Realizing holonomic constraints

in classical and quantum mechanics

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Abstract

We consider the problem of constraining a particle to a submanifold Σ of configuration space using a sequence of increasing potentials. We compare the classical and quantum versions of this procedure. This leads to new results in both cases: an unbounded energy theorem in the classical case, and a quantum averaging theorem. Our two step approach, consisting of an expansion in a dilation parameter, followed by averaging in normal directions, emphasizes the role of the normal bundle of Σ, and shows when the limiting phase space will be larger (or different) than expected.

Introduction

Consider a system of non-relativistic particles in an Euclidean configuration space $\mathbb{R}^{n+m}$ whose motion is governed by the Hamiltonian

$$H = \frac{1}{2}\langle p, p\rangle + V(x). \tag{1.1}$$

We are interested in the motion of these particles when their positions are constrained to lie on some n-dimensional submanifold $\Sigma \subset \mathbb{R}^{n+m}$. In both classical and quantum mechanics there are accepted notions about what the constrained motion should be.

In classical mechanics, the Hamiltonian for the constrained motion still has the form (1.1), but whereas p and x originally denoted variables on the phase space $T^*\mathbb{R}^{n+m} = \mathbb{R}^{n+m} \times \mathbb{R}^{n+m}$, they now are variables on the cotangent bundle $T^*\Sigma$. The inner product $\langle p, p\rangle$ is now computed using the metric that Σ inherits from $\mathbb{R}^{n+m}$, and V now denotes the restriction of V to Σ.

In quantum mechanics, $\langle p, p\rangle$ is interpreted to mean the Laplace operator Δ, and $V(x)$ is the operator of multiplication by V. For unconstrained motion Δ is the Euclidean Laplacian on $\mathbb{R}^{n+m}$, and the Hamiltonian acts $L^2(\mathbb{R}^{n+m})$. For constrained motion, the Laplace operator for Σ with the inherited metric is used, and the Hilbert space is $L^2(\Sigma, d\mathrm{vol})$.

In both cases the description of the constrained motion is intrinsic: it depends only on the Riemannian structure that Σ inherits from $\mathbb{R}^{n+m}$, but not on other details of the imbedding.

Of course, a constrained system of particles is an idealization. Instead of particles moving exactly on Σ, one might imagine there is a strong force pushing the particles onto the submanifold. The motion of the particles would then be governed by the Hamiltonian

$$H_\lambda = \frac{1}{2}\langle p, p\rangle + V(z) + \lambda^4 W(z) \tag{1.2}$$

where W is a positive potential vanishing exactly on Σ and λ is large. (The fourth power is just for notational convenience later on.) Does the motion described by H_λ converge to the intrinsic constrained motion as λ tends to infinity? Surprisingly, the answer to this question depends on exactly how it is asked, and is often no.

A situation in classical mechanics where the answer is yes is described by Rubin and Ungar [RU]. An initial position on Σ and an initial velocity tangent to Σ are fixed. Then, for a sequence of λ's tending to infinity, the subsequent motions under H_λ are computed. As λ becomes large, these motions converge to the intrinsic constrained motion on Σ. This result is widely known, since it appears in Arnold's book [A1] on classical mechanics. However, from the physical point of view, it is neither completely natural to require that initial position lies exactly on Σ, nor that the initial velocity be exactly tangent. Rubin and Ungar also consider what happens if initial velocity has a component in the direction normal to Σ. In this case, the motion in the normal direction is highly oscillatory, and there is an extra potential term, depending on the initial condition, in the Hamiltonian for the limiting motion on Σ. A more complete result is given by Takens [T]. Here the initial conditions are allowed to depend on λ in such a way that the initial position converges to a point on Σ and the initial energy remains bounded. (We will give precise assumptions below.) Once again, the limiting motion on Σ is governed by a Hamiltonian with an additional potential. Takens noticed that a non-resonance condition on the eigenvalues of the Hessian of the constraining potential W along Σ is required to prove convergence. He also gave an example showing that if the Hessian of W does have an eigenvalue crossing, then there may not be a good notion of limiting motion. In his example, he constructs two sequences of orbits, each one converging to an limiting orbit on Σ. These limiting orbits are identical until they hit the point on Σ

where the eigenvalues cross. After that, they are different. This means there is no differential equation on Σ governing the limiting motion. For other discussions of the question of realizing constraints see [A2] and [G]. A modern survey of the classical mechanical results that emphasizes the systematic use of weak convergence is given by Bornemann and Schütte [BS].

The quantum case was considered previously by Tolar [T], da Costa [dC1, dC2] and in the path integral literature (see Anderson and Driver [AD]). Related work can also be found in Helffer and Sjöstrand [HS1] [HS2], who obtained WKB expansions for the ground state, and in Duclos and Exner [DE], Figotin and Kuchment [FK] and Schatzman [S]. There are really two aspects to the problem of realizing constraints: a large λ expansion followed by an averaging procedure to deal with highly oscillatory normal motion. Previous work in quantum mechanics concentrated on the first aspect (although a related averaging procedure for classical paths with a vanishingly small random perturbation can be found in [F]). Already a formal large λ expansion reveals the interesting feature that the limiting Hamiltonian has an extra potential term depending on scalar and the mean curvatures. Since the mean curvature is not intrinsic, this potential does depend on the imbedding of Σ in $\mathbb{R}^{n+m}$. It is not completely straightforward to formulate a theorem in the quantum case. We have chosen a formulation, modelled on the classical mechanical theorems, tracking a sequence of orbits with initial positions concentrating on Σ via dilations in the normal direction. Actually we consider the equivalent problem of tracking the evolution of H_λ conjugated by dilations, acting on a fixed initial vector. In order to obtain a limiting orbit we must assume that all the eigenvalues of the Hessian of the constraining potential W are constant on Σ. In fact we will assume that W is exactly quadratic. When the eigenvalues are all different (and non-resonant) we are able to prove the existence of a limiting motion in $L^2(\Sigma)$. Surprisingly, for very symmetrical restraining potentials, the Hilbert space need not be $L^2(\Sigma)$, but may be the space of L^2 sections of a vector bundle over Σ.

Our formulation of the quantum theorems invites comparison with the classical mechanical case. It turns out that extra potentials that appear in the two cases are quite different, and there is no obvious connection. Upon reflection, the reason for this difference is clear. If we have a sequence of initial quantum states whose position distribution is being squeezed to lie close to Σ, then by the uncertainty principle, the distribution of initial momenta will be spreading out, and thus the initial energy will be unbounded. However, the classical mechanical convergence theorems above all deal with bounded energies. As Bornemann and Schütte point out, if the energies are unbounded, it may happen that the weak limit of the orbits does not even lie on Σ. However, in situations where we can obtain a quantum mechanical theorem, we can also obtain an analogous classical theorem with unbounded energies.

The present note contains the statements of our results. Proofs will be given in [FH].

Classical mechanics: bounded energy

To give a precise statement of our results we must introduce some notation. The normal bundle to Σ is the subset of $\mathbb{R}^{n+m} \times \mathbb{R}^{n+m}$ given by

$$N\Sigma = \{(\sigma, n) : \sigma \in \Sigma,\, n \in N_\sigma \Sigma\}$$

Here $N_\sigma \Sigma$ denotes the normal space to Σ at σ, identified with a subspace of $\mathbb{R}^{n+m}$.

There is a natural map from $N\Sigma$ into $\mathbb{R}^{n+m}$ given by

$$\iota : (\sigma, n) \mapsto \sigma + n.$$

We now fix a sufficiently small δ so that this map is a diffeomorphism of $N\Sigma_\delta = \{(\sigma, n) : \|n\| < \delta\}$ onto a tubular neigbourhood of Σ in $\mathbb{R}^{n+m}$. Then we can pull back the Euclidean metric from $\mathbb{R}^{n+m}$ to $N\Sigma_\delta$. Since we are interested in the motion close to Σ we may use $N\Sigma_\delta$ as the classical configuration space. This will be convenient in what follows, and is justified below.

We will want to decompose vectors in the cotangent spaces of $N\Sigma_\delta$ into horizontal and vertical vectors, so we now explain this decomposition. Let $\pi : N\Sigma \to \Sigma$ denote the projection of the normal bundle onto the base given by $\pi : (\sigma, n) \mapsto \sigma$. The vertical subspace of $T_{\sigma,n} N\Sigma$ is defined to be the kernel of $d\pi : T_{\sigma,n} N\Sigma \to T_\sigma \Sigma$. The horizontal subspace is then defined to be the orthogonal complement (in the pulled back metric) of the vertical subspace. Using the identification of $T_{\sigma,n} N\Sigma$ with $T^*_{\sigma,n} N\Sigma$ given by the metric we obtain a decomposition of cotangent vectors into horizontal and vertical components as well. We will denote by (ξ, η) the horizontal and vertical components of a vector in $T^*_{(\sigma,n)} N\Sigma$.

The decomposition can be explained more concretely as follows. For each point $\sigma \in \Sigma$, we may decompose $T_\sigma \mathbb{R}^{n+m} = T_\sigma \Sigma \oplus N_\sigma \Sigma$ into the tangent and normal space. Using the natural identification of all tangent spaces with $\mathbb{R}^{n+m}$, we may regard this as a decomposition of $\mathbb{R}^{n+m}$. Let P^T_σ and P^N_σ be the corresponding orthogonal projections. Since we are thinking of $N\Sigma$ as an $n+m$–dimensional submanifold of $\mathbb{R}^{n+m} \times \mathbb{R}^{n+m}$, we can identify $T_{(\sigma,n)} N\Sigma$ with the $n+m$–dimensional subspace of $\mathbb{R}^{n+m} \times \mathbb{R}^{n+m}$ given by all vectors of the form $(X, Y) = (\dot\sigma(0), \dot n(0))$, where $(\sigma(t), n(t))$ is a curve in $N\Sigma$ passing through (σ, n) at time $t = 0$. The inner product of two such tangent vectors is

$$\langle (X_1, Y_1), (X_2, Y_2) \rangle = \langle X_1 + Y_1, X_2 + Y_2 \rangle$$

where the inner product on the right is the usual Euclidean inner product. For a tangent vector (X, Y), the decomposition into horizontal and vertical vectors is given by

$$(X, Y) = (X, P^T_\sigma Y) + (0, P^N_\sigma Y)$$

For each point (σ, n) in the normal bundle, the map $d\pi : T_{\sigma,n}N\Sigma \to T_\sigma\Sigma$ is an isomorphism when restricted to the horizontal subspace of $T_{\sigma,n}N\Sigma$. Its adjoint $d\pi^*$ is an isomorphism of $T^*_\sigma\Sigma$ onto the horizontal subspace of $T^*_{\sigma,n}N\Sigma$. The map $d\pi^{*-1}$ appears in the definition of the bundle hamiltonian H_B below.

We will assume that the constraining potential is a C^∞ function of the form

$$W(\sigma, n) = \frac{1}{2}\langle n, A(\sigma)n\rangle \tag{2.1}$$

where for each σ, $A(\sigma)$ is a positive definite linear transformation on $N_\sigma\Sigma$. The Hamiltonian (1.2) can then be written

$$H_\lambda(\sigma, n, \xi, \eta) = \frac{1}{2}\langle \xi, \xi\rangle + \frac{1}{2}\langle \eta, \eta\rangle + V(\sigma + n) + \frac{\lambda^4}{2}\langle n, A(\sigma)n\rangle \tag{2.2}$$

Notice that on the boundary of $N\Sigma_\delta$

$$H_\lambda(\sigma, n, \xi, \eta) \geq c_1\lambda^4 - c_2$$

with

$$c_1 = \inf_{(\sigma,\mathbf{n}):\sigma\in\Sigma, \|\mathbf{n}\|=\delta} W(\sigma + \mathbf{n}) > 0$$
$$c_2 = \sup_{(\sigma,\mathbf{n}):\sigma\in\Sigma, \|\mathbf{n}\|=\delta} V(\sigma + \mathbf{n})$$

By conservation of energy, this implies that an orbit under H_λ that starts out in $N\Sigma_\delta$ with initial energy less than $c_1\lambda^4 - c_2$ can never cross the boundary, and therefore stays in $N\Sigma_\delta$. We will only consider such orbits in this section, and therefore are justified in taking our phase space to be $T^*N\Sigma_\delta$, or even $T^*N\Sigma$ if we extend H_λ in some arbitrary way.

Since we expect the motion in the normal directions to consist of rapid harmonic oscillations, it is natural to introduce action variables for this motion. There is one for each distinct eigenvalue $\omega^2_\alpha(\sigma)$ of $A(\sigma)$. Let $P_\alpha(\sigma)$ be the projection onto the eigenspace of $\omega^2_\alpha(\sigma)$. This projection is defined on $N_\sigma\Sigma$, which we may think of as the range of P^N_σ in $\mathbb{R}^{n+m}$. Thus the projection is defined on vertical vectors in $T_{(\sigma,n)}N\Sigma$ and, via the natural identification, on vertical vectors in $T^*_{(\sigma,n)}N\Sigma$. With this notation, the corresponding action variable, multiplied by λ^2 for notational convenience, is given by

$$I^\lambda_\alpha(\sigma, n, \xi, \eta) = \frac{1}{2\omega_\alpha(\sigma)}\langle \eta, P_\alpha\eta\rangle + \frac{\lambda^4\omega_\alpha(\sigma)}{2}\langle n, P_\alpha n\rangle \tag{2.3}$$

Notice that the total normal energy is given by $\sum_\alpha \omega_a I^\lambda_\alpha$. The following is a version of the theorem of Takens and Rubin, Ungar.

Theorem 2.1 *Let the Hamiltonian H_λ be given by (1.2) where W has the form (2.1) and satisfies*

(i) The eigenvalues $\omega^2_\alpha(\sigma)$ of $A(\sigma)$ have constant multiplicity.

Suppose that $(\sigma_\lambda, n_\lambda, \xi_\lambda, \eta_\lambda)$ are initial conditions in $T^*N\Sigma_\delta$ satisfying

(a) $\sigma_\lambda \to \sigma_0$,

(b) $\xi_\lambda \to \xi_0$,

(c) $I^\lambda_\alpha(\sigma_\lambda, n_\lambda, \xi_\lambda, \eta_\lambda) \to I^0_\alpha > 0$,

as $\lambda \to \infty$. *Let* $(\sigma_\lambda(t), n_\lambda(t), \xi_\lambda(t), \eta_\lambda(t))$ *denote the subsequent orbit in* $T^*N\Sigma_\delta$ *under the Hamiltonian* H_λ.

Suppose that $(\sigma(t), \xi(t))$ *is the orbit in* $T^*\Sigma$ *with initial conditions* (σ_0, ξ_0) *governed by the Hamiltonian*

$$h(\sigma, \xi) = \frac{1}{2}\langle \xi, \xi \rangle_\sigma + V(\sigma) + \sum_\alpha I^0_\alpha \omega_\alpha(\sigma).$$

Then for any $T \geq 0$

$$\sup_{0 \leq t \leq T} |\sigma_\lambda(t) - \sigma(t)| + |\xi_\lambda(t) - \xi(t)| \to 0$$

as $\lambda \to \infty$.

Implicit in this statement is the fact that the approximating orbit stays in the tubular neighbourhood for $0 \leq t \leq T$, provided λ is sufficiently large. This theorem is actually true in greater generality. We can consider smooth restraining potentials W where $\frac{1}{2}\langle n, A(\sigma)n \rangle$ is the first term in an expansion. If we choose our tubular neighbourhood so that $W(\sigma + n) \geq c|n|^2$ and impose the non-resonance condition $\omega_\alpha(\sigma) \neq \omega_\beta(\sigma) + \omega_\gamma(\sigma)$ for every choice of α, β and γ and for every σ, then the same conclusion holds. This theorem is also really a local theorem: if we impose the conditions on W and the non-resonance condition locally, and take T to be the time where the orbit leaves the set where all the conditions are true, then the same conclusion holds as well.

Classical mechanics: unbounded energy

We now describe our theorems in classical mechanics where the initial energies are diverging as they do in the quantum case. Our assumptions will imply that the initial value of the action variables I^λ_α scales like $\lambda^2 I^0_\alpha$, and thus the initial normal energy diverges like λ^2. Examining the effective Hamiltonian $h(\sigma, \xi)$ in Theorem 2.1, one would expect there to be a diverging $\lambda^2 \sum_\alpha I^0_\alpha \omega_\alpha(\sigma)$ potential term that forces the particles to the local minima of $\sum_\alpha I^0_\alpha \omega_\alpha(\sigma)$. If these local minima (called mini-wells in [HS1, HS2]) exist, we would expect the limiting motion to take place there. We want to consider the case where the limiting motion takes place on all of Σ. Therefore we will assume that there are no mini-wells, i.e., the frequencies ω_α are constant.

The first step in our analysis is a large λ expansion. It is convenient to implement this expansion using dilations in the fibre of the normal bundle. It is also convenient to assume that our configuration space is all of $N\Sigma$. This makes no difference, since the orbits we are considering never leave $N\Sigma_\delta$.

The dilation $d_\lambda : N\Sigma \to N\Sigma$ is defined by

$$d_\lambda(\sigma, n) = (\sigma, \lambda n)$$

It has a symplectic lift D_λ to the cotangent bundle given by

$$D_\lambda = d_\lambda^{-1*} = d^*_{\lambda^{-1}}$$

Instead of the original Hamiltonian H_λ we may now consider the equivalent pulled back Hamiltonian $H_\lambda \circ D_\lambda^{-1}$. A large λ expansion yields

$$H_\lambda \circ D_\lambda^{-1} = H_B + \lambda^2 H_O + O(\lambda^{-2})$$

where H_O is the harmonic oscillator Hamiltonian

$$H_O(\sigma, n, \xi, \eta) = \frac{1}{2}\langle \eta, \eta \rangle + \frac{1}{2}\langle n, An \rangle$$

and H_B is the bundle Hamiltonian given by

$$H_B(\sigma, n, \xi, \eta) = \frac{1}{2}\langle d\pi^{*-1}\xi + f(\sigma, n, \eta), d\pi^{*-1}\xi + f(\sigma, n, \eta)\rangle_\sigma + V(\sigma)$$

The inner product $\langle \cdot, \cdot \rangle_\sigma$ is the inner product on $T^*\Sigma$ defined by the imbedding. Here $f \in T^*_\sigma \Sigma$ is defined locally as follows. Choose a local co-ordinate system $x \mapsto \sigma(x)$ for Σ and local frame $n_1(\sigma), \ldots, n_m(\sigma)$ for the normal bundle. Then we obtain local co-ordinates for $N\Sigma$ by sending $(x, y) \mapsto (\sigma(x), \sum y_k n_k)$. (Here n_k denotes $n_k(\sigma(x))$.) Associated with the frame is the connection one-form. This is the antisymmetric matrix valued one-form given by

$$b_{k,l}[\cdot] = \langle n_k, dn_l[\cdot] \rangle \tag{3.1}$$

(Here we are thinking of n_k as a map from Σ to $\mathbb{R}^{n+m}$, and the inner product is in R^{n+m}.) With this notation,

$$f(\sigma(x), \sum y_k n_k, \sum r_k dy_k)[\cdot] = \sum_{k,l} y_k b_{k,l}[\cdot] r_l.$$

The following theorem describes a sequence of orbits with initial conditions obeying

$$D_\lambda(\sigma_\lambda, n_\lambda, \xi_\lambda, \eta_\lambda) \to (\sigma_0, n_0, \xi_0, \eta_0).$$

This condition implies that

(a) $\sigma_\lambda \to \sigma_0$,

(b) $\lambda n_\lambda \to n_0$,

(c) $\xi_\lambda \to d\pi^{*-1}\xi_0 + f(\sigma_0, n_0, \eta_0)$,

(d) $\lambda^{-1}\eta_\lambda \to \eta_0$.

(Here we are thinking of σ, n as vectors in $\mathbb{R}^{n+m}$ and ξ, η as vectors in $\mathbb{R}^{2(n+m)}$.) So, although the initial position is converging to a point on Σ, the initial normal energy $\sum I^\lambda_\alpha$ is diverging like λ^2.

Theorem 3.1 *Let the Hamiltonian H_λ be given by (2.2) where W has the form (2.1) and satisfies*

(i) The eigenvalues ω_α^2 of $A(\sigma)$ do not depend on σ.

Suppose that $(\sigma_\lambda, n_\lambda, \xi_\lambda, \eta_\lambda)$ are initial conditions in $T^*N\Sigma_\delta$ with $D_\lambda(\sigma_\lambda, n_\lambda, \xi_\lambda, \eta_\lambda) \to (\sigma_0, n_0, \xi_0, \eta_0)$ as $\lambda \to \infty$. Let $(\sigma_\lambda(t), n_\lambda(t), \xi_\lambda(t), \eta_\lambda(t))$ denote the subsequent orbit in $T^*N\Sigma_\delta$ under the Hamiltonian H_λ.

Suppose that $(\sigma^\lambda(t), n^\lambda(t), \xi^\lambda(t), \eta^\lambda(t))$ is the orbit in $T^*N\Sigma$ with initial conditions $(\sigma_0, n_0, \xi_0, \eta_0)$ governed by the Hamiltonian $H_B + \lambda^2 H_O$ defined above.

Then for any $T \geq 0$

$$\sup_{0\leq t\leq T} \left| D_\lambda\Big(\sigma_\lambda(t), n_\lambda(t), \xi_\lambda(t), \eta_\lambda(t)\Big) - \Big(\sigma^\lambda(t), n^\lambda(t), \xi^\lambda(t), \eta^\lambda(t)\Big)\right| \to 0$$

as $\lambda \to \infty$.

This theorem gives a satisfactory description of the limiting motion if the Poisson bracket of H_B and H_O vanishes. Then the flows generated by H_B and H_O commute and the motion is given by the rapid oscillations generated by $\lambda^2 H_O$ superimposed on the flow generated by H_B. In this situation we can perform averaging by simply ignoring the oscillations.

An example where $\{H_B, H_O\}$ is zero is when Σ has codimension one, or, more generally, if the connection form vanishes. Then H_B only involves variables on $T^*\Sigma$, so the limiting motion is a motion on Σ with independent oscillations in the normal variables.

The Poisson bracket $\{H_B, H_O\}$ also vanishes if all the frequencies ω_α are equal. In this case the motion generated by H_B need not only involve the variables on $T^*\Sigma$. It can be thought of as a generalized minimal coupling type flow. (See [GS] for a description of the geometry of this sort of flow.) The flow has the property that the trajectories in $N\Sigma$ are parallel along their projections onto Σ. In particular, $|n|^2$ is preserved by this motion. In certain situations there may be other, angular momentum like, conserved quantities for H_B, which would show up as adiabatic invariants for the original flow.

In general, when the frequencies are not all equal, the flows generated by H_B and $\lambda^2 H_O$ interact, and their interaction produces an extra potential term in the limiting Hamiltonian. To describe the limiting motion, we must perform an averaging. This requires non-resonance conditions. In this note, we only consider the extreme case where all the eigenvalues are distinct. (We will treat the more general case where some, but not all, the frequencies are equal in our forthcoming paper [FH].) We have the following theorem.

Theorem 3.2 *Let the Hamiltonian H_λ be given by (1.2) where W has the form (2.1) and satisfies*

(i) The eigenvalues $\omega_1^2, \ldots, \omega_m^2$ of $A(\sigma)$ do not depend on σ,

(ii) If $j \neq k$ then $\omega_j \pm \omega_k \neq 0$,

(iii) If $j \neq k$ and $l \neq m$ then $\omega_j \pm \omega_k \pm \omega_l \pm \omega_m \neq 0$.

Suppose that $(\sigma_\lambda, n_\lambda, \xi_\lambda, \eta_\lambda)$ are initial conditions in $T^*N\Sigma_\delta$ satisfying

(a) $\sigma_\lambda \to \sigma_0$,

(b) $\xi_\lambda \to \xi_0$,

(c) $\lambda^{-2} I_k^\lambda(\sigma_\lambda, n_\lambda, \xi_\lambda, \eta_\lambda) \to I_k^0 > 0$,

as $\lambda \to \infty$. *Let* $(\sigma_\lambda(t), n_\lambda(t), \xi_\lambda(t), \eta_\lambda(t))$ *denote the subsequent orbit in* $T^*N\Sigma_\delta$ *under the Hamiltonian* H_λ.

Suppose that $(\sigma(t), \xi(t))$ *is the orbit in* $T^*\Sigma$ *with initial conditions* (σ_0, ξ_0) *governed by the Hamiltonian*

$$h(\sigma, \xi) = \frac{1}{2}\langle \xi, \xi \rangle_\sigma + V(\sigma) + V_1(\sigma),$$

where V_1 *is described below. Then for any* $T \geq 0$

$$\sup_{0 \leq t \leq T} |\sigma_\lambda(t) - \sigma(t)| + |\xi_\lambda(t) - \xi(t)| \to 0$$

as $\lambda \to \infty$.

To complete the statement of the theorem, we must define the potential V_1. The normalized eigenvectors of $A(\sigma)$ provide an orthonormal frame $n_1(\sigma), \ldots, n_m(\sigma)$ for the normal bundle. (Each n_k is defined up to a choice of sign.) Let $b_{k,l}$ be the associated connection one-form given by (3.1). Then

$$V_1(\sigma) = \sum_{k,l} \frac{I_k^0 I_l^0 \omega_l}{\omega_k} \|b_{k,l}\|^2. \tag{3.2}$$

Notice that the norm $\|b_{k,l}\|$ is insensitive to the choice of signs for the frame.

Quantum mechanics

In quantum mechanics, it is also convenient to work with the normal bundle $N\Sigma$. If we consider initial conditions in $L^2(\mathbb{R}^{n+m})$ that are supported near Σ then, to a good approximation for large λ, the time evolution stays near Σ. Thus we lose nothing by inserting Dirichlet boundary conditions on the boundary of the tubular neighbourhood of Σ, and may transfer our considerations to $L^2(N\Sigma_\delta, d\mathrm{vol})$, where $d\mathrm{vol}$ is computed using the pulled back metric. If we extend the pulled back metric, and make a suitable definition of H_λ in the complement of $N\Sigma_\delta$, we may remove the boundary condition. Thus we may assume that that the Hamiltonian H_λ acts in $L^2(N\Sigma, d\mathrm{vol})$.

We now introduce the group of dilations in the normal directions by defining

$$(D_\lambda \psi)(\sigma, n) = \lambda^{m/2} \psi(\sigma, \lambda n).$$

This is a unitary operator from $L^2(N\Sigma, d\mathrm{vol}_\lambda)$ to $L^2(N\Sigma, d\mathrm{vol})$ where $d\mathrm{vol}_\lambda$ denotes the pulled back density $d\mathrm{vol}_\lambda(\sigma, n) = d\mathrm{vol}(\sigma, \lambda^{-1} n)$. Since the spaces $L^2(N\Sigma, d\mathrm{vol}_\lambda)$ depend on λ, and we want to deal with a fixed Hilbert space as $\lambda \to \infty$, we perform an an additional unitary transformation. Let

$$d\mathrm{vol}_{N\Sigma} = \lim_{\lambda \to \infty} d\mathrm{vol}_\lambda = d\mathrm{vol}_\Sigma \otimes d\mathrm{vol}_{\mathbb{R}^{n+m}}$$

Then the quotient of densities $d\mathrm{vol}_{N\Sigma}/d\mathrm{vol}_\lambda$ is a function on $N\Sigma$ and we may define M_λ to be the operator of multiplication by $\sqrt{d\mathrm{vol}_{N\Sigma}/d\mathrm{vol}_\lambda}$. The operator M_λ is unitary from $L^2(N\Sigma, d\mathrm{vol}_{N\Sigma})$ to $L^2(N\Sigma, d\mathrm{vol}_\lambda)$. Let

$$U_\lambda = D_\lambda M_\lambda.$$

Notice that the support of a family of initial conditions of the form $U_\lambda\psi_0$ is being squeezed close to Σ as $\lambda \to \infty$. We want to consider a such a sequence of initial conditions. Therefore it is natural to consider the conjugated Hamiltonian

$$L_\lambda = U_\lambda^* H_\lambda U_\lambda,$$

since the evolution generated by L_λ acting on ψ_0 is unitarily equivalent to the evolution generated by H_λ acting on $U_\lambda\psi_0$.

As a first step we perform a large λ expansion. This yields

$$L_\lambda = H_B + \lambda^2 H_O + O(\lambda^{-1})$$

where H_O and H_B are defined in the local co-ordinates (x, y) associated to some local frame (as introduced above) as follows. Let

$$D_x = \begin{bmatrix} D_{x_1} \\ \vdots \\ D_{x_n} \end{bmatrix}, \quad D_y = \begin{bmatrix} D_{y_1} \\ \vdots \\ D_{y_m} \end{bmatrix}$$

and let $H = [\langle \partial/\partial x_i, \partial/\partial x_j \rangle]$ be the local expression for the metric on Σ. Define $h = \det(H)$. Define the operator F_i by

$$F_i = \sum_{k,l} y_k b_{k,l} [\partial/\partial x_i] D_{y_l},$$

where $b_{k,l}$ is the connection form defined by (3.1), and let

$$F = \begin{bmatrix} F_1 \\ \vdots \\ F_n \end{bmatrix}.$$

Then

$$H_O = D_y^* D_y$$

is the harmonic oscillator Hamiltonian in the normal variables, and

$$H_B = (D_x + F)^* H^{-1} (D_x + F) + K + V(\sigma).$$

Here the adjoints are taken with respect to $d\mathrm{vol}_{N\Sigma}$, given locally by $\sqrt{h}|d^n x|d^m y|$. In other words, $D_y^* = -D_y^t$ and $D_x^* = -(1/\sqrt{(}h))D_x^t\sqrt{h}$. The additional potential K is given by

$$K = \frac{n(n-1)}{2} s - \frac{n^2}{4}\mathbf{h}^2$$

where s is the scalar curvature and $\mathbf{h}$ is the mean curvature vector. Notice that this extra potential does depend on the imbedding of Σ in $\mathbb{R}^{n+m}$, since the mean curvature does.

Theorem 4.1 *Let H_λ be the Hamiltonian (1.2), considered to be acting in $L^2(N\Sigma, d\mathrm{vol})$, as explained above, where $V, W \in C^\infty$, W has the form (2.1) and satisfies*

(i) the eigenvalues of ω_α^2 of $A(\sigma)$ do not depend on σ.

Let $L_\lambda = U_\lambda^* H_\lambda U_\lambda$ acting in $L^2(N\Sigma, d\mathrm{vol}_{N\Sigma})$. Then

$$\operatorname*{s-lim}_{\lambda\to\infty} \left(e^{-itL_\lambda} - e^{-it(H_B + \lambda^2 H_O)} \right) = 0$$

Just as in the classical case, this theorem provides a satisfactory description of the motion if $[H_B, H_O] = 0$, so that $\exp(-it(H_B + \lambda^2 H_O)) = \exp(-itH_B)\exp(-it\lambda^2 H_O)$. As before, this will happen, for example, if Σ has co-dimension one, or if all the frequencies ω_α are equal.

If Σ has co-dimension one, then the normal bundle is trivial. (We are assuming that Σ is compact.) Then we have $L^2(N\Sigma, d\mathrm{vol}_{N\Sigma}) = L^2(\Sigma, d\mathrm{vol}_\Sigma) \otimes L^2(\mathbb{R}, dy)$ and $H_B = h_B \otimes I$ for a Schrödinger operator h_B acting in $L^2(\Sigma, d\mathrm{vol}_\Sigma)$. Since $H_O = I \otimes h_O$ we have that $\exp(-it(H_B + \lambda^2 H_O)) = \exp(-ith_B) \otimes \exp(-it\lambda^2 h_O)$. This can be interpreted as a motion in $L^2(\Sigma, d\mathrm{vol}_\Sigma)$ with superimposed normal oscillations.

In the case where the frequencies ω_α are all equal, the normal bundle may be non-trivial, and there is not such a simple tensor product decomposition of $L^2(N\Sigma, d\mathrm{vol}_{N\Sigma})$. However, there is a geometric interpretation, which we now explain briefly. Consider the normal frame bundle $F\Sigma$ for Σ. Concretely, this may be thought of as a subset of $\mathbb{R}^{n+m} \times \mathbb{R}^{(n+m)m}$ given by

$$F\Sigma = \{\sigma, n_1, \ldots, n_m : \sigma \in \Sigma \quad \text{and} \quad n_1, \ldots, n_m \quad \text{is an orthonormal basis for } N_\sigma\Sigma\}.$$

The bundle $F\Sigma$ is a principal bundle with structure group the orthogonal group $O(m)$. Given a representation of $O(m)$ on a vector space V there is an associated vector bundle with fibre V. For example, $N\Sigma$ is the vector bundle associated to the identity representation of $O(m)$ by $m \times m$ matrices. It turns out that $L^2(N\Sigma, d\mathrm{vol}_{N\Sigma})$ is the vector bundle with fibre $L^2(\mathbb{R}^m, d^m y)$ associated with the left regular representation of $O(m)$. With this interpretation, the operator $D_x + F$ is a covariant derivative.

For some initial conditions (i.e., the vector on which $\exp(-itL_\lambda)$ acts,) the limiting motion may again be thought of as taking place in $L^2(\Sigma, d\mathrm{vol}_\Sigma)$ with superimposed oscillations. For example, consider the subspace of functions in $L^2(N\Sigma, d\mathrm{vol}_{N\Sigma})$ that are radially symmetric in the fibre variable n. This subspace does have a tensor product decomposition $L^2(\Sigma, d\mathrm{vol}_\Sigma) \otimes L^2_{\mathrm{radial}}(\mathbb{R}^m, d^m y)$. It is an invariant subspace for H_B. Furthermore, $F = 0$ on this subspace, so the restriction of H_B has the form $h_B \otimes I$. Thus, if ψ_0 is a radial function in n, then $\exp(-itL_\lambda)\psi_0 = \exp(-ith_B) \otimes \exp(-it\lambda^2 h_O)\psi_0$. As above, we interpret this as motion in $L^2(\Sigma, d\mathrm{vol}_\Sigma)$ with superimposed normal oscillations.

On the other hand, if $N\Sigma$ is non-trivial, it may happen that the limiting motion takes place on a space of sections of a vector bundle over Σ. Instead of giving more details about the general case, we offer the following illustrative example. Instead of a normal bundle, consider the Möbius band $\mathcal{B}$ defined by $\mathbb{R} \times \mathbb{R} / \sim$, where $(x, y) \sim (x + 1, -y)$. This an $O(1)$ bundle over S^1 with fibre $\mathbb{R}$. An L^2

function ψ on $\mathcal{B}$ can be thought of as a function on $\mathbb{R}\times\mathbb{R}$ satisfying $\psi(x+1,-y)=\psi(x,y)$. If we decompose $\psi(x,y)$, for fixed x, into odd and even functions of y

$$\psi(x,y)=\psi_{\rm even}(x,y)+\psi_{\rm odd}(x,y)$$

then $\psi_{\rm even}(x+1,y)=\psi_{\rm even}(x,y)$ and $\psi_{\rm odd}(x+1,y)=-\psi_{\rm odd}(x,y)$. (Notice that these are eigenfunctions for the left regular representation of $O(1)$ on $L^2(\mathbb{R})$.) Thus $\psi_{\rm even}$ can be thought of as an $L^2(\mathbb{R},dy)$ valued function on S^1, while $\psi_{\rm odd}$ can be thought of as an $L^2(\mathbb{R},dy)$ valued section of a line bundle over S^1 (which happens to be $\mathcal{B}$ itself). In this way we obtain the decomposition

$$L^2(\mathcal{B})=L^2(S^1,dx)\otimes L^2_{\rm even}(\mathbb{R},dy)\ \oplus\ \Gamma(S^1,dx)\otimes L^2_{\rm odd}(\mathbb{R},dy)$$

where Γ is the space of L^2 sections of $\mathcal{B}$.

In this example, the bundle is flat, so $F=0$, $H_B=-D_x^2+V(x)$ and $H_O=-D_y^2$ acting in $L^2(\mathcal{B},dxdy)$. Let $h_+=-D_x^2+V(x)$ acting in $L^2(S^1,dx)$ and $h_-=-D_x^2+V(x)$ acting in $\Gamma(S^1,dx)$. Let $h_0=-D_y^2$ acting in $L^2(\mathbb{R},dy)$, with $L^2_{\rm even}(\mathbb{R},dy)$ and $L^2_{\rm odd}(\mathbb{R},dy)$ as invariant subspaces. Then

$$e^{-it(H_B+\lambda^2H_O)}=e^{-ith_+}\otimes e^{-it\lambda^2h_O}\ \oplus\ e^{-ith_-}\otimes e^{-it\lambda^2h_O}$$

So if the initial condition happens to lie in $\Gamma\otimes L^2_{\rm odd}$, then we would think of the limiting motion as taking place in Γ, with superimposed oscillations in $L^2_{\rm odd}$.

Finally, we consider the case where the eigenvalues $\omega_1,\dots,\omega_m$ of $A(\sigma)$ are all different. (For the case when some eigenvalues, but not all, are the same, see [FH].) For simplicity we will assume that we can make a global choice of sign for the eigenvectors, thereby obtaining a global frame $n_1,\dots,n_m$ for $N\Sigma$. Then the bundle $N\Sigma$ is trivial, with the map from $\Sigma\times\mathbb{R}^m\to N\Sigma$ sending $(\sigma,y)\mapsto(\sigma,\sum y_kn_k)$ providing the trivialization. Thus $L^2(N\Sigma,d{\rm vol}_{N\Sigma})=L^2(\Sigma,d{\rm vol}_\Sigma)\otimes L^2(\mathbb{R}^m,d^my)$.

In this situation, $[H_B,H_O]\neq0$, so to determine the limiting motion we must perform a quantum version of averaging. We have the following theorem.

Theorem 4.2 *Let H_λ be the Hamiltonian (1.2), considered to be acting in $L^2(N\Sigma,{\rm dvol})$, as explained above, where $V,W\in C^\infty$, W has the form (2.1) and satisfies*

(i) the eigenvalues of $\omega_1^2,\dots,\omega_m^2$ of $A(\sigma)$ do not depend on σ.

(ii) If $j\neq k$ then $\omega_j\pm\omega_k\neq0$,

(iii) If $j\neq k$ and $l\neq m$ then $\omega_j\pm\omega_k\pm\omega_l\pm\omega_m\neq0$

Let $L_\lambda=U_\lambda^*H_\lambda U_\lambda$ acting in $L^2(N\Sigma,d{\rm vol}_{N\Sigma})=L^2(\Sigma,d{\rm vol}_\Sigma)\otimes L^2(\mathbb{R}^m,d^my)$. Let

$$h_B=-\Delta_\Sigma+K+V(\sigma)+V_1(\sigma)$$

acting in $L^2(\Sigma,d{\rm vol}_\Sigma)$, where V_1 is defined by (3.2) above. Let h_O be the harmonic oscillator Hamiltonian acting in $L^2(\mathbb{R}^m,d^my)$. Then

$$\operatorname*{s-lim}_{\lambda\to\infty}\left(e^{-itL_\lambda}-e^{-ith_B}\otimes e^{-it\lambda^2h_O}\right)=0$$

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