Omega_{\sigma,j}^j)^2 \right]^{1/2}, \quad (37)$$

and

$$R = \sum_{\sigma=1}^p (\Omega_{\sigma;k}^l \Omega_{\sigma,l}^k - \Omega_{\sigma,l}^l \Omega_{\sigma,k}^k), \quad (38)$$

are, respectively, the mean and total curvatures of V_N as embedded in R_{N+p} . For the particular case of a single-particle subject to one constraint (that is, moving on a surface) we can, using appropriate coordinates, write $\Omega_{\sigma,k}^l = k_\sigma \delta_k^l$, where k_1 and k_2 are the principal curvatures of the surface V_2 in our ordinary space R_3 . From (37) and (38) we have $R = -2k_1k_2$, $M^2 = (k_1 + k_2)^2$, and from (36)

$$U_i(q^1, q^2) = -\frac{\hbar^2}{8m}(k_1 - k_2)^2, \quad (39)$$

which agrees with previous results.¹ Although R depends only on the intrinsic properties of V_N , this is not the case of the mean curvature M , so that two isometric subspaces V_N and V_N^* of R_{N+p} (for which correspondent points can be found with the same g_{ij} 's) will have different internal potentials, and, therefore, different quantum mechanics. As already mentioned in the introduction this result is in strong disagreement with the usual quantization procedures which start from the Lagrangian of the classical motion.

One last remark that must be made about Eq. (3) is as follows: As we have just proved it provides a sufficient condition, in the sense that whenever it holds we can, using a relatively ample class of potentials $V_\lambda(u^1, \dots, u^p)$, obtain a unique Schrödinger equation for the constrained system. Nothing was said, however, on whether (3) was or was not necessary, that is, if a Schrödinger equation can still be obtained even when (3) is not satisfied. Although we do not have a full analytic demonstration there are good reasons to believe that (3) [or (12)] is both necessary and sufficient to obtain a unique Schrödinger equation (at least within the context of the present work). The first reason is based on the fact that if (3) is not satisfied there will appear in (27) crossed terms of the type $\partial^2\psi/\partial q^i\partial u^\alpha$ preventing the separation of the wave function, which seems to be essential in order to have a meaningful limit process. We must also remember that even when the coefficients of the crossed terms vanish in the limit $u^\alpha \rightarrow 0$ [as is the case with the coordinates (21)], the derivatives with respect to external variables go to infinity so that we cannot show, *a priori*, that those terms can be disregarded (as a matter of fact, elementary calculations based on harmonic constraining potentials V_λ predict a finite limit). This same problem can also be seen from the point of view of classical mechanics. In fact, the total energy in terms of

the coordinates (21) is written as

$$E = \frac{1}{2}m \sum_{\alpha=1}^{N+p} (\dot{x}^\alpha)^2 + V_\lambda = \frac{1}{2}m G_{ij} \dot{q}^i \dot{q}^j + \frac{1}{2}m \sum_{\alpha=1}^p (\dot{u}^\alpha)^2 + V_\lambda, \quad (40)$$

where the G_{ij} 's given in (24) depend on both q^i 's and u^β 's. Taking $u^\beta \rightarrow 0$ in the coefficients of the kinetic energy, as required by the constraining process, transforms (40) into

$$E = \frac{1}{2}m g_{ij}(q^1, \dots, q^N) \dot{q}^i \dot{q}^j - \frac{1}{2}m \sum_{\alpha=1}^p (\dot{u}^\alpha)^2 + V_\lambda(u^1, \dots, u^p). \quad (41)$$

Equation (41) is readily separated as

$$E_i = \frac{1}{2}m g_{ki}(q^1, \dots, q^N) \dot{q}^k \dot{q}^l, \quad (42)$$

$$E_e = \frac{1}{2}m \sum_{\alpha=1}^p (\dot{u}^\alpha)^2 + V_\lambda(u^1, \dots, u^p),$$

where each of the equations (42) contain only one kind of coordinate (internal or external). Let us consider what happens when the u^β 's and g^i 's are no longer orthogonal. The result will be the same as in (40) with the term

$$m \sum_{i,\alpha} G_{i,N+\alpha} \dot{q}^i \dot{u}^\alpha$$

added to its last member. The same separation obtained in (41) is still feasible in classical mechanics where we can take $u_\alpha \rightarrow 0$ irrespective of the value taken by \dot{u}_α (or take both of them going to zero if we so desire). However, as is well known, this is no longer possible in quantum mechanics because of the uncertainty relations, and, therefore, we cannot associate separation energies to the internal and external motions.

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¹R. C. T. da Costa, Phys. Rev. A **23**, 1982 (1981).

²For a review of the quantization methods which start from the classical Lagrangian or Hamiltonian, see B. de Witt, Rev. Mod. Phys. **29**, 377 (1957).

³Results found in the literature [e.g., K. S. Cheng, J. Math. Phys. **13**, 1723 (1972)] stating that the limit process employed here gives infinite or meaningless results are due to the disregard of this orthogonality condition.

⁴D. Laugwitz, *Differential and Riemannian Geometry* (Academic, New York, 1965), p. 225.

⁵L. P. Eisenhart, *Riemannian Geometry* (Princeton University Press, Princeton, New Jersey, 1949), p. 190.

⁶Examples where condition (19) [or (12)] cannot be satisfied can be found in every textbook on classical mechanics. Consider, for example, the well-known double pendulum, $x_1 = \cos\theta$, $y_1 = \sin\theta$, $x_2 = \cos\theta + \cos\phi$, $y_2 = \sin\theta + \sin\phi$, as the result of the introduction of two spatial constraints on the four-

dimensional Euclidean space (x_1, y_1, x_2, y_2) . Using the unit normals $\hat{n}_1 = (\cos\theta, \sin\theta, 0, 0)$ and

$$\hat{n}_2 = [1 + \sin^2(\theta - \phi)]^{-1/2}$$

$$\times [\sin(\phi - \theta)\sin\theta, -\sin(\phi - \theta)\cos\theta, \cos\phi, \sin\phi]$$

it is not difficult to show that

$$A_{12,12} = [1 + \sin^2(\phi - \theta)]^{-3/2} \cos(\phi - \theta) \neq 0.$$

⁷See Ref. 5, p. 189.

⁸The case where the particles have different masses m_i can be treated by the change of coordinates $\vec{r}'_i = (m_i/M)^{1/2}\vec{r}_i$, where \vec{r}_i is the vector position of the i th particle, and M the mean mass, leading to the same expression (26) with m substituted by M . The only thing we must keep in mind is that the numbers M/m_i will appear in the diagonal of the metric tensor of R_{N+p} referred to the primed Cartesian coordinates.