On a Quantum Mechanical d'Alembert Principle

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1 Introduction

In classical mechanics, constraints in the configuration space of a mechanical system can be treated using d'Alembert's principle [1]. The procedure of Lagrange which eliminates holonomic time-independent constraints by introducing generalized coordinates can be given natural geometric interpretation in terms of an imbedding $i: M \to \mathbf{R}^n$ of a manifold M (defined as the locus of the constraints) in the original configuration manifold $\mathbf{R}^n$.

As a rule, the d'Alembert principle is considered as an axiom which is a posteriori empirically justified by its successful application to mechanical systems. It can, however, be given theoretical derivation by replacing constraints by a potential which grows large when the system deviates from M [2].

In quantum mechanics, it is apparently impossible to eliminate constraints in this way. However, on the basis of the given holomomic time-independent constraints

$$q^y = 0, \quad y = D+1, \ldots, n, \tag{1}$$

we expect that the Schrödinger equation can be separated into two parts: the first part depending only on Lagrange's generalized coordinates q^b, $b = 1, \ldots, D$, while the other on the mechanically redundant coordinates q^y. The second part would describe arbitrarily rapid oscillations of small amplitude relative to the constraint submanifold M. From the strict quantum mechanical standpoint these oscillations cannot be let frozen like in classical mechanics, since then the Heisenberg uncertainty relations would be violated.

In our note we describe a model situation where a quantum mechanical system in $\mathbf{R}^n$ is confined by a strong potential force to a tubular neighborhood W_ε of constant radius ε of a given submanifold M in $\mathbf{R}^n$. Since the quantal system cannot be strictly localized on M, we investigate whether the restoring forces in the neighbourhood of M would affect the motion of the system along M. We find that the quantum mechanical coupling of transversal motion with the constrained motion leads to a peculiar dependence of the constrained Schrödinger equation (in the zeroth approximation in ε) on the internal as well as external curvature of the submanifold M in $\mathbf{R}^n$. The additional "quantum potential" $-(h^2/2m)U$ vanishes in the classical limit, so it cannot be obtained via the correspondence principle - it represents a purely quantal effect.

We derive the quantum potential in the general case of a compact submanifold M of dimension D embedded in $\mathbf{R}^n$, $D < n$. The cases $D = 1$, $n = 2$, and $D = 2$, $n = 3$ were considered in [3], $D = 1$, $n = 3$ in [4]. Our general resulting U reduces exactly to the results obtained for those special values of D and n.

In order to expose the essential idea in a simple setting, we first consider the case of a particle moving along a planar curve [3] (Sect. 2), and then turn to the general case in Sect.3.

2 Quantum Potential for a Particle Bound to a Planar curve

Let a C^∞ curve C in $\mathbf{R}^2$ be given in parametric form

$$\vec{r} = (x_1, x_2) = \vec{a}(q^1), \tag{2}$$

where q^1 is the Euclidean length $(d\vec{r})^2 = (dq^1)^2$. We assume that C admits a tubular neighbourhood W_ε of constant radius ε. Points of W_ε can be parametrized by (q^1, q^2), $|q^2| < \varepsilon$, such that

$$\vec{r} = \vec{a}(q^1) + q^2\vec{n}(q^1), \tag{3}$$

where $\vec{n}(q)$ denotes the unit normal of C at q^1. The constraining potential with infinitely high equidistant walls

$$V(q^1, q^2) = \begin{cases} 0 & |q^2| < d < \varepsilon \\ \infty & |q^2| > d \end{cases} \tag{4}$$

will be replaced by the boundary conditions

$$\Psi(q^1, d) = 0 = \Psi(q^1, -d), \tag{5}$$

satisfied by $\Psi \in \mathrm{L}^2(W_\varepsilon, dx_1 dx_2)$ – solution of the Schrödinger equation

$$-\frac{\hbar^2}{2m}\triangle\Psi = E\Psi \tag{6}$$

The Laplacian $\triangle = (\partial^2/\partial x_1^2) + (\partial^2/\partial\ x_2^2)$ and the Lebesgue measure $dx_1 dx_2$ will be transformed from Cartesian coordinates (x_1, x_2) to orthogonal curvilinear coordinates (q^1, q^2) in W_ε. For this, we calculate the components g_{ij} of the metric tensor in new coordinates [5]. Using differential equations for the tangent vector $\vec{t} = d\vec{a}/dq^1$ and the normal $\vec{n}$,

$$\frac{d\vec{t}}{dq^1} = -\eta\vec{n}, \quad \frac{d\vec{n}}{dq^1} = \eta\vec{t}, \qquad \vec{t}\cdot\vec{n} = 0, \tag{7}$$

in terms of the curvature $\eta = 1/R$, R being the radius of curvature, we obtain

$$\begin{aligned} g_{11} &= \left(\frac{\partial\vec{r}}{\partial q^1}\right)^2 = \left(\frac{\partial\vec{a}}{\partial q^1} + q^2\frac{\partial\vec{n}}{\partial q^1}\right)^2 = (\vec{t} + q^2\eta\vec{t})^2 = (1 + q^2\eta)^2, \\ g_{22} &= \left(\frac{\partial\vec{r}}{\partial q^2}\right)^2 = \vec{n}^2 = 1, \quad g_{12} = g_{21} = \frac{\partial\vec{r}}{\partial q^1}\cdot\frac{\partial\vec{r}}{\partial q^2} = 0. \end{aligned} \tag{8}$$

Then, denoting $g = \det(g_{ij})$, $\partial_i = \partial/\partial q^i$, we have $g^{1/2} = 1 + q^2\eta$ in W_ε where $|q^2\eta(q^1)| < 1$ and

$$\begin{aligned} \triangle &= g^{-1/2}\partial_1(g^{-1/2}\partial_1) + g^{-1/2}\partial_2(g^{1/2}\partial_2), \\ dx_1 dx_2 &= (g_{11}g_{22})^{1/2}dq^1 dq^2 = g^{1/2}dq^1 dq^2. \end{aligned} \tag{9}$$

In order to have consistent probabilistic interpretation along the curve

$$\int |\Psi|^2 dx_1 dx_2 = \int \left(\int_{-d}^{d} |\Phi|^2 dq^2 \right) dq^1 \tag{10}$$

after integrating over the transversal parameter q^2, we perform the unitary transformation

$$\Phi = g^{1/4}\Psi. \tag{11}$$

Then also the singular term $\partial_2 \Psi$ is eliminated from the Schrödinger equation; we obtain

$$\begin{aligned} g^{1/4}\triangle(g^{-1/4}\Phi) &= \frac{1}{g}\frac{\partial^2\Phi}{(\partial q^1)^2} - \frac{2q^2\eta'}{g^{3/2}}\frac{\partial\Phi}{\partial q^1} - \\ &\quad -\frac{q^2\eta''}{2g^{3/2}}\Phi + \frac{5(q^2\eta')^2}{4g^2}\Phi + \frac{\partial^2\Phi}{(\partial q^2)^2} + \frac{\eta^2}{4g}\Phi. \end{aligned} \tag{12}$$

In the limit $d \to 0$, i. e. $q^2 \to 0$, $g \to 1$, only three terms of zeroth order in q^2 survive, resulting in an approximate separated Schrödinger equation

$$-\frac{\hbar^2}{2m}\left(\partial_1^2 + \frac{1}{4}\eta(q^1)^2\right)\Phi - \frac{\hbar^2}{2m}\partial_2^2\Phi = E\Phi. \tag{13}$$

Solving (13), (5) by the separation of variables $\Phi(q^1, q^2) = \chi(q^1)\varphi(q^2)$ yields

$$\begin{aligned} -\frac{\hbar^2}{2m}\chi'' - \frac{\hbar^2}{2m}U_\chi &= E_1\chi, \\ -\frac{\hbar^2}{2m}\varphi'' &= E_2\varphi, \end{aligned} \tag{14}$$

where $\varphi(\pm d) = 0$, $E = E_1 + E_2$, and the quantum potential is

$$-\frac{\hbar^2}{2m}U = -\frac{\hbar^2\eta(q^1)^2}{8m}. \tag{15}$$

The probability density to find the particle somewhere along C is given (if φ is normalized) by

$$|\chi(q_1)|^2 \int_{-d}^{d} \left|\varphi(q^2)\right|^2 dq^2 = |\chi|^2. \tag{16}$$

For instance, the normalized ground state wave function of transversal oscillation is

$$\varphi = d^{-1/2}\cos(\pi q^2/2d) \tag{17}$$

with divergent behaviour of $\varphi'(\pm d) \sim d^{-3/2}$ when $d \to 0$, and

$$E_2 = -\frac{\hbar^2}{2m}\left(\frac{\pi}{2d}\right)^2. \tag{18}$$

Let us note that similar results can be obtained with a constraining oscillator potential $U = \frac{1}{2}\omega^2(q^2)^2$ in the limit $\omega \to \infty$.

3 Quantum Potential for a General Submanifold

Let a C^∞ manifold M of dimension $D < n$ be isometrically embedded in a bigger configuration space $\mathbf{R}^n$ equipped with Euclidean metric. We also assume that M admits a tubular neighbourhood W_ε of constant radius ε (W_ε excists for some $\varepsilon > 0$ whenever M is compact).

If x_μ, $\mu = 1, \ldots, n$, are Cartesian coordinates in $\mathbf{R}^n$, and M is covered by a system of coordinate neighbourhoods $(V, q^a,\ a = 1, \ldots, D)$, then the points of M can be represented locally by

$$x_\mu = a_\mu(q^b), \quad \text{or} \quad \vec{r} = \vec{a}(q^b) \tag{19}$$

in vector notation. We shall identify vector fields X in M and their images $i_* X$ under the embedding $i\colon M \to \mathbf{R}^n$; if $X \in \mathcal{X}(M)$ and is locally given by $X = X^a \partial_a$, $\partial_a = \partial/\partial q^a$, then X can also be expressed in $\mathcal{X}(\mathbf{R}^n)$ as

$$X = B^\mu_b X^b \partial_\mu, \quad \text{where} \quad \partial_\mu = \partial/\partial x_\mu, \quad B^\mu_b = \partial_b a_\mu. \tag{20}$$

For the Euclidean metric $\delta_{\mu\nu}$, the induced metric $\mathring{g}$ on M is

$$\mathring{g}_{ba} = \delta_{\mu\lambda} \frac{\partial a_\mu}{\partial q^b} \frac{\partial a_\lambda}{\partial q^a} = \delta_{\mu\lambda} B^\mu_b B^\lambda_a = \vec{B}_b \cdot \vec{B}_a. \tag{21}$$

In $W_\varepsilon \subset \mathbf{R}^n$ we introduce special local coordinates q^i, $i = 1, \ldots, n$, based on M [6]:

$$x_\mu = a_\mu(q^a) + q^y \underset{y}{n}_\mu \quad (y = D+1, \ldots, n) \tag{22}$$

where $\{\underset{y}{\vec{n}}\}$ is a moving orthonormal frame in the normal bundle over M,

$$\underset{y}{\vec{n}} \cdot \frac{\partial \vec{a}}{\partial q^a} = 0, \quad \underset{y}{\vec{n}} \cdot \underset{x}{\vec{n}} = \delta_{yx}. \tag{23}$$

In these coordinates, the metric tensor g takes the form

$$(g_{ji}) = \begin{pmatrix} g_{ba} & 0 \\ 0 & \delta_{yx} \end{pmatrix} \tag{24}$$

where

$$g_{ba} = \frac{\partial x_\mu}{\partial q^b} \frac{\partial x_\lambda}{\partial q^a} \delta_{\mu\lambda} = \left(\partial_b \vec{a} + q^y \partial_b \underset{y}{\vec{n}} \right) \cdot \left(\partial_a \vec{a} + q^x \partial_a \underset{x}{\vec{n}} \right). \tag{25}$$

The constraining potential with infinitely high equidistant walls is replaced by the boundary condition

$$\Psi(q^i) = 0 \quad \text{whenever} \quad q^y q_y = d^2,\ d < \varepsilon, \tag{26}$$

imposed on $\Psi \in \mathrm{L}^2(W_\varepsilon, d^n x)$ – solution of the Schrödinger equation

$$-\frac{\hbar^2}{2m} \triangle \Psi = E\psi. \tag{27}$$

The Laplacian $\triangle = \partial_\mu \partial_\mu$ and the Lebesgue measure $d^n x$ are transformed from Cartesian coordinates x_μ to the coordinates q^i in W_ε:

$$\begin{gathered}\triangle\Psi = g^{-1/2}\partial_b\left(g^{ba}g^{1/2}\partial_a\Psi\right) + g^{-1/2}\partial_y\left(g^{1/2}\partial_y\Psi\right),\\ d^n x = g^{1/2}d^n q\end{gathered} \tag{28}$$

where $g = \det(g_{ba})$, $(g^{ba}) = (g_{ba})^{-1}$.

For a consistent probabilistic interpretation on M we factorize $g = \mathring{g}\gamma$ and perform a unitary transformation

$$\Phi = \gamma^{1/4}\Psi \tag{29}$$

so that

$$\int |\Psi|^2 d^n x = \int \left(\int_{q_y q_y \le d^2} |\Phi|^2 dq^{D+1}\dots dq^n \right) \mathring{g}^{1/2} dq^1 \dots dq^D. \tag{30}$$

This transformation also eliminates the terms $\partial_y \Psi$ in the Schrödinger equation which are divergent in the limit $d \to 0$. Using (24), (28), the Schrödinger equation (27) takes the form

$$\begin{gathered}-\frac{\hbar^2}{2m}\mathring{g}^{-1/2}\gamma^{-1/4}\partial_b\left(g^{ba}\mathring{g}^{1/2}\gamma^{1/2}\partial_a(\gamma^{-1/4}\Phi)\right) -\\ -\frac{\hbar^2}{2m}\sum_y\left(\partial_y^2\Phi + \left[-\frac{1}{4}\partial_y^2\ln\gamma - \frac{1}{16}(\partial_y\ln\gamma)^2\right]\Phi\right) = E\Phi,\end{gathered} \tag{31}$$

which separates in the limit $q^y \to 0$:

$$-\frac{\hbar^2}{2m}\mathring{\triangle}\Phi - \frac{\hbar^2}{2m}U\Phi - \frac{\hbar^2}{2m}\sum_y \partial_y^2\Phi = E\Phi. \tag{32}$$

Here the quantum potential is given by

$$-\frac{\hbar^2}{2m}U = \frac{\hbar^2}{8m}\lim_{q_y\to 0}\sum\left[\partial_y^2\ln\gamma + \frac{1}{4}(\partial_y\ln\gamma)^2\right] \tag{33}$$

where

$$\gamma = \mathring{g}^{-1}\det\left[\left(\partial_b\vec{a} + q^y\partial_b\underset{y}{\vec{n}}\right)\cdot\left(\partial_a\vec{a} + q^x\partial_a\underset{x}{\vec{n}}\right)\right]. \tag{34}$$

Further calculation of (33) uses the Weingarten formula [7] for $X \in TM$, $\xi \in TM^\perp$, decomposing $\nabla_X\xi$ uniquely into its tangent and normal parts,

$$\nabla_X\xi = -A_\xi X + D_X\xi \tag{35}$$

with

$$\mathring{g}(A_\xi X, Y) = g(H(X,Y),\xi), \tag{36}$$

$H(X,Y) = (\nabla_X Y)_n$ being the second fundamental form of M in $\mathbf{R}^n$:

$$H: TM \times TM \to TM^\perp : (\underset{b}{\vec{e}}, \underset{a}{\vec{e}}) \mapsto \vec{H}_{ba} = \underset{y}{H}{}_{ba}\underset{y}{\vec{n}}. \tag{37}$$

Since all normal fields $\underset{y}{\vec{n}}$ can be chosen parallel in the normal bundle, $D_X\underset{y}{\vec{n}} = 0$, we find in our local coordinates

$$\partial_c\underset{y}{\vec{n}} = -\underset{y}{H}{}_{cb}\vec{B}^b, \tag{38}$$

where the coefficients of the second fundamental form are given by

$$\underset{y}{H}_{cb} = (\partial_c \partial_b \vec{a}) \cdot \underset{y}{\vec{n}}. \tag{39}$$

We calculate

$$\begin{aligned} \partial_y g_{ba} &= -2\underset{y}{H}_{ba} + (\underset{y}{H}_b{}^c \underset{x}{H}_{ac} + \underset{x}{H}_b{}^c \underset{y}{H}_{ac}) q^x, \\ \partial_y^2 g_{ba} &= 2\underset{y}{H}_b{}^c H_{ac}, \end{aligned} \tag{40}$$

so, since $\partial_y \ln g = g^{ba} \partial_y g_{ba}$, we obtain

$$\begin{aligned} \lim_{q_y \to 0} \partial_y \ln g &= -2 \mathrm{Tr}\, \underset{y}{H}, \quad \underset{y}{H} = (\underset{y}{H}_{ba}) \\ \lim_{q_y \to 0} \sum_y (\partial_y \ln g)^2 &= 4 \sum_y (\mathrm{Tr}\, \underset{y}{H})^2, \\ \lim_{q_y \to 0} \sum_y \partial_y^2 \ln g &= -2 \sum_y \mathrm{Tr}\, (\underset{y}{H}^2). \end{aligned} \tag{41}$$

Inserting this into (33) we finally have the quantum potential

$$-\frac{\hbar^2}{2m} U = -\frac{\hbar^2}{2m} \sum_y \left[\tfrac{1}{2} \mathrm{Tr}\, (\underset{y}{H}^2) - \frac{1}{4} (\mathrm{Tr}\, \underset{y}{H})^2 \right]. \tag{42}$$

It can be expressed in terms of the intrinsic *scalar curvature* of M

$$R = \underset{y}{H}_b{}^b \underset{y}{H}_a{}^a - \underset{y}{H}_{ba} \underset{y}{H}^{ba} \tag{43}$$

and the extrinsic *mean curvature* of M in $\mathbf{R}^n$ $\eta = (\vec{\eta} \cdot \vec{\eta})^{1/2}$, or the mean curvature vector

$$\vec{\eta} = \frac{1}{D} \underset{y}{H}_a{}^a \underset{y}{\vec{n}} \tag{44}$$

as

$$\boxed{-\frac{\hbar^2}{2m} U = \frac{\hbar^2}{4m} R - \frac{\hbar^2}{8m} D^2 \eta^2.} \tag{45}$$

Upon using the separation Ansatz $\Phi = \chi(q^a) \varphi(q^y)$ we get

$$\begin{aligned} -\frac{\hbar^2}{2m} \mathring{\Delta} \chi - \frac{\hbar^2}{2m} U \chi &= E_1 \chi, \\ -\frac{\hbar^2}{2m} \sum_y \partial_y^2 \Phi &= E_2 \Phi, \quad E = E_1 + E_2. \end{aligned} \tag{46}$$

Then the probability to find the system localized in a subset B of M is given by

$$\int_B |\chi(q^a)|^2 \mathring{g}^{1/2} d^D q \int |\varphi(q^y)|^2 dq^{D+1} \ldots dq^n = \int_B |\chi|^2 \mathring{g}^{1/2} d^D q \tag{47}$$

depending only on the embedding of M (provided φ is normalized).

Table 1: Quantum potential in special cases

(R_b = principal radii of curvature)

D	n	$-\frac{\hbar^2}{2m}U$
1	n	$-\frac{\hbar^2}{8m}\eta^2$
2	3	$-\frac{\hbar^2}{8m}\left(\frac{1}{R_1}-\frac{1}{R_2}\right)^2$
$n-1$	n	$-\frac{\hbar^2}{4m}\sum_{b=1}^{D}\frac{1}{R_b^2}+\frac{\hbar^2}{8m}\left(\sum_{b=1}^{D}\frac{1}{R_b}\right)^2$
S^{n-1}	R^n	$(n-1)(n-3)\frac{\hbar^2}{8mR^2}$
S^2	R^3	0

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