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A complete perturbative expansion for quantum mechanics with constraints

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Abstract. We discuss the motion of a quantum-mechanical system constrained to move on an arbitrary submanifold M of its configuration space R^n by a real confining potential. A complete perturbative expansion for the Hamiltonian describing the dynamics of the system is obtained in terms of the quantities characterizing the *intrinsic* and *extrinsic geometric properties* of the constraint's surface M. In accordance with Heisenberg's principle the zeroth-order term of the expansion represents strong fluctuations of the system in directions normal to M, whereas the first-order term is naturally interpreted as the Hamiltonian describing the effective dynamics along the constraint's surface. The effective motion on M results in coupling with *Abelian/non-Abelian gauge fields* and *quantum potentials*. The rest of the perturbative expansion allows one to take into account further interactions between normal and effective degrees of freedom. As a concrete example we consider the dynamics of an electron constrained on a circle by a hypothetical semiconductor device. Dunham's expansion for the rotovibrational energy of a rigid diatom is also obtained.

1. Introduction

The quantum-mechanical description of constrained systems is extremely important in physics and since the early days of quantum mechanics several techniques have been developed to deal with this matter. A fundamental contribution was made by Dirac [1]. His idea, geometrical in nature, consists of removing the redundant degrees of freedom by the construction of a consistent Hamiltonian formalism for the constrained classical theory and proceeding then to its quantization. Other noteworthy approaches have been developed by Schwinger, Peierls by using variational arguments and by De Witt, Faddeev, Popov by means of a Lagrangian formalism and path integral techniques. The common feature to all these methods is that the reduction of the dynamics is studied without considering the physical mechanism, if there is one, producing the confinement to the constraint's surface. Nevertheless, in the study of a constrained quantum-mechanical system we have to distinguish between the kind of constraints which may appear in the formulation of a dynamical theory, which we will refer to as *formal constraints*, and the constraints which may be produced by a real potential confining the motion of the system to a submanifold of its configuration space, which we will call *real constrains*. Concrete examples of the latter are electrons constrained to move on a plane or on a line by a semiconductor device of the same kind of that used in the quantum Hall effect, or a rigid molecule in which the Born–Oppenheimer potential behaves as a potential confining the motion from the nuclear configuration space R^{3N} to the submanifold $SO(3)$. Whereas the method of Dirac and

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followers is probably indispensable for the treatment of formal constraints, ordinary quantum mechanics is sufficient to give an accurate description of real constraints. Furthermore, the techniques developed for *formal constrains* turn out to be inadequate for the treatment of *real constraints,* introducing non-physical ambiguities and causing some effects to be ignored.

Let us consider, for example, a particle constrained to move on an arbitrary surface Σ embedded in the three-dimensional Euclidean space R^3. The reduction of the classical theory is straightforward. Introducing coordinates x^1, x^2 parametrizing the surface and denoting the metric induced on Σ from R^3 by $g_{\mu\nu}$, $\mu, \nu = 1, 2$, the system is described by the Lagrangian $\mathcal{L} = \frac{1}{2} g_{\mu\nu} \dot{x}^\mu \dot{x}^\nu$. Defining the generalized momenta $p_\mu = \partial \mathcal{L} / \partial \dot{x}^\mu$, we obtain the Hamiltonian $\mathcal{H} = \frac{1}{2} g^{\mu\nu} p_\mu p_\nu$, where $g^{\mu\nu}$ denotes the inverse of the metric. The quantization of $\mathcal{H}$ contains ordering ambiguities which are not completely removed by the required covariance of the theory. As was first observed by De Witt [2], in constructing the Hamiltonian operator we are free to add to minus one half the Laplacian Δ a term proportional to the scalar curvature R of the surface,

$$\mathcal{H} = -\tfrac{1}{2}\Delta + \alpha R. \tag{1}$$

Different quantization schemes produces different values for the constant α. α may not be determined unambiguously, as it depends essentially on a choice of ordering. On the other hand, the reduction of the motion of a particle to a surface is by no means an academic problem. Devices producing the confinement of electrons on a plane are widely studied in physics [3], and we may consider using the same techniques to constrain a particle on an arbitrary surface Σ. How then do we determine then the constant α? In addressing the solution of the problem, it is convenient to abandon the formal treatment of the constraint, thinking instead of the physical mechanism producing the confinement of the particle on the surface. The analysis of devices used in the quantum Hall effect suggests that the confinement is produced by a potential presenting a deep minimum relative to the constraint surface and depending only on the coordinate normal to it [4–6]. Proceeding along these lines, Jensen and Koppe [7] first gave a realistic description of the motion of a particle on a surface embedded in R^3. In accordance with Heisenberg's principle, the confinement causes the particle to fluctuate very strongly in the direction normal to the surface so that the spectrum of the system is described to a first approximation by that of the confining potential. Relative to each level the effective Hamiltonian describing the motion along the surface may then be unambiguously obtained as (see [7] and the discussion below)

$$\mathcal{H} = -\tfrac{1}{2}\Delta + \tfrac{1}{4}R - \tfrac{1}{8}\xi^2 \tag{2}$$

where ξ is the extrinsic mean curvature of the surface Σ. The analysis has to be completed by considering the interactions between the degrees of freedom normal to the surface and those parallel to it. The case of a wire embedded in R^3 has also been considered by many authors [8].

From this simple example we learn that in the treatment of a real constraint we cannot disregard the physical mechanism producing the confinement to the constraint's surface. A formal treatment of the constraint produces the appearance of unphysical ambiguities and neglects contributions connected with the extrinsic geometrical properties of the constraint's surface.

In this paper we present a complete perturbative description of a system constrained to move on a submanifold of its configuration space R^n by a confining potential V_C. Generalizing the example of the surface embedded in R^3 we require V_C to satisfy two very general conditions:

(C1) V_C presents a deep minimum relative to the constraint's surface,
(C2) V_C depends only on coordinates normal to the constraint's surface.

Adapting coordinates to the constraint in section 2, a complete perturbative expansion for the Hamiltonian describing the motion of the system is obtained in section 3. In accordance with Heisenberg's principle, the zeroth-order term of the expansion takes into account the fluctuations of the system in the directions normal to the constraint's surface. The first-order term, already discussed in [5,6,9], describes the effective constrained dynamics while the rest of the perturbative expansion describes the interactions between normal and effective degrees of freedom. The effective dynamics results in being coupled with Abelian/non-Abelian gauge fields and quantum potentials induced by the intrinsic and extrinsic geometrical properties of the constraint's surface. This phenomenon very much resemble Berry's analysis of the adiabatic approximation [10] and considering the reduction of motion to a submanifold M by means of a confining potential is an adiabatic approximation after all, the coordinates normal and tangential to the constraint's surface being considered as *fast* and *slow* degrees of freedom. Nevertheless, the mechanism producing the coupling with gauge fields and quantum potentials in the discussion of a real constraint is different from that considered by Moody, Shapere and Wilczek [11], Jackiw [12] and Berry [13]. In that context the embedding of the slow-coordinate space in the total configuration space is geometrically trivial, whereas this non-triviality lies at the heart of the mechanism appearing in the treatment of real constraints.

We want to point out that the constrained quantum dynamics is characterized by the whole perturbative expansion, the effective dynamics on the constraint surface representing only the leading term. In contrast to what happens in the classical description, the explicit form of the potential realizing the constraint leaves traces in the effective dynamics and in the spectrum of the system and therefore may not be neglected. This is illustrated by two examples in sections 5 and 6. Section 7 contains our conclusions.

2. Geometrical preliminaries

In what follows we identify the constraint surface with a smooth m-dimensional submanifold M of the configuration space R^n. Denoting by $\Phi : M \to R^n$ the embedding of M in R^n and by $n^1(x), n^2(x), \ldots, n^{n-m}(x)$ a smooth assignment of $(n-m)$ orthonormal vectors normal to M in every point $x \in M$, an *adapted-coordinate frame* may be introduced by using coordinates $x^\mu, \mu = 1, \ldots, m$, on M, plus the distances $y^i, i = m+1, \ldots, n$, along the geodetics leaving M with speed n^i. In a 'sufficently close' neighbourhood of M the frame $\{x^\mu, y^i; \mu = 1, \ldots, m, i = i = m+1, \ldots, n\}$ is well defined and its relation with the Cartesian coordinates $r = (r^1, \ldots, r^n)$ of R^n is given by

$$r = \Phi(x^\mu) + y^i n^i(x^\mu). \tag{3}$$

It is important to realize that the embedding of M in R^n is completely characterized by the assignment of some tensorial quantities on M [14]. In an adapted-coordinate frame these may be easily constructed as follows:

$$g_{\mu\nu} = t_\mu \cdot t_\nu \qquad \textit{induced metric (first fundamental form)}$$
$$\alpha^i_{\mu\nu} = n^i \cdot \partial_\nu t_\mu \qquad \textit{second fundamental form}$$
$$A^{ij}_\mu = n^i \cdot \partial_\mu n^j \qquad \textit{normal fundamental form}$$

where the $t_\mu = \partial_\mu \Phi$ denote the tangent vectors to M associated with the chosen coordinate frame and the dot denotes the standard scalar product in R^n.

The choice of an adapted-coordinate frame is obviously not unique. An arbitrary-coordinate transformation on M as well as a point-dependent rotation of the normal vectors $n^i(x)$ transforms an adapted-coordinate frame into an adapted-coordinate frame. Whereas varying the choice of the coordinates x^μ causes $g_{\mu\nu}$, $\alpha^i_{\mu\nu}$ and A^{ij}_μ to transform as tensors of M, the variation of normal vectors $n^i(x)$ by a rotation $R^{kl}(x)$ makes $\alpha^i_{\mu\nu}$ to transform as a $SO(n-m)$ vector but A^{ij}_μ as a $SO(n-m)$ gauge connection

$$A^{ij}_\mu \longrightarrow \mathcal{R}^{ik}A^{kl}_\mu\mathcal{R}^{jl} + \mathcal{R}^{ik}\partial_\mu\mathcal{R}^{jk}. \tag{4}$$

The normal fundamental form A^{ij}_μ actually represents the connection induced by R^n on the normal bundle of M, $TM^\perp$.

The metric G_{IJ}, $I, J = 1, \ldots, n$ of R^n in the adapted-coordinate frame $\{x^\mu, y^i\}$ is written as

$$G_{IJ} = \begin{pmatrix} \gamma_{\mu\nu} + y^k y^l A^{kh}_\mu A^{lh}_\nu & y^k A^{jk}_\mu \\ y^k A^{ik}_\nu & \delta^{ij} \end{pmatrix} \tag{5}$$

where, introducing the matrix η by $\eta^\mu_\nu = y^i g^{\mu\rho}\alpha^i_{\rho\nu}$, the matrix γ may be written as

$$\gamma_{\mu\nu} = g_{\mu\rho}(\mathbb{1} - \eta)^\rho_\sigma(\mathbb{1} - \eta)^\sigma_\nu. \tag{6}$$

The determinant $|G|$ of G_{IJ} coincides with that of the matrix γ, $|\gamma|$, and the inverse of the metric tensor may be calculated as

$$G^{IJ} = \begin{pmatrix} \gamma^{\mu\nu} & \gamma^{\mu\rho}y^k A^{kj}_\rho \\ \gamma^{\nu\rho}y^k A^{ki}_\rho & \delta^{ij} + y^k y^l A^{ik}_\rho A^{jl}_\sigma \gamma^{\rho\sigma} \end{pmatrix}. \tag{7}$$

3. The perturbative expansion

We come now to the dynamical aspect of the problem. The quantization of the system is performed very easily and unambiguously in R^n, before considering the constraint. In a Cartesian-coordinate frame $\{r^I; I = 1, \ldots, n\}$, dynamics is described by

$$\mathcal{H} = -\tfrac{1}{2}\partial_I\partial_I + V_C \tag{8}$$

where V_C is the potential realizing the constraint. $\mathcal{H}$ acts on wavefunctions $\psi \in \mathcal{L}^2(R^n)$ normalized with the condition

$$\int |\psi|^2 \, \mathrm{d}r^n = 1. \tag{9}$$

In an *adapted-coordinate frame* $\{x^\mu, y^i; \mu = 1, \ldots, m, i = m+1, \ldots, n\}$ the Hamiltonian (8) takes the form

$$\mathcal{H} = -\frac{1}{2|G|^{1/2}}\partial_I G^{IJ}|G|^{1/2}\partial_J + V_C \tag{10}$$

and the normalization condition (9) transforms to

$$\int |\psi|^2 |G|^{1/2} \, \mathrm{d}x^m \, \mathrm{d}y^{(n-m)} = 1. \tag{11}$$

Since we are looking for an effective dynamics on the submanifold M we find it natural to perform a similitude transformation in such a way that the wavefunctions are correctly normalized in $\mathcal{L}^2(M)$ instead of $\mathcal{L}^2(R^n)$. The aim is achieved by

$$\psi \to \frac{|G|^{1/4}}{|g|^{1/4}}\psi \qquad \mathcal{H} \to \frac{|G|^{1/4}}{|g|^{1/4}}\mathcal{H}\frac{|g|^{1/4}}{|G|^{1/4}} \tag{12}$$

where $|g|$ denotes the determinant of the metric $g_{\mu\nu}$ induced on M. Considering the explicit form (7) of the inverse metric G^{IJ} and introducing $\hat{\partial}_\mu = \partial_\mu + iA^{ij}_\mu L_{ij}/2$, where $L_{ij} = -i(y^i\partial_j - y^j\partial_i)$ are the $SO(n-m)$ generators, the Hamiltonian (10) takes the quite complicated form

$$\mathcal{H} = -\frac{1}{2|\gamma|^{1/4}}\partial_i|\gamma|^{1/2}\partial_i\frac{1}{|\gamma|^{1/4}} - \frac{1}{2|g|^{1/4}|\gamma|^{1/4}}\hat{\partial}_\mu\gamma^{\mu\nu}|\gamma|^{1/2}\hat{\partial}_\nu\frac{|g|^{1/4}}{|\gamma|^{1/4}} + V_C. \tag{13}$$

At this point, and only at this point, the constraint is imposed by considering conditions C1 and C2. Condition C1 ensures that the potential V_C may be replaced by its power expansion around the minimum $\vec{y} = 0$. Condition C2 states that there exists an adapted-coordinate frame in which V_C only depends on the normal coordinates $\vec{y}$. Without loss of generality the constant term of the expansion may be neglected and the quadratic term diagonalized by means of a point-independent rotation in the normal space

$$V_C(\vec{y}) = \frac{1}{2\epsilon^2}\omega^{i2}y^{i2} + a_{ijk}y^iy^jy^k + b_{ijkl}y^iy^jy^ky^l + \cdots . \tag{14}$$

The scale of the proper frequencies ω^i has been readsorbed in the dimensionless parameter ϵ^{-1}. The smaller ϵ the deeper is the minimum of V_C and the more the system is squeezed on the constraint's surface.

The parameter ϵ appears as a natural perturbative parameter in the theory and, rescaled the normal coordinates by $\vec{y} \to \epsilon^{1/2}\vec{y}$, a perturbative theory may be set up by expanding the Hamiltonian (13) in powers of ϵ

$$\epsilon\mathcal{H} = H^{(0)} + \epsilon H^{(1)} + \epsilon^{3/2}H^{(3/2)} + \epsilon^2 H^{(2)} + \cdots$$
$$+\epsilon^{5/2}a_{ijk}y^iy^jy^k + \epsilon^3 b_{ijkl}y^iy^jy^ky^l + \cdots . \tag{15}$$

The constants $a_{ijk}, b_{ijkl}, \ldots$, appearing in the expansion of the confining potential are such that the second, third and further terms of the right-hand side of (14) are small compared to the first term and in this sense are ϵ-dependent. In practical applications they appear in the perturbative expansion as independent parameter so that, for example, $\epsilon^{5/2}a_{ijk}y^iy^jy^k$ is not in general of order $\epsilon^{5/2}$, its magnitude depending on the explicit form of the potential V_C. The zeroth- and first-order terms of the expansion (15) has been extensively discussed in [5].

In accordance with Heisenberg principle the zeroth-order dynamics depends only on the normal degrees of freedom

$$H^{(0)} = \tfrac{1}{2}\left(-\partial_i\partial_i + \omega^{i2}y^{i2}\right) \tag{16}$$

describing a system of $(n-m)$ uncoupled harmonic oscillators with frequencies $\omega^{m+1}, \ldots, \omega^n$.

More surprising results follow from the analysis of the first-order term

$$H^{(1)} = -\frac{1}{2|g|^{1/2}}\left(\partial_\mu + \frac{i}{2}A^{ij}_\mu L_{ij}\right)g^{\mu\nu}|g|^{1/2}\left(\partial_\nu + \frac{i}{2}A^{kl}_\nu L_{kl}\right) + Q^{(1)}(x) \tag{17}$$

where the potential $Q^{(1)}$ may be expressed in terms of the intrinsic scalar curvature R and the extrinsic mean curvature ξ as

$$Q^{(1)}(x) = \tfrac{1}{4}R(x) - \frac{m^2}{8}\xi^2(x). \tag{18}$$

Apart from the potential term $Q^{(1)}$, $H^{(1)}$ is proportional to the Laplace operator on M coupled to the motion in normal directions by means of the minimal interaction with the

gauge field $A_\mu^{ij}L_{ij}/2$. It is therefore resonable to expect that in a perturbative picture $H^{(1)}$ describes the effective dynamics on M. This has actually been found in [5]. The surprising result, unexpected and unrecoverable by means of a formal treatment of constraints, is that the effective dynamics is coupled with gauge fields and quantum potentials induced by the intrinsic and extrinsic geometrical properties of the constraint's surface. The physical relevance of such a geometry-induced dynamical structure has recently been discussed in [6], showing how this phenomenon is observable in the effective rotational motion of some simple polyatomic molecules.

Since we are interested in a realistic description of a constrained microscopic system we never consider the limit $\epsilon \to 0$. ϵ is a small but finite parameter, its magnitude depending on the characteristics of the system under consideration. It is therefore very important to know the explicit expression of further terms of the expansion (15) in order to predict the spectrum of the system with adequate precision.

To evaluate the explicit expression of the generic term of the expansion (15), we start by observing that the first and second terms of the Hamiltonian (13) may be rewritten solely in terms of $\gamma^{\mu\nu}$ and $\ln|\mathbb{1}-\eta|$ as

$$-\frac{1}{2|\gamma|^{1/4}}\partial_i|\gamma|^{1/2}\partial_i\frac{1}{|\gamma|^{1/4}} = -\tfrac{1}{2}\partial_i\partial_i + \tfrac{1}{4}(\partial_i\partial_i \ln|\mathbb{1}-\eta|) + \tfrac{1}{8}(\partial_i \ln|\mathbb{1}-\eta|)(\partial_i \ln|\mathbb{1}-\eta|)$$

and

$$-\frac{1}{2|g|^{1/4}|\gamma|^{1/4}}\hat{\partial}_\mu\gamma^{\mu\nu}|\gamma|^{1/2}\hat{\partial}_\nu\frac{|g|^{1/4}}{|\gamma|^{1/4}} = -\tfrac{1}{2}\hat{\nabla}_\mu\gamma^{\mu\nu}\hat{\nabla}_\nu + \tfrac{1}{4}\left(\hat{\nabla}_\mu\gamma^{\mu\nu}\hat{\nabla}_\nu \ln|\mathbb{1}-\eta|\right)$$
$$+\tfrac{1}{8}\gamma^{\mu\nu}\left(\hat{\nabla}_\mu \ln|\mathbb{1}-\eta|\right)\left(\hat{\nabla}_\nu \ln|\mathbb{1}-\eta|\right)$$

where, denoting by ∇_μ the covariant derivative associated with the connection induced on M,

$$\hat{\nabla}_\mu = \nabla_\mu + \frac{\mathrm{i}}{2}A_\mu^{ij}L_{ij}. \tag{19}$$

It is very convenient to introduce the matrices

$$\eta_{(N)}^{\mu\nu} = (N+1)g^{\mu\rho_1}y^{i_1}\alpha_{\rho_1\sigma_1}^{i_1}g^{\sigma_1\rho_2}\cdots y^{i_N}\alpha_{\rho_N\sigma_N}^{i_N}g^{\sigma_N\nu} \tag{20}$$

$\eta_{(0)}^{\mu\nu} = g^{\mu\nu}$. The expansion in ϵ of $\gamma^{\mu\nu}$ and $\ln|\mathbb{1}-\eta|$ may then be computed as

$$\gamma^{\mu\nu} = \sum_{N=0}^{\infty}\epsilon^{N/2}\eta_{(N)}^{\mu\nu} \tag{21}$$

$$\ln|\mathbb{1}-\eta| = -\sum_{N=1}^{\infty}\frac{\epsilon^{N/2}}{N}\operatorname{tr}\left[\eta^N\right]. \tag{22}$$

The evaluation of the $N/2$-order term of the perturbative expansion (15) thus reduces to a matter of simple algebra, yielding

$$H^{(N/2)} = -\tfrac{1}{2}\hat{\nabla}_\mu\eta_{(N-2)}^{\mu\nu}\hat{\nabla}_\nu + Q^{(N/2)} \tag{23}$$

$N \geqslant 2$, where the potentials $Q^{(N/2)}$ may be written as

$$Q^{(1)} = \tfrac{1}{8}\operatorname{tr}[\partial_i\eta]\operatorname{tr}[\partial_i\eta] - \tfrac{1}{4}\operatorname{tr}[\partial_i\eta\partial_i\eta]$$

$$Q^{(3/2)} = \tfrac{1}{4}\operatorname{tr}[\partial_i\eta]\operatorname{tr}[\eta\partial_i\eta] - \tfrac{1}{2}\operatorname{tr}[\eta\partial_i\eta\partial_i\eta] - \tfrac{1}{4}\operatorname{tr}\left[\hat{\nabla}_\mu g^{\mu\nu}\hat{\nabla}_\nu\eta\right]$$

and for $N \geqslant 4$

$$Q^{(N/2)} = \sum_{K=0}^{N-2} \left\{ \tfrac{1}{8} \operatorname{tr}\left[\eta^K \partial_i \eta\right] \operatorname{tr}\left[\eta^{N-K-2} \partial_i \eta\right] - \tfrac{1}{4} \operatorname{tr}\left[\eta^{N-2} \partial_i \eta \partial_i \eta\right] \right\}$$

$$- \sum_{K=0}^{N-3} \tfrac{1}{4} \operatorname{tr}\left[\eta^{N-K-3} \hat{\nabla}_\mu \eta_{(K)}^{\mu\nu} \hat{\nabla}_\nu \eta + (N-K-3) \eta_{(K)}^{\mu\nu} \eta^{N-K-4} (\hat{\nabla}_\mu \eta)(\hat{\nabla}_\nu \eta)\right]$$

$$+ \sum_{K=0}^{N-4} \sum_{L=1}^{N-K-3} \tfrac{1}{8} \eta_{(K)}^{\mu\nu} \operatorname{tr}\left[\eta^{L-1} (\hat{\nabla}_\mu \eta)\right] \operatorname{tr}\left[\eta^{N-K-L-3} (\hat{\nabla}_\nu \eta)\right].$$

It is remarkable that the perturbative expansion of the Hamiltonian of the system is completely written in terms of the induced metric $g_{\mu\nu}$, the second fundamental form $\alpha_{\mu\nu}^i$, its first and second covariant derivative $\nabla_\rho \alpha_{\mu\nu}^i$, $\nabla_\sigma \nabla_\rho \alpha_{\mu\nu}^i$ and the normal fundamental form A_μ^{ij}. A_μ^{ij} appears in the perturbative expansion only by means of the minimal coupling (19).

4. Spectrum and effective dynamics

To evaluate the spectrum of the system we now proceed by means of the standard Raleigh–Schrödinger perturbation theory. We identify $H^{(0)}$ with the unperturbed Hamiltonian and the rest of expansion (15) with the perturbation $\mathcal{P}_\epsilon$,

$$\epsilon \mathcal{H} = H^{(0)} + \mathcal{P}_\epsilon. \tag{24}$$

As was stated in the previous section, $H^{(0)}$ represents a system of $(n-m)$ uncoupled harmonic oscillator. We denote by $\chi_{\mathcal{N}}(\vec{y})$ its eigenfunctions, having collected the harmonic oscillator quantum numbers $n_{m+1}, \ldots, n_n$ in the multi-index $\mathcal{N} = (n_{m+1}, \ldots, n_n)$. The corresponding eigenvalues are given by $E^{(0)} = \sum_i \omega^i (n_i + \frac{1}{2})$. The spectrum is degenerate every time the frequencies ω^i satisfy linear conditions in the integer field. The zeroth-order eigenfunctions corresponding to an energy $E^{(0)}$ are given by

$$\psi_{\mathcal{N}}^{(0)}(\vec{x}, \vec{y}) = \phi_{\mathcal{N}}(\vec{x}) \chi_{\mathcal{N}}(\vec{y}) \tag{25}$$

and present an infinite degeneracy given by the presence of the arbitrary function of $\vec{x}$, $\phi_{\mathcal{N}}(\vec{x})$, besides that labelled by the multi-index corresponding to the energy $E^{(0)}$.

The first-order correction to $E^{(0)}$, $E^{(1)}$, is obtained by diagonalizing the perturbation on degenerate states, that is by solving the Schrödinger equation

$$\mathcal{H}^{E^{(0)}} \phi(\vec{x}) = E^{(1)} \phi(\vec{x}) \tag{26}$$

where the Hamiltonian $\mathcal{H}^{E^{(0)}}$ is obtained by bracketing the order ϵ term of $\mathcal{P}_\epsilon$, $H^{(1)}$, between the harmonic oscillator states corresponding to $E^{(0)}$ and $\phi(\vec{x})$ is a vector wavefunction having as component the $\phi_{\mathcal{N}}(\vec{x})$ with energy $E^{(0)}$. The explicit expression of $\mathcal{H}^{E^{(0)}}$ is

$$\mathcal{H}^{E^{(0)}} = -\frac{1}{2|g|^{1/2}} (\mathbb{1} \partial_\mu + \mathrm{i} A_\mu) g^{\mu\nu} |g|^{1/2} (\mathbb{1} \partial_\nu + \mathrm{i} A_\nu) + Q^{(1)}(\vec{x}) + \bar{Q}^{(1)}(\vec{x}) \tag{27}$$

with

$$A_\mu = \tfrac{1}{2} A_\mu^{ij} \langle L_{ij} \rangle, \tag{28}$$

$$\bar{Q}^{(1)} = \tfrac{1}{8} g^{\mu\nu} A_\mu^{ij} A_\nu^{kl} \left(\langle L_{ij} L_{kl} \rangle - \langle L_{ij} \rangle \langle L_{kl} \rangle \right) \tag{29}$$

where $\langle L_{ij} \rangle$ and $\langle L_{ij} L_{kl} \rangle$ denote the matrices obtained by bracketing L_{ij} and $L_{ij} L_{kl}$ between the harmonic oscillator states corresponding to $E^{(0)}$ and $\mathbb{1}$ is the identity matrix with the dimension of the degenerate space. $\mathcal{H}^{E^{(0)}}$ appears as a free Hamiltonian on the constraint's

surface coupled with the geometry induced gauge fields (28) and the potentials (18) and (29). Equation (26) therefore has to be interpreted as the Schrödinger equation describing the effective dynamics induced on the constraint's surface. Note that for a surface Σ embedded in the three-dimensional Euclidean space R^3 the Hamiltonian (27) reduces to (2). The potentials (28) and (29) produces a gauge structure which resembles the *geometric electromagnetism* discussed in the context of the adiabatic approximation [10]. It is, however, important to note that the mechanism producing the coupling with gauge fields and quantum potentials in the effective dynamics of a constrained system is distinct from that explored by Berry, its origin having to be found in the non-trivial geometry of the constraint's surface M.

Denoting by $\mathcal{K}$ the quantum numbers labelling the eigenfunctions of $\mathcal{H}^{E^{(0)}}$ and supposing the degeneracy to be completely removed, the eigenvalues of $\epsilon\mathcal{H}$ are evaluated by means of the standard formula

$$\epsilon\mathcal{E}_{\mathcal{N},\mathcal{K}} = E^{(0)} + \langle\mathcal{N},\mathcal{K}|\mathcal{P}_\epsilon|\mathcal{N},\mathcal{K}\rangle + \sum_{(\mathcal{N}'\mathcal{K}')\neq(\mathcal{N},\mathcal{K})} \frac{|\langle\mathcal{N},\mathcal{K}|\mathcal{P}_\epsilon|\mathcal{N}',\mathcal{K}'\rangle|^2}{E^{(0)} - E^{(0)'}} + \cdots . \tag{30}$$

This allows us to calculate the spectrum of the system with an arbitrary accuracy as a power series in the parameter ϵ.

5. Particle constrained on a circle

As a very simple, but non-trivial, example we consider a particle constrained to move on a circle embedded in R^3 by a harmonic potential. This allows us to illustrate some peculiarities of constrained quantum-mechanical systems which are systematically ignored in formal treatments. Therefore let $c : [0, 2\pi R] \to R^3$, $c(x) = (R\cos(x/R), R\sin(x/R), 0)$ be the embedding map of the circle in the three-dimensional Euclidean space R^3. The curve is parametrized by the arc length x, so that its tangent, normal and binormal may immediately be evaluated as $t(x) = (-\sin(x/R), \cos(x/R), 0)$, $n(x) = (\cos(x/R), \sin(x/R), 0)$ and $b(x) = (0, 0, 1)$. Every smooth assignment of an orthonormal basis of the normal space to c in x may be obtained by rotating the normal and binormal by a point-dependent angle $w(x)$

$$\begin{aligned} n^2 &= \cos w\ n + \sin w\ b \\ n^3 &= -\sin w\ n + \cos w\ b \end{aligned} \tag{31}$$

where $w(0) = w(2\pi R) + 2\pi z$, z being an integer. The induced metric, the second fundamental form and the normal fundamental form of the embedding read

$$\begin{aligned} &g_{11} = 1 \\ &\alpha^2_{11} = \frac{1}{R}\cos w \qquad \alpha^3_{11} = -\frac{1}{R}\sin w \\ &A^{23}_1 = -\dot{w}. \end{aligned} \tag{32}$$

The one-by-one matrix η is written as $\eta = (y^2/R)\cos w - (y^3/R)\sin w$, whereas the covariant derivative (19) on c reads $\hat{\nabla}_x = \partial_x - i\dot{w}L_{23}$. Direct calculation shows that

$\hat{\nabla}_x \eta = 0$, so that the whole perturbative expansion (15) may be easily evaluated as

$$\begin{aligned} H^{(0)} &= \tfrac{1}{2}\left(-\partial_2^2 + \omega^{2^2} y^{2^2}\right) + \tfrac{1}{2}\left(-\partial_3^2 + \omega^{3^2} y^{3^2}\right) \\ H^{(1)} &= -\tfrac{1}{2}\left(\partial_x - \mathrm{i}\dot{w} L_{23}\right)^2 - \frac{1}{8R^2} \\ &\vdots \qquad\qquad \vdots \\ H^{(N/2)} &= (N-1)\left(\frac{y^2}{R}\cos w - \frac{y^3}{R}\sin w\right)^{N-2} H^{(1)} \\ &\vdots \qquad\qquad \vdots . \end{aligned} \tag{33}$$

The spectrum of the system may now be calculated by means of perturbation theory. As in the general case the infinite degeneracy of the zeroth-order states is removed by solving the Schrödinger equation (26) for the effective dynamics on the constraint's surface. In correspondence to the zeroth-order state labelled by the harmonic oscillator quantum numbers (n_2, n_3) the effective Hamiltonian on the circle is written as

$$\mathcal{H}^{(n_2,n_3)} = -\tfrac{1}{2}\left(\partial_x - \mathrm{i}\dot{w}\langle L_{23}\rangle\right)^2 + \tfrac{1}{2}\left(\langle L_{23}^2\rangle - \langle L_{23}\rangle^2\right)\dot{w}^2 - \frac{1}{8R^2} \tag{34}$$

where the angular brackets again denote expectation values between harmonic oscillator states corresponding to the energy $E^{(0)} = \omega^2(n_2 + \frac{1}{2}) + \omega^3(n_3 + \frac{1}{2})$.

Let us now discuss the physical meaning of the function $w(x)$. If the confining potential is symmetric, that is $\omega^2 = \omega^3$, it is possible to choose the harmonic oscillator basis is such a way that L_{23} is diagonal. The effective potential $(\langle L_{23}^2\rangle - \langle L_{23}\rangle^2)\dot{w}^2/2$ then vanishes identically and $\langle L_{23}\rangle\dot{w}$ then appears as a pure gauge field in the theory and may be removed by a different choice of normal coordinates y^2, y^3. The effective dynamics on the circle and the whole perturbative expansion are then considerably simplified. In contrast, if the confining potential is not symmetric, $\omega^2 \neq \omega^3$, $\langle L_{23}\rangle = 0$, $\langle L_{23}^2\rangle \neq 0$ and a different choice of normal coordinates would cause the confining potential to be x-dependent. The effects produced by $w(x)$ may therefore not be eliminated. Pictorially we may liken our model to a particle moving in a ring with a small ellipsoidal section. The function $w(x)$ describes then how the section wraps up when moving along the ring. If the ring's section reduces to a circle $(\omega^2 = \omega^3)$ it then does not matter how the wrapping is done and we can always recover the case $w = 0$. On the contrary the wrapping produces observable effects when the ring's section is not circular $(\omega^2 \neq \omega^3)$.

As the $\omega^2 = \omega^3$ case is straightforward, we concentrate on $\omega^2 \neq \omega^3$. The effective Hamiltonian describing the dynamics on the circle then reduces to

$$\mathcal{H}^{(n_2,n_3)} = -\tfrac{1}{2}\partial_x^2 + \tfrac{1}{2}\left[\left(\frac{\omega^2}{\omega^3} + \frac{\omega^3}{\omega^2}\right)\left(n_2 + \tfrac{1}{2}\right)\left(n_3 + \tfrac{1}{2}\right) - \tfrac{1}{2}\right]\dot{w}^2 - \frac{1}{8R^2}. \tag{35}$$

Different choices of the *wrapping function* $w(x)$ produce a completely different effective dynamics. An arbitrary positive, and everywhere finite, smooth potential may be reproduced by a suitable choice of w.

The simpler case we may consider is that in which the potential wraps us uniformly, say z times, $w(x) = zx/R$. The effective Schrödinger equation on the circle is then immediately solved by $\phi_{(n_2,n_3),k}(x) = \exp\left(\mathrm{i}\frac{k}{R}x\right)/\sqrt{2\pi R}$, k any integer, and

$$E^{(1)} = \frac{1}{2R^2}\left\{k^2 + z^2\left[\left(\frac{\omega^2}{\omega^3} + \frac{\omega^3}{\omega^2}\right)\left(n_2 + \tfrac{1}{2}\right)\left(n_3 + \tfrac{1}{2}\right) - \tfrac{1}{2}\right] - \tfrac{1}{4}\right\}. \tag{36}$$

Finer corrections to the spectrum may be evaluated by going over in perturbation theory. As this matter is not particulary interesting for this model, examination of the matter is postponed to the next example which is physically more significant. The remarkable fact we learn from this example is that the realization of the constraint, i.e. the particular form of the confining potential V_C, characterizes the spectrum and the effective dynamics of the constrained quantum system. Such information is completely lost within a formal treatment of the constraint.

6. Particle constrained on a sphere (the rigid diatom)

As a second example of a constrained quantum-mechanical system we consider the motion of a particle on a sphere embedded in R^3. To get some physical grasp of what we are dealing with, let us consider a diatom. Apart from effects connected with the geometric phase [11], the effective Hamiltonian describing the rotovibrational degrees of freedom of the molecule is written in the adiabatic approximation as

$$\mathcal{H}_{\text{nuc}} = -\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+V_{\text{BO}}(|r|) \tag{37}$$

where $r=(x,y,z)$ is the relative position of the nuclei, μ the reduced mass of the system and V_{BO} is the Born–Oppenheimer potential. It is usual to assume that:

(i) V_{BO} presents a deep minimum in correspondence of the molecular equilibrium length r_0, and

(ii) V_{BO} depends only on the relative distance of the nuclei $r=|r|$ and not on the orientation of the molecule in space.

That is, V_{BO} behaves as a potential confining the motion from the rotovibrational configuration space R^3 to the sphere of radius r_0. The Hamiltonian (37) describes therefore a constrained quantum-mechanical system in the sense we specified before, cf equation (8).

In order to adapt coordinates we introduce the usual angles θ and ϕ parametrizing the sphere and the normal coordinate $y=(1/r_0)\sqrt{(I\omega/\hbar)}\,(r-r_0)$. $I=\mu r_0^2$ is the moment of inertia of the diatom and ω the frequency introduced by the Born–Oppenheimer potential

$$\omega=\sqrt{(2/\mu)(\partial^2 V_{\text{BO}}/\partial r^2)|_{r=r_0}}.$$

The dimensionless scaling factor $\epsilon=\hbar/I\omega$ appears naturally in the definition of y once the zeroth-order energy $\hbar\omega$ is factorized from the Hamiltonian. From most diatoms ϵ is a very small parameter, $\epsilon\simeq 10^{-2}$–10^{-4}, and, as our notation anticipates, gives a measure of the rigidity of the molecule. The metric of R^3 in the adapted-coordinate frame reads

$$G_{IJ}=\frac{1}{\hbar\omega\epsilon}\begin{pmatrix}(1+\epsilon^{1/2}y)^2 & 0 & 0\\ 0 & (1+\epsilon^{1/2}y)^2\sin^2\theta & 0\\ 0 & 0 & \epsilon\end{pmatrix} \tag{38}$$

while the Born–Oppenheimer potential is written as

$$V_{\text{BO}}=\hbar\omega\left(\tfrac{1}{2}y^2+\hat{a}y^3+\hat{b}y^4+\cdots\right) \tag{39}$$

where $\hat{a}=a\hbar^{1/2}/\mu^{3/2}\omega^{5/2}$ and $\hat{b}=b\hbar/\mu^2\omega^3$, a and b being the usual spectroscopic parameters. The rigidity parameter $\hbar/I\omega$ therefore plays the role of the parameter ϵ we introduced in section 3 for a generic constraint†. A comparison of equation (38) with

† Note that the normal coordinate y appears as already rescaled.

equations (5) and (6) allows us to write down immediately the induced metric and the second fundamental form on the sphere as

$$g_{\mu\nu} = \frac{1}{\hbar\omega\epsilon}\begin{pmatrix} 1 & 0 \\ 0 & \sin^2\theta \end{pmatrix} \tag{40}$$

and

$$\alpha_{\mu\nu} = -\frac{\epsilon^{1/2}}{\hbar\omega}\begin{pmatrix} 1 & 0 \\ 0 & \sin^2\theta \end{pmatrix}. \tag{41}$$

As the codimension of the constraint's surface is one, the normal fundamental form vanishes identically. The embedding of the sphere in R^3 is standard and the perturbative expansion $\mathcal{H}/\hbar\omega = H^{(0)} + \epsilon H^{(1)} + \cdots + \hat{a}y^3 + \hat{b}y^4 + \cdots$ is easily evaluated as

$$\begin{aligned} H^{(0)} &= \tfrac{1}{2}(-\partial_y^2 + y^2) \\ H^{(1)} &= -\tfrac{1}{2}\left(\frac{1}{\sin\theta}\partial_\theta \sin\theta \partial_\theta + \frac{1}{\sin^2\theta}\partial_\phi^2\right) \\ &\vdots \qquad\qquad\qquad \vdots \\ H^{(N/2)} &= (-1)^N (N-1) y^{N-2} H^{(1)} \\ &\vdots \qquad\qquad\qquad \vdots . \end{aligned} \tag{42}$$

The zeroth-order Hamiltonian $H^{(0)}$ takes into account the vibrational motion of the diatom. $H^{(1)}$ is the angular momentum operator describing the effective rotational dynamics as that of a spherical top. The rest of the perturbative expansion reproduces Dunham's expansion [15] of the non-rigid rotor taking into account rotovibrational interactions. The rotovibrational spectrum of the diatom therefore finds a very natural interpretation in terms of constrained quantum mechanics. Having abandoned the classical idea of constraint ($\epsilon \to 0$) the rotovibrational structure appears naturally as a consequence of the physical structure of the constraint. The algorithm we present in this paper gives an automatic way of computing rotovibrational interactions, and may be of use in the analysis of rigid polyatomic molecules [6]. For the moment we conclude by evaluating the spectrum of the particle constrained on a sphere. Having introduced creation/destruction operators relative to the normal coordinate, the computation becomes algebraic in nature, and may be performed to arbitrary order in perturbation theory by means of computer algebraic manipulation. Here we report that the expansion of the energy $\mathcal{E}_{n,l}$ to third order in perturbation theory is

$$\begin{aligned} \frac{\mathcal{E}_{n,l}}{\hbar\omega} &= \left(n+\tfrac{1}{2}\right) + \epsilon\tfrac{1}{2}\left[l(l+1)\right] + \epsilon^2\tfrac{3}{2}\left[l(l+1)\right]\left(n+\tfrac{1}{2}\right) \\ &\quad + \epsilon^3\left\{\tfrac{15}{8}\left[l(l+1)\right] + \tfrac{15}{2}\left[l(l+1)\right]\left(n+\tfrac{1}{2}\right)^2 - \tfrac{1}{2}\left[l(l+1)\right]^2\right\} \\ &\quad + \left(\tfrac{3}{2}\hat{b} - 3\epsilon^{3/2}\hat{a} - \tfrac{15}{4}\hat{a}^2\right)\left(n+\tfrac{1}{2}\right)^2. \end{aligned} \tag{43}$$

Replacing the values of ϵ, $\hat{a}$ and $\hat{b}$, equation (43) reproduces the standard expression for the rotovibrational energies of diatoms [16].

7. Concluding remarks

The reduction of the motion of a quantum-mechanical system from its configuration space to a submanifold is by no means unique, in the sense that it is impossible to perform this

operation by completely disregarding the motion in the directions normal to the constraint's surface. Quantum mechanics is a field theory, after all, and the wavefunction of the system keeps on exploring the whole configuration space even if it is squeezed on the constraint's surface. When the system is in an eigenstate of the confining potential we can obtain an effective Hamiltonian describing the dynamics on the constraint's surface. As is clearly illustrated by the examples of sections 5 and 6, this effective dynamics, described by $\mathcal{H}^{E^{(0)}}$, depends both on the specific normal eigenstate and on the explicit form of the confining potential. In any case the eigenvalues of the effective Hamiltonian give only the first-order corrections to the spectrum of the system at finite ϵ. An accurate description also requires the analysis of the interaction between the motion normal and along the constraint's surface. The perturbative expansion (15) we present in this paper takes this effect into account.

Taking the limit $\epsilon \to 0$ after subtracting the divergent zeroth-order energies of the system produces a well defined description of the motion on the constraint's surface. Nevertheless we consider this operation to be artificial, the physical nature of the constraint lying in the small but finite value of ϵ (cf the discussion of the diatom). The whole perturbative expansion (15) is therefore necessary to characterize the dynamics of the constrained system.

Apart from its conceptual importance, the perturbative expansion (15) may be of practical importance in the analysis of electrons confined on arbitrary surfaces and wires, as well as in the analysis of polyatomic molecular spectra. The effective rotational dynamics of some simple polyatomic molecules has already been considered in [6], demonstrating the physical relevance of the induced gauge structure and quantum potentials (28), (18) and (29). Our hope is that the expansion (15) may serve as an unifying tool in understanding the fine-structure spectra of rigid polyatomic molecules.

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References

[1] Dirac P A M 1964 *Lectures notes on Quantum Mechanics* (New York: Yeshiva)
[2] De Witt B 1952 *Phys. Rev.* **85** 635
[3] See, for example:
Bastard G 1990 *Wave Mechanics Applied to Semiconductor and Heterostructures* (Les Ulis: Editions de Physique)
[4] For a review see:
Prange R E and Girvin S M (ed) 1989 *The Quantum Hall Effect* (Berlin: Springer)
[5] Maraner P and Destri C 1993 *Mod. Phys. Lett.* A **8** 861
[6] Maraner P 1994 *Parma University Preprint* UPRF-94-400
[7] Jensen H and Koppe H 1971 *Ann. Phys.* **63** 586
[8] Marcus R A 1966 *J. Chem. Phys.* **45** 4493
Kugler M and Shtrikman S 1988 *Phys. Rev.* D **37** 934
da Costa R C T 1981 *Phys. Rev.* A **23** 1982
Exner P, Seba P and Stovicek P 1990 *Phys. Lett.* **150A** 179
Nagoshi Y and Takagi S 1991 *J. Phys. A: Math. Gen.* **24** 4093
Takagi S and Tanzawa T 1992 *Prog. Theor. Phys.* **87** 561
[9] Fujii K and Ogawa N 1993 *Prog. Theor. Phys.* **89** 575
[10] Shapere A and Wilczek F (ed) 1989 *Geometric Phases in Physics* (Singapore: World Scientific)
[11] Moody J, Shapere A and Wilczek F 1986 *Phys. Rev. Lett.* **56** 199
[12] Jackiw R 1988 *Int. J. Mod. Phys.* A **3** 285
[13] Berry M V 1989 *Geometric Phases in Physics* ed A Shapere and F Wilczek (Singapore: World Scientific) pp 7–28

[14] See, for example:
Spivak M 1975 *Differential Geometry* vol IV (Boston, MA: Publish or Perish)
[15] Dunham J L 1932 *Phys. Rev.* **41** 721
[16] Herzberg G 1945 *Molecular Spectra and Molecular Structure, I. Spectra of Diatomic Molecules* (Princeton, NJ: Van Nostrand)