Killling vector fields and quantisation of natural Hamiltonians

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Abstract

The usual canonical prescription ordinarily made for the obtention of the quantum Hamiltonian operator for a classical system leads to some ambiguities in situations beyond the simplest ones and these ambiguities arise unavoidably when the configuration space has non-zero curvature, as well as in systems in Euclidean space but with a position-dependent mass. A recently proposed method to circumvent this difficulty for natural Hamiltonians will be described. The idea is not to quantise the coordinates and their (classical) conjugate momenta (which is where the ambiguities could arise), but to work directly with Killing vector fields and associated Noether momenta in order to get in some unambiguous way the corresponding Hamiltonian operator. The example of one-dimensional position-dependent mass systems will be used to illustrate the method.

This is a report on previous collaborations with:

M.F. Rañada and M.Santander

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Introduction

I meet Giuseppe for the first time at Genth in July of 1986, during the

1st Workshop on Diff. Geom. Methods in Classical Mechanics.

This was the beginning of a series of meetings.

The second was organized by myself in Jaca (1987) and the third one in Ferrara (1998)

by Giuseppe, of course!!!

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José F. Cariñena Alberto Ibort Giuseppe Marmo Giuseppe Morandi

Geometry from Dynamics, Classical and Quantum



A long collaboration

The book is devoted to establish a geometric approach to both Classical and Quantum Mechanics and the transition from Classical to Quantum Mechanics.

Symplectic geometry is the common framework for dealing with both types of systems

The geometric framework for the description of classical mechanical systems is the theory of Hamiltonian dynamical systems.

A symplectic structure ω on a differentiable manifold M, or more generally a Poisson structure, is the basic concept.

It is then possible to define an associated Poisson bracket endowing the set of functions on M with a real Lie algebra structure.

The dynamics is given by the Hamiltonian vector field X_H defined by the Hamiltonian $H \in C^\infty(M)$ by means of

$$i(X_H)\omega = dH.$$

The system of differential equations determining the integral curves of X_H in Darboux coordinates are Hamilton equations.

A particularly interesting case is when the manifold is the cotangent bundle of the configuration space Q, $M=T^*Q$, endowed with its natural symplectic structure.

The states are the points of M, and the observables are the functions $F \in C^{\infty}(M)$. The measure of an observable F in a state x is given by the evaluation map, the result being F(x)

On the other side, the mathematical model for Quantum Theories is different. In Quantum Mechanics in Schrödinger picture:

- \square (pure) states are (rays rather than) vectors ψ of a Hilbert space $(\mathcal{H}, \langle \cdot, \cdot \rangle)$
- \square observables are selfadjoint operators in ${\mathcal H}$
- \Box the results of the measure of the observable A on the pure state ψ may be any eigenvalue of A but with probabilities such that the mean value is given by

$$e(\psi) = \frac{\langle \psi, A\psi \rangle}{\langle \psi, \psi \rangle}$$

☐ dynamics is given by Schrödinger equation

The framework unifying both approaches is the theory of Hamiltonian dynamical systems.

Hamiltonian dynamical systems

A symplectic manifold is a pair (M,ω) where M is a differentiable manifold and ω is a symplectic form, i.e. a non-degenerate closed 2-form in M, $\omega \in Z^2(M)$: $d\omega = 0$.

Non-degeneracy of ω means that for every point $u \in M$ the map $\widehat{\omega}_u : T_uM \to T_u^*M$:

$$\langle \widehat{\omega}_u(v), v' \rangle = \omega_u(v, v') , \qquad v, v' \in T_u M,$$

is a bijection. This implies that the dimension of M is even, $\dim M = 2n$.

 $\widehat{\omega}:TM\to T^*M$ is a base-preserving fibred map, i.e. the following diagram :

$$TM \xrightarrow{\widehat{\omega}} T^*M$$

$$\downarrow^{\tau} \qquad \qquad \downarrow^{\pi}$$

$$M \xrightarrow{\mathrm{id}_M} M$$

is commutative and induces a \mathbb{R} -linear map between the spaces of sections of both bundles which, with a slight abuse of notation, we also write $\widehat{\omega}:\mathfrak{X}(M)\to \bigwedge^1(M)$.

The vector fields corresponding to closed forms are called locally-Hamiltonian vector fields and those corresponding to exact forms are said to be Hamiltonian vector fields.

$$\widehat{\omega}(\mathfrak{X}_{\mathrm{H}}(M,\omega)) = B^1(M), \qquad \widehat{\omega}(\mathfrak{X}_{\mathrm{LH}}(M,\omega)) = Z^1(M).$$

If $H \in C^{\infty}(M)$, the Hamiltonian vector field X_H is defined by the vector field s.t.

$$i(X_H)\omega = dH$$

 (M,ω,H) is a Hamiltonian system whenever (M,ω) is a symplectic manifold and $H\in C^\infty(M)$: the dynamical vector field is X_H

Cartan identity, $\mathcal{L}_X = i(X) \circ d + d \circ i(X)$, shows that $X \in \mathfrak{X}_{LH}(M,\omega)$ if and only if $\mathcal{L}_X \omega = 0$.

Darboux proved that $d\omega=0$ and regularity of ω imply that around each point $u\in M$ there is a local chart (U,ϕ) such that if $\phi=(q^1,\ldots,q^n;p_1,\ldots,p_n)$, then

$$\omega|_{U} = \sum_{i=1}^{n} dq^{i} \wedge dp_{i}.$$

Such coordinates are said to be Darboux coordinates. The expression of X_H in Darboux coordinates is given by

$$X_H = \sum_{i=1}^n \left(\frac{\partial H}{\partial p_i} \frac{\partial}{\partial q^i} - \frac{\partial H}{\partial q^i} \frac{\partial}{\partial p_i} \right) ,$$

and therefore, the local equations determining its integral curves are similar to Hamilton equations.

$$\begin{cases} \dot{q}^i &=& \frac{\partial H}{\partial p_i} \\ \dot{p}_i &=& -\frac{\partial H}{\partial q^i} \end{cases}$$

Define the $Poisson\ bracket$ of two functions $f,g\in C^\infty(M)$ as being the function $\{f,g\}$ given by:

$$\{f,g\} = \omega(X_f,X_g) = df(X_g) = -dg(X_f) \ .$$

In Darboux coordinates for ω the expression for $\{f,g\}$ is the usual one:

$$\{f,g\} = \sum_{i=1}^{n} \left(\frac{\partial f}{\partial q^{i}} \frac{\partial g}{\partial p_{i}} - \frac{\partial f}{\partial p_{i}} \frac{\partial g}{\partial q^{i}} \right).$$

If X,Y are locally Hamiltonian vector fields, then [X,Y] is a Hamiltonian vector field, its Hamiltonian being $\omega(Y,X)$.

It is a consequence of the relation $i(X)\mathcal{L}_Y\alpha - \mathcal{L}_Yi(X)\alpha = i([X,Y])\alpha$, which is valid for any form α . We then obtain:

$$i([X,Y])\omega = i(X)\mathcal{L}_Y\omega - \mathcal{L}_Y i(X)\omega = -\mathcal{L}_Y i(X)\omega = -i(Y)d[i(X)\omega] - d[i(Y)i(X)\omega] = -d[\omega(X,Y)] .$$

In particular, when $X = X_f$ and $Y = X_g$ in the previous relation:

$$d\{f,g\} = -i([X_f, X_g])\omega ,$$

i.e.,

$$[X_f, X_g] = X_{\{g,f\}}.$$

This shows that the set of Hamiltonian vector fields, to be denoted $\mathfrak{X}_{\mathrm{H}}(M,\omega)$, is an ideal of the Lie algebra of locally-Hamiltonian vector fields $\mathfrak{X}_{\mathrm{LH}}(M,\omega)$ and that

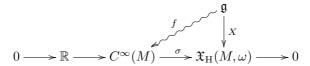
$$0 \longrightarrow \mathbb{R} \longrightarrow C^{\infty}(M) \xrightarrow{\sigma} \mathfrak{X}_{H}(M,\omega) \longrightarrow 0$$

with $\sigma = -\widehat{\omega}^{-1} \circ d$, is an exact sequence of Lie algebras.

An action Φ of a Lie group G on M defines a set of fundamental vector fields $X_a \in \mathfrak{X}(M), \ a \in \mathfrak{g}, \ \text{by} \ X_a(m) = \Phi_{m*e}(-a)$ and the map $X: \mathfrak{g} \to \mathfrak{X}(M), \ a \in \mathfrak{g} \to X_a$ is a Lie algebra homomorphism,

$$[X_a, X_b] = X_{[a,b]}.$$

If the action of G is strongly symplectic, $X(\mathfrak{g})\subset \mathfrak{X}_{\mathrm{H}}(M,\omega)$, then X is a Lie algebra homomorphism $X:\mathfrak{g}\to \mathfrak{X}_{\mathrm{H}}(M,\omega)$, and then there exists a linear map $f:\mathfrak{g}\to C^\infty(M)$, called comomentum map, making commutative the following diagram:



The corresponding momentum map introduced by Souriau, is the map $P:M\to \mathfrak{g}^*$, defined by

$$\langle P(m), a \rangle = f_a(m), \quad \forall m \in M, a \in \mathfrak{g}.$$

It is not uniquely defined but two possible comomentum map differ by a linear map $r:\mathfrak{g}\to\mathbb{R},$

$$f_a'(m) = f_a(m) + r(a).$$

In case of exact symplectic actions on exact symplectic manifolds (M,θ) , namely, $g^*\theta=\theta, \forall g\in G$, the fundamental vector fields X_a are Hamiltonian and a comomentum map can be defined as $f_a=-i(X_a)\theta$. This is the case of an action of a Lie group G on a cotangent bundle T^*Q lifted from an action of G on its base manifold.

Recall that if $X=\xi^i(q)\partial/\partial q^i\in\mathfrak{X}(Q)$, its cotangent lift $\widetilde{X}\in\mathfrak{X}(T^*Q)$ (satisfying $\mathcal{L}_{\widetilde{X}}\theta=0$, with θ the Liouville 1-form), $\theta=p_i\,dq^i$, is

$$\widetilde{X} = \xi^i \frac{\partial}{\partial q^i} - p_i \frac{\partial \xi^i}{\partial q^j} \frac{\partial}{\partial p_j}.$$

As an instance if the configuration space is $Q=\mathbb{R}^3$ we can consider vector fields generating translations on $Q=\mathbb{R}^3$, and their corresponding lift in $T^*\mathbb{R}^3$, the fundamental vector fields in \mathbb{R}^3 being $X_a=-a^i\,\partial/\partial q^i$, with canonical lifts \widetilde{X}_a a $T^*\mathbb{R}^3$

$$\widetilde{X}_a = -a^i \frac{\partial}{\partial q^i} \ .$$

The functions $f_a \in C^{\infty}(T^*\mathbb{R}^3)$ are defined by

$$f_a(q,p) = -[i(\widetilde{X}_a)\theta](q,p) = a^i p_i$$
.

Using $f_a(q,p) = \langle \vec{P}(q,p), a \rangle$ and identifying \mathbb{R}^3 , as Lie algebra of translations, with its dual, we obtain

$$\vec{P}(q,p) = \vec{p}.$$

If consider the action of $SO(3,\mathbb{R})$ on \mathbb{R}^3 and the induced action on $T^*\mathbb{R}^3$, the fundamental vector fields in \mathbb{R}^3 are

$$X_i = -\epsilon_{ijk} \, q^j \frac{\partial}{\partial q^k} \,,$$

with canonical lifts

$$\widetilde{X}_i = -\epsilon_{ijk} \left(q^j \frac{\partial}{\partial q^k} + p_j \frac{\partial}{\partial p_k} \right),$$

and consequently a comomentum map is

$$f_{\vec{n}}(q,p) = n_i \, \epsilon_{ijk} \, q^j \, p_k = \vec{n} \cdot (\vec{q} \times \vec{p}) \, .$$

Using the identification of \mathbb{R}^3 with its dual space we see that

$$\vec{P}(q,p) = \vec{q} \times \vec{p},$$

i.e. the associated momentum is the angular momentum

Dynamical systems of mechanical type

A regular natural Lagrangian system is given by a non-degenerate symmetric (0,2)-tensor field g on the configuration space Q and a function V on Q: The Lagrangian function $L \in C^{\infty}(TQ)$ is given by

$$L_{g,V}(v) = \frac{1}{2}(\tau_Q^*g)(v,v) + \tau^*V,$$

where $\tau_Q: TQ \to Q$ is the tangent bundle.

Nondegeneracy means that the map $\widehat{g}: TQ \to T^*Q$ from the tangent bundle $\tau_Q: TQ \to Q$ to the cotangent bundle $\pi_Q: T^*Q \to Q$, defined by $\langle \widehat{g}(v), w \rangle = g(v, w)$, where $v, w \in T_xQ$, is regular.

 \widehat{g} is a fibred map over the identity on Q and induces a map between the spaces of sections $\widehat{g}:\mathfrak{X}(Q)\to\Omega^1(Q)$: $\langle\widehat{g}(X),Y\rangle=g(X,Y)$.

The vector field corresponding to the exact 1-form df is called $\operatorname{grad} f$, i.e.

$$\widehat{g}(\operatorname{grad} f) = df, \quad \forall f \in C^{\infty}(Q).$$

The case V=0 corresponds to free motion on the Riemann manifold (Q,g), the Lagrangian then being given by the kinetic energy defined by the metric g:

$$T_g(v) = \frac{1}{2}(\tau_Q^*g)(v, v), \qquad v \in TQ,$$

which can be rewritten as the following function on TQ:

$$T_g = \frac{1}{2} g(T\tau_Q \circ D, T\tau_Q \circ D),$$

with D being any second order differential equation vector field, i.e. a vector field on TQ, and therefore $\tau_{TQ} \circ D = \mathrm{id}_{TQ}$, such that also $T\tau_Q \circ D = \mathrm{id}_{TQ}$.

If (U,q^1,\ldots,q^n) is a local chart on Q we consider the coordinate basis of $\mathfrak{X}(U)$ denoted $\{\partial/\partial q^j\mid j=1,\ldots,n\}$ and its dual basis for $\Omega^1(U)$, $\{dq^j\mid j=1,\ldots,n\}$.

A vector and a covector in a point $q \in U$ are $v = v^j (\partial/\partial q^j)_q$ and $\zeta = p_j (dq^j)_q$, with $v^j = \langle dq^j, v \rangle$ and $p_j = \langle \zeta, \partial/\partial q^j \rangle$. The local expressions for g and T_g are:

$$g = g_{ij}(q) dq^i \otimes dq^j, \qquad T_g(v) = \frac{1}{2} g_{ij}(\tau_Q(v)) v^i v^j,$$

while the coordinate expression for the gradient of a function $f \in C^\infty(Q)$ is:

$$(\operatorname{grad} f)^i = g^{ij} \frac{\partial f}{\partial q^j}, \quad \text{with} \quad \sum_{k=1}^n g^{ik}(q) \, g_{kj}(q) = \delta^i_j.$$

The dynamics is then given by a vector field Γ_L solution of the dynamical equation

$$i(\Gamma_L)\omega_L = dE_L.$$

where the energy E_L of the Lagrangian system is defined by $E_L = \Delta L - L$, with Δ being the Liouville vector field, generator of dilations along the fibres, given by

$$\Delta f(v) = \frac{d}{dt} f(e^t v)|_{t=0},$$

for all $v \in TQ$ and $f \in C^{\infty}(TQ)$.

As $\Delta(T_g)=2\,T_g$ and $\Delta(V)=0$, the total energy is $E_L=T_g+V$.

The Cartan 1-form $\theta_L=dL\circ S$, where S is the vertical endomorphism, gives us an exact 2-form $\omega_L=-d\theta_L$ which is non-degenerate when the Lagrangian is regular and then (TQ,ω_L,E_L) is a Hamiltonian dynamical system.

The coordinate expressions of $\theta_L = dL \circ S$ and ω_L are:

$$\theta_L(q,v) = g_{ij}(q) v^j dq^i, \qquad \omega_L = g_{ij} dq^i \wedge dv^j + \frac{1}{2} \left(\frac{\partial g_{ij}}{\partial q^k} v^j - \frac{\partial g_{kj}}{\partial q^i} v^j \right) dq^i \wedge dq^k.$$

To be remarked that ω_L only depends on T_g and not on V, and we can use ω_T instead of ω_L .

Moreover, it can be proved that if $X \in \mathfrak{X}(Q)$ and $X^c \in \mathfrak{X}(TQ)$ is its complete lift,

$$X^c T_g = T_{\mathcal{L}_X g},$$

and this property can be used to prove that the lifts of the flow of X are symplectomorphisms if and only if $\mathcal{L}_X g=0$, i.e. X is a Killing vector field. Actually,

$$\mathcal{L}_{X^c}\omega_L = \mathcal{L}_{X^c}\omega_{T_g} = \omega_{X^c(T_g)} = \omega_{T_{\mathcal{L}_{X^g}}},$$

and consequently, if X is a Killing vector field, $\mathcal{L}_{X^c}\omega_L=0$.

Recall also that Killing vector fields close under commutators on a Lie algebra.

Legendre transformation is regular because the (0,2)-symmetric tensor g is assumed to be non-degenerate: $v \in T_qQ \mapsto \alpha \in T_q^*Q$ such that $\langle \alpha, w \rangle = g(v,w)$.

In the above mentioned local coordinates

$$p_i = \frac{\partial T}{\partial v^i} = g_{ik}(q) v^k \iff v^i = g^{ij}(q) p_j,$$

with $g^{ik}(q) g_{kj}(q) = \delta^i_j$.

The Hamiltonian is the kinetic energy of the free system in terms of momenta:

$$H = \frac{1}{2}g(\widehat{g}^{-1}(p), \widehat{g}^{-1}(p)) = \frac{1}{2}g^{ij} p_i p_j.$$

If we consider the exact symplectic action of a Lie group G on the bundle T^*Q defined by lifting an action of G on the base Q, if $X_a=\xi^i_a(q)\,\partial/\partial q^i$ is the infinitesimal generator of $a\in\mathfrak{g}$ in the action on Q its lifting is given in the induced coordinate system by

$$\widetilde{X}_a = \xi_a^i(q) \frac{\partial}{\partial q^i} - p_i \frac{\partial \xi_a^i}{\partial q^j} \frac{\partial}{\partial p_j}.$$

If \widetilde{X}_a is Hamiltonian, as $\theta = p_i \, dq^i$ we have that $f_a(q,p) = -p_i \, \xi_a^i(q)$.

In the particular case of a natural Lagrangian system as the complete lift $X^c \in \mathfrak{X}(TQ)$ of a Killing vector field $X \in \mathfrak{X}(Q)$ is a Hamiltonian vector field, we have an exact action of the Lie algebra of Killing vector fields on TQ and the momentum map $P:TQ \to \mathfrak{kill}^*$ is defined by

$$\langle P(x,v),a\rangle = f_a(x,v) = -\theta_{T_q}(X_a^c) = -g_{ij}v^j\xi_a^i, \qquad (x,v)\in TQ, a\in \mathfrak{kil}.$$

and in the corresponding Hamiltonian formalism, $P: T^*Q \to \mathfrak{kill}^*$ by

$$\langle P(x,p),a\rangle = f_a(x,p) = -\theta_o(\widetilde{X}_a) = -p_i\,\xi_a^i, \qquad (x,p)\in T^*Q, a\in \mathfrak{kil}.$$

Geometric approach to Quantum Mechanics

The Schrödinger picture of Quantum mechanics admits a geometric interpretation similar to that of classical mechanics.

A separable complex Hilbert space $(\mathcal{H}, \langle \cdot, \cdot \rangle)$ can be considered as a real linear space, to be then denoted $\mathcal{H}_{\mathbb{R}}$. The norm in \mathcal{H} defines a norm in $\mathcal{H}_{\mathbb{R}}$, where $\|\psi\|_{\mathbb{R}} = \|\psi\|_{\mathbb{C}}$.

The linear real space $\mathcal{H}_{\mathbb{R}}$ is endowed with a natural symplectic structure as follows:

$$\omega(\psi_1, \psi_2) = 2 \operatorname{Imag} \langle \psi_1, \psi_2 \rangle.$$

The Hilbert $\mathcal{H}_{\mathbb{R}}$ can be considered as a real manifold modelled by a Banach space admitting a global chart.

The tangent space $T_{\phi}\mathcal{H}_{\mathbb{R}}$ at any point $\phi \in \mathcal{H}_{\mathbb{R}}$ can be identified with $\mathcal{H}_{\mathbb{R}}$ itself: the isomorphism associates $\psi \in \mathcal{H}_{\mathbb{R}}$ with the vector $\dot{\psi} \in T_{\phi}\mathcal{H}_{\mathbb{R}}$ given by:

$$\dot{\psi}f(\phi) := \left(\frac{d}{dt}f(\phi + t\psi)\right)_{|t=0}, \quad \forall f \in C^{\infty}(\mathcal{H}_{\mathbb{R}}).$$

The real manifold can be endowed with a symplectic 2-form ω :

$$\omega_{\phi}(\dot{\psi}, \dot{\psi}') = 2 \operatorname{Imag} \langle \psi, \psi' \rangle$$
.

One can see that the constant symplectic structure ω in $\mathcal{H}_{\mathbb{R}}$, considered as a Banach manifold, is exact, i.e., there exists a 1-form $\theta \in \bigwedge^1(\mathcal{H}_{\mathbb{R}})$ such that $\omega = -d\theta$. Such a 1-form $\theta \in \bigwedge^1(\mathcal{H})$ is, for instance, the one defined by

$$\theta(\psi_1)[\dot{\psi}_2] = -\operatorname{Imag}\langle \psi_1, \psi_2 \rangle.$$

This shows that the geometric framework for usual Schrödinger picture is that of symplectic mechanics, as in the classical case.

A continuous vector field in $\mathcal{H}_{\mathbb{R}}$ is a continuous map $X \colon \mathcal{H}_{\mathbb{R}} \to \mathcal{H}_{\mathbb{R}}$. For instance for each $\phi \in \mathcal{H}$, the constant vector field X_{ϕ} defined by

$$X_{\phi}(\psi) = \dot{\phi}.$$

It is the generator of the one-parameter subgroup of transformations of $\mathcal{H}_{\mathbb{R}}$ given by

$$\Phi(t,\psi) = \psi + t \,\phi.$$

As another particular example of vector field consider the vector field X_A defined by the \mathbb{C} -linear map $A: \mathcal{H} \to \mathcal{H}$, and in particular when A is skew-selfadjoint.

With the natural identification natural of $T\mathcal{H}_{\mathbb{R}} \approx \mathcal{H}_{\mathbb{R}} \times \mathcal{H}_{\mathbb{R}}$, X_A is given by

$$X_A: \phi \mapsto (\phi, A\phi) \in \mathcal{H}_{\mathbb{R}} \times \mathcal{H}_{\mathbb{R}}$$
.

When A=I the vector field X_I is the Liouville generator of dilations along the fibres, $\Delta=X_I$, usually denoted Δ given by $\Delta(\phi)=(\phi,\phi)$.

Given a selfadjoint operator A in $\mathcal H$ we can define a real function in $\mathcal H_\mathbb R$ by

$$a(\phi) = \langle \phi, A\phi \rangle,$$

i.e.,

$$a = \langle \Delta, X_A \rangle$$
.

Then,

$$da_{\phi}(\psi) = \frac{d}{dt}a(\phi + t\psi)_{t=0} = \frac{d}{dt} \left[\langle \phi + t\psi, A(\phi + t\psi) \rangle \right]_{|t=0}$$
$$= 2\operatorname{Re} \langle \psi, A\phi \rangle = 2\operatorname{Imag} \langle -i A\phi, \psi \rangle = \omega(-i A\phi, \psi).$$

If we recall that the Hamiltonian vector field defined by the function a is such that for each $\psi \in T_\phi \mathcal{H} = \mathcal{H}$,

$$da_{\phi}(\psi) = \omega(X_a(\phi), \psi),$$

we see that

$$X_a(\phi) = -\mathrm{i} A\phi$$
.

Therefore if A is the Hamiltonian H of a quantum system, the Schrödinger equation describing time-evolution plays the rôle of 'Hamilton equations' for the Hamiltonian dynamical system (\mathcal{H}, ω, h) , where $h(\phi) = \langle \phi, H\phi \rangle$: the integral curves of X_h satisfy

$$\dot{\phi} = X_h(\phi) = -i H \phi$$
.

The real functions $a(\phi)=\langle \phi,A\phi\rangle$ and $b(\phi)=\langle \phi,B\phi\rangle$ corresponding to two selfadjoint operators A and B satisfy

$${a,b}(\phi) = -i \langle \phi, [A,B]\phi \rangle,$$

because

$$\{a,b\}(\phi) = [\omega(X_a,X_b)](\phi) = \omega_{\phi}(X_a(\phi),X_b(\phi)) = 2\operatorname{Imag}\langle A\phi,B\phi\rangle,$$

and taking into account that

$$2\operatorname{Imag}\langle A\phi, B\phi\rangle = -\mathrm{i}\left[\langle A\phi, B\phi\rangle - \langle B\phi, A\phi\rangle\right] = -\mathrm{i}\left[\langle \phi, AB\phi\rangle - \langle \phi, BA\phi\rangle\right],$$

we find the above result.

In particular, on the integral curves of the vector field X_h defined by a Hamiltonian H,

$$\dot{a}(\phi) = \{a, h\}(\phi) = -i \langle \phi, [A, H]\phi \rangle,$$

what is usually known as Ehrenfest theorem:

$$\frac{d}{dt}\langle\phi,A\phi\rangle = -\mathrm{i}\langle\phi,[A,H]\phi\rangle.$$

There is another relevant symmetric (0,2) tensor field which is given by the Real part of the inner product. It endows $\mathcal{H}_{\mathbb{R}}$ with a Riemann structure and we have also a complex structure J such that

$$g(v_1, v_2) = -\omega(Jv_1, v_2), \qquad \omega(v_1, v_2) = g(Jv_1, v_2),$$

together with

$$g(Jv_1, Jv_2) = g(v_1, v_2), \qquad \omega(Jv_1, Jv_2) = \omega(v_1, v_2).$$

The triplet (g,J,ω) defines a Kähler structure in $\mathcal{H}_{\mathbb{R}}$ and the symmetry group of the theory must be the unitary group $U(\mathcal{H})$ whose elements preserve the inner product, or in an alternative but equivalent way (in the finite-dimensional case), by the intersection of the orthogonal group $O(2n,\mathbb{R})$ and the symplectic group $Sp(2n,\mathbb{R})$.

On the other hand, as the fundamental concept for measurements is the expectation value of observables, two vector fields such that

$$\frac{\langle \psi_2, A\psi_2 \rangle}{\langle \psi_2, \psi_2 \rangle} = \frac{\langle \psi_1, A\psi_1 \rangle}{\langle \psi_1, \psi_1 \rangle}, \quad \forall A \in \text{Her}(\mathcal{H})$$

should be considered as indistinguishable.

This is only possible when ψ_2 is proportional to ψ_1 . In fact it suffices to take as observable A the orthogonal projection on ψ_1 in the preceding relation.

Therefore we must consider rays rather than vectors the elements describing the quantum states.

The space of states is not \mathbb{C}^n but the projective space \mathbb{CP}^{n-1} .

It is possible to define a Kähler structure on \mathbb{CP}^{n-1} and therefore to study Lie-Kähler systems leading to superposition rules and to study time evolution in this projective space.

How to find a quantum model for a classical one?

In general the problem of 'quantisation' of a system is, given a classical Hamiltonian system (M,ω,H) , to find a Hilbert space $\mathcal H$ and to choose the selfadjoint operator $\widehat F$ corresponding to the relevant observables F.

In the simplest case of an Euclidean configuration space, the prescription is that

- \square $\mathcal H$ is the space of square integrable functions with respect to the Lebesgue measure
- \square position \widehat{x}_i have associated multiplication by x_i operators and
- ☐ the momentum operators are the differential operators

$$\widehat{p}_k = -\mathrm{i} \; \frac{\partial}{\partial x_k}.$$

There will be some ordering ambiguities for other observables because functions of x_i commute with those of p_k , but \hat{x}_i does not commute with \hat{p}_k but

$$[\widehat{x}_i, \widehat{p}_j] = i \, \delta_{ik}, \quad \text{versus} \quad \{x_i, p_k\} = \delta_{ik}.$$

Many textbooks warn that this is only valid using Euclidean coordinates.

This is very restrictive, because:

What happens in other coordinates and even worse when there are no global preferred coordinates (for instance Q is compact)?

What about position-dependent mass for which mass operator does not commute with momentum operators?

Generalising previous procedure for a more general case of a Hamiltonian dynamical system, Dirac assertion is that Quantisation is to be understood as a a map ζ : $C^{\infty}(M) \to \mathcal{A}(\mathcal{H})$ such that

$$-i\zeta(\{F,G\}) = [\zeta(F),\zeta(G)]$$

Several meanings for p_i

	assical mechanics, if the configuration space is an Euclidean space \mathbb{R}^n , p_i denotes different and inequivalent objects:
	p_i is the i -th coordinate of a covector in a point of the configuration space
	p_i is a real function in $T^*\mathbb{R}^n$: $p_i(lpha)=lpha(\partial/\partial x_i)$
	the real function p_i is the infinitesimal generator of translations along the i -th coordinate axis, which are canonical transformations for $(T^*\mathbb{R}^n, \omega_0)$
lnan	nore general case, $Q eq T^*\mathbb{R}^n$,
	there is not a global chart,
	the momentum coordinates are local and depend on the choice of base manifold coordinates,
	translations are not defined.

Recall however that translations and rotations are isometries of the Euclidean space.

For natural Lagrangians defined on TQ, with Q an arbitrary Riemann manifold, we can consider the isometries of the Riemann metric, whose cotangent lifts are Hamiltonian vector fields and in this way we define a strongly symplectic action of the group of isometries, with Lie algebra \mathfrak{til} , on T^*Q .

We are then able to define an associated momentum. The components P_i of this map are the objects to be quantised instead of the p_i which is not an intrinsic but a coordinate dependent ingredient.

This allows us to quantise functions of the momentum map by associating the function P_k with $\hat{P}_k = -\mathrm{i}\,X_k$ acting on an appropriate Hilbert space.

Consequently we can quantise functions of the momentum map.

Position dependent mass systems

Consider a 1-dimensional system described in terms of a coordinate x by a Lagrangian

$$L = \frac{1}{2} m(x) \dot{x}^2 - V(x), \quad x \in \mathbb{R}, \quad m(x) > 0,$$

that leads to the following nonlinear differential equation

$$m(x) \ddot{x} + \frac{1}{2} m'(x) \dot{x}^2 = 0,$$

with associated Hamiltonian H given by

$$H(x,p) = \frac{1}{2} \frac{1}{m(x)} p^2 + V(x).$$

There is an important problem with the construction of the quantum version of H, $H\to \widehat{H}$ from the classical system to the quantum one, because if the mass m becomes a function of the spatial coordinate, m=m(x), then the quantum version of the mass no longer commutes with the momentum.

Different forms of presenting the kinetic term in the Hamiltonian H, as for example

$$T = \frac{1}{4} \left[\frac{1}{m(x)} p^2 + p^2 \frac{1}{m(x)} \right], \quad T = \frac{1}{2} \left[\frac{1}{\sqrt{m(x)}} p^2 \frac{1}{\sqrt{m(x)}} \right], \quad T = \frac{1}{2} \left[p \frac{1}{m(x)} p \right],$$

are equivalent at the classical level but they lead to different and nonequivalent Schrödinger equations.

This problem is important mainly for two reasons.

- (i) There are a certain number of important areas, mainly related with problems on condensed-matter physics (electronic properties of semiconductors, liquid crystals, quantum dots, etc), in which the behaviour of the system depends of an effective mass that is position-dependent.
- (ii) From a more conceptual viewpoint, the ordering of factors in the transition from a commutative to a noncommutative formalism is an old question that remains as an important open problem in the theory of quantization.

(iii) The free motion along a simple regular curve C looks like a position–dependent mass system. If C is given in parametric form by $\mathbf{x}:I\to\mathbb{R}^n$, $u\mapsto\mathbf{x}(u)$, its arc-length function s(u) is an intrinsic parameter given by

$$\frac{ds}{du} = \sqrt{\frac{d\mathbf{x}}{du} \cdot \frac{d\mathbf{x}}{du}} = f(u) > 0 ,$$

and therefore

$$s(u) = \int^{u} \sqrt{\dot{\mathbf{x}}(\zeta) \cdot \dot{\mathbf{x}}(\zeta)} \ d\zeta.$$

The geodesics of this metric coincide, up to reparametrisation, with the curves solution of the Euler–Lagrange equation of the Lagrangian

$$L_0(u, v_u) = \frac{1}{2} m_0 f(u) v_u^2,$$

where m_0 is a constant with mass dimension, i.e.

$$\frac{d}{dt}(f(u)\dot{u}) = \frac{1}{2}f'(u)\dot{u}^2 \Longrightarrow f(u)\ddot{u} + \frac{1}{2}f'(u)\dot{u}^2 = 0,$$

where f'(u) = df/du.

Quantisation of position dependent mass

The usual approach make uses of the formalism (α, β, γ) : T has the following expression introduced by von Roos (generalizing a previous study by BenDaniel $et\ al.$

$$T_{\alpha\beta\gamma} = \frac{1}{4} \left(m^{\alpha} p m^{\beta} p m^{\gamma} + m^{\gamma} p m^{\beta} p m^{\alpha} \right), \quad \alpha + \beta + \gamma = -1.$$

It is important to remark that in order to study a quantum system (in the Schrödinger picture) we should first fix the Hilbert space \mathcal{H} and then the (essentially) selfadjoint operators corresponding to the relevant observables to be quantized.

Therefore the quantization of the Hamiltonian of a system means first to define the appropriate Hilbert space of pure states, and then construction of the quantum Hamiltonian.

In the problem of quantization of a Hamiltonian system with a PDM the definition of the measure $d\mu$ defining the Hilbert space $L^2(\mathbb{R}, d\mu)$ strongly depends on the characteristics of the function m(x).

The kinetic Lagrangian T possesses an exact Noether symmetry. The function T is not invariant under translations but under the action of the vector field X given by

$$X(x) = \frac{1}{\sqrt{m(x)}} \frac{\partial}{\partial x},$$

(displacement $\delta x = \epsilon(m(x))^{-1/2}$, in the physicists language), i.e. we have $X^t(T) = 0$, where X^t denotes the tangent lift to the velocity phase space $\mathbb{R} \times \mathbb{R}$ (that, in differential geometric terms, is the tangent bundle TQ of the configuration space $Q = \mathbb{R}$) of the vector field $X \in \mathfrak{X}(\mathbb{R})$,

$$X^{t}(x,v) = \frac{1}{\sqrt{m(x)}} \left(\frac{\partial}{\partial x} - \left(\frac{1}{2} \frac{m'(x)}{m(x)} \right) v \frac{\partial}{\partial v} \right).$$

Recall that given a Riemannian space (M,g), a Killing vector field X defined on M is a symmetry of the metric g (in the sense that it satisfies $\mathcal{L}_X g = 0$ where \mathcal{L}_X denotes the Lie derivative with respect to X). Killing vector fields also preserve the volume Ω_g determined by the metric, that is,

$$\Omega_g = \sqrt{|g|} dx^1 \wedge dx^2 \wedge \cdots \wedge dx^n, \qquad \mathcal{L}_X \Omega_g = 0,$$

where |g| denotes the determinant of the matrix g defining the Riemann structure.

One can show that if $T_g(x,v) = \frac{1}{2}g_{ij}(x)v^iv^j$, then

$$X^t(T_g) = T_{\widetilde{g}}, \quad \widetilde{g} = \mathcal{L}_X g.$$

Consequently, X is a Killing vector field for g iff X^t is a symmetry for the associated kinetic energy function T_g . The above X is a Killing vector field. In fact it is a Killing vector field of the one-dimensional m-dependent metric

$$g = m(x) dx \otimes dx$$
, $ds^2 = m(x) dx^2$.

The line element is invariant under the flow of the vector field $X = f(x)\partial/\partial x$ when

$$f\,m'+2\,m\,f'=0\,\,,$$

and, therefore, in order to the vector field X to be a Killing vector, it should be proportional to the vector field X, which represents (the infinitesimal generator of) an exact Noether symmetry for the geodesic motion. If we denote by θ_L the 1-form

$$\theta_L = \left(\frac{\partial L}{\partial v}\right) dx = m(x)v dx,$$

the associated Noether constant of the motion ${\cal P}$ for the free (geodesic) motion, called Noether momentum is

$$P = i(X^t) \theta_L = \sqrt{m(x)} v.$$

Quasi-regular representation

The Hilbert space for a quantum system with a configuration space M is the linear space of square integrable functions on M with respect to an appropriate measure, $L^2(M,d\mu)$.

In the case of a natural system the measure to be considered must be invariant under the the Killing vector fields of the metric. The reason is the following:

If $\Phi:G\times M\to M$ denotes the action of a Lie group G on a differentiable manifold M, then the associated quasi-regular representation is given by the following action of G on the set of complex functions on M:

$$(U(g)\psi)(x) = \psi(\Phi(g^{-1}, x)).$$

If M admits an invariant measure $d\mu$ we can restrict the action on the set $L^2(M,d\mu)$ and if $d\mu$ is G-invariant, the representation so obtained is a unitary representation.

If a one-parameter subgroup $\gamma(t)=\exp(at)$, $a\in\mathfrak{g}$, is considered, then the fundamental vector field $X_a\in\mathfrak{g}$, which is given by

$$(X\psi)(x) = \frac{d}{dt}\psi(\Phi(\exp(-ta), x))_{|t=0},$$

when restricted to the subspace $L^2(M,d\mu)$ is a skew-selfadjoint operator provided that the measure μ is $\gamma(t)$ -invariant, because $U(\gamma(t))$ is a one-parameter group of unitary transformations.

The infinitesimal generator in the regular representation is a generator for a 1-parameter group of unitary transformations, and consequently it is skew-self-adjoint operator. Of course if we want the generators of several one-parameter groups be skew-self-adjoint, the measure defining the Hilbert space must be invariant under each 1-parameter subgroup.

For the one-dimensional PDM system, the quantum system must be described by the Hilbert space $L^2(\mathbb{R}, d\mu_x)$ of square integrable functions w,r,t. an invariant under X measure, $d\mu_x$, therefore determined by the metric.

The Lebesgue measure dx is not invariant under $X=f(x)\partial/\partial x$, the invariance condition for the measure $d\mu_x=\rho(x)\,dx$ being

$$f \, \rho' + \rho f' = 0 \, .$$

Then, the only measure invariant under X for $f(x) = (m(x))^{-1/2}$ is a multiple of

$$d\mu_x = \sqrt{m(x)} \, dx.$$

This automatically implies that the first-order linear operator X is skew-symmetric. This means that the operator \widehat{P} representing the quantum version of the Noether momentum P must be selfadjoint, not in the standard space $L^2(\mathbb{R}) \equiv L^2(\mathbb{R}, dx)$, but in the space $L^2(\mathbb{R}, d\mu_x)$ of square integrable functions with respect the PDM measure $d\mu_x$.

Using the Legendre transformation the momentum p and velocity v are related by $p=m(x)\,v$, so that the expressions of the Noether momenta and the Hamiltonian (kinetic term plus a potential) in the phase space are

$$P = \frac{1}{\sqrt{m(x)}} \, p \,,$$

and

$$H = \frac{1}{2}P^2 + V(x) \,.$$

As we have pointed out, the generator of the infinitesimal 'translation' symmetry, $(1/\sqrt{m(x)})\,d/dx$, is skew-Hermitian in the space $L^2(\mathbb{R},d\mu_x)$ and therefore the translation's

sition from the classical system to the quantum one is given by defining the operator \widehat{P} as follows

$$P \ \mapsto \ \widehat{P} = \frac{1}{\sqrt{m(x)}} \Big(-i \, \hbar \, \frac{d}{dx} \Big) \, ,$$

so that

$$\frac{1}{m} \, p^2 \ \to \ - \, \hbar^2 \, \Big(\frac{1}{\sqrt{m(x)}} \, \frac{d}{dx} \Big) \Big(\frac{1}{\sqrt{m(x)}} \, \frac{d}{dx} \Big) \, ,$$

in such a way that the quantum Hamiltonian \widehat{H} is represented by the following Hermitian (defined on the space $L^2(\mathbb{R},d\mu_x)$) operator

$$\hat{H} = -\frac{\hbar^2}{2} \left(\frac{1}{\sqrt{m(x)}} \frac{d}{dx} \right) \left(\frac{1}{\sqrt{m(x)}} \frac{d}{dx} \right) + V(x),$$

$$= -\frac{\hbar^2}{2} \frac{1}{m(x)} \frac{d^2}{dx^2} + \frac{\hbar^2}{4} \left(\frac{m'(x)}{m^2(x)} \right) \frac{d}{dx} + V(x),$$

and then the Schrödinger equation $\widehat{H}\,\Psi=E\,\Psi$ becomes

$$-\frac{\hbar^2}{2} \frac{1}{m(x)} \frac{d^2 \Psi}{dx^2} + \frac{\hbar^2}{4} \left(\frac{m'(x)}{m^2(x)} \right) \frac{d\Psi}{dx} + V(x) \Psi = E \Psi.$$

Motion on a cycloid: A case study

Consider the motion of a particle of mass m_0 moving on a gravitational field along a cycloid inverted in such a way that the origin is sited in the lowest point, namely:

$$\mathbf{x}(\vartheta) = (x(\vartheta + \pi), -y(\vartheta + \pi)) + (0, 2R) = (R(\vartheta + \pi + \sin \vartheta), R(1 - \cos \vartheta)),$$

i.e.,

$$\mathbf{x}(\vartheta) = \left(R(\vartheta + \pi + \sin \vartheta), 2R \sin^2 \frac{\vartheta}{2}\right), \qquad \theta \in (-\pi, \pi).$$

Consequently,

$$\dot{\mathbf{x}}(\vartheta) = (R(1 + \cos \vartheta), R\sin \vartheta),$$

and then,

$$\|\dot{\mathbf{x}}\|^2 = R^2(1 + \cos^2\vartheta + 2\cos\vartheta + \sin^2\vartheta) = 2R^2(1 + \cos\vartheta) = 4R^2\cos^2\frac{\vartheta}{2},$$

from which we obtain (recall that $\theta \in (-\pi, \pi)$ and therefore $\cos(\vartheta/2) > 0$)

$$\frac{ds}{d\vartheta} = 2R\cos\frac{\vartheta}{2} \Longrightarrow s(\vartheta) = 4R\left[\sin\frac{\zeta}{2}\right]_0^{\vartheta} = 4R\sin\frac{\vartheta}{2}.$$

The expression of the metric in these coordinates is

$$g = 2R \cos \frac{\vartheta}{2} \, d\vartheta^2,$$

i.e. the free motion is described by the Lagrangian with a position-dependent mass given by $m(\vartheta)=2m_0\,R\,\cos\frac{\theta}{2}$:

$$L_0(\vartheta, \dot{\vartheta}) = m_0 R \cos \frac{\vartheta}{2} \dot{\vartheta}^2.$$

The potential function describing the action of the gravity in terms of the arc–length \boldsymbol{s} is:

$$V(\vartheta) = m_0 g y(\vartheta) = 2m_0 g R \sin^2 \frac{\vartheta}{2} = 2m_0 g R \frac{s^2}{16R^2} = \frac{1}{2} m_0 \frac{g}{4R} s^2,$$

and then the Lagrangian is given by

$$L(\vartheta, \dot{\vartheta}) = m_0 R \cos \frac{\vartheta}{2} \dot{\vartheta}^2 - 2m_0 g R \sin^2 \frac{\vartheta}{2},$$

or in terms of the canonical coordinate

$$L(s, \dot{s}) = \frac{1}{2}m_0 \dot{s}^2 - \frac{1}{2}m_0 \frac{g}{4R} s^2.$$

Correspondingly, the tangent vector to the curve is

$$\mathbf{t}(\vartheta) = \frac{1}{2R\cos\frac{\vartheta}{2}}(R(1+\cos\vartheta), R\sin\vartheta) = \left(\cos\frac{\vartheta}{2}, \sin\frac{\vartheta}{2}\right),$$

which shows that the tangential force is given by

$$F_t = \mathbf{F} \cdot \mathbf{t} = -m_0 \operatorname{g} \sin \frac{\vartheta}{2} = -\frac{m_0 \operatorname{g}}{4R} s,$$

while the tangential component of $\ddot{\mathbf{x}}$ is \ddot{s} , and then Newton's second law is

$$\ddot{s} = -\frac{m_0 \,\mathrm{g}}{4R} \,s.$$

Both expressions show that the motion along the inverted cycloid in terms of the arc-length s is oscillatory with a constant period function

$$\tau = \frac{2\pi}{\omega} = 4\pi\sqrt{\frac{R}{g}}.$$

The quantum model for a particle of mass m_0 living on a cycloid as configuration space, under the action of a gravitational force, in terms of the arc-length parameter is like that of a harmonic oscillator with mass m_0 and $\omega^2 = m_0 \, {\rm g}/(4R)$, for $-4R \le s \le 4R$.

The Hilbert space of the corresponding quantum system will be $\mathcal{L}_0^2(-L,L)$ of square integrable functions in the interval (-L,L), with L=4R, satisfying the boundary conditions $\psi(-L)=\psi(L)=0$, and the quantum Hamiltonian operator is given by

$$H = -\frac{\hbar^2}{2m_0} \frac{d^2}{ds^2} + V(s),$$

where

$$V(s) = \begin{cases} \frac{1}{2} m_0 \omega^2 s^2 & \text{if } |s| \le R \\ \infty & \text{if } |s| \ge 4R \end{cases}.$$

This problem of a confined harmonic oscillator has been studied by Ghosh. The Hamiltonian is parity invariant and consequently the eigenfunctions are either even or odd functions. The time-independent Schrödinger equation is

$$\left(-\frac{\hbar^2}{2m_0}\frac{d^2}{ds^2} + \frac{1}{2}m_0\omega^2 s^2\right)\psi(s) = E\,\psi(s),$$

which can be rewritten as

$$\frac{d^2}{dz^2} + \left(\varepsilon - \frac{z^2}{4}\right)\psi(z) = 0,$$

where

$$z = \sqrt{\frac{2m_0\omega}{\hbar}}, \qquad E = \varepsilon \,\hbar\omega.$$

It is common to write $\varepsilon=\nu+1/2$, by similarity with the usual harmonic oscillator, i.e. $E=(\nu+1/2)\,\hbar\omega$.

If we introduce now the change

$$\psi(z) = e^{-z^2/4}\phi(z),$$

and redefine the independent variable as $y=\frac{1}{2}z^2$, the new function $\phi(y)$ satisfies the confluent hypergeometric equation (Abramowitz and Stegun, p 504):

$$y\frac{d^2\phi}{dy^2} + (b-y)\frac{d\phi}{dy} - ay,$$

with $b=\frac{1}{2}$ and $a=-\frac{\nu}{2}$, i.e.

$$y\frac{d^2\phi}{dy^2} + \left(\frac{1}{2} - y\right)\frac{d\phi}{dy} + \frac{\nu}{2}y.$$

The point y=0 is a regular singular point while $y=\infty$ is an irregular singularity. A basis of the linear space of solutions for $b \notin \mathbb{Z}$ is given by the confluent hypergeometric function, also called Kummer function M(a,b,y) and its related function U(a,b,y)

with power expansions (see e.g. Abramowitz and Stegun, p 504):

$$M(a,b,y) = {}_{1}F_{1}(a,b,y) = \sum_{n=0}^{\infty} \frac{(a)_{n}}{(b)_{n}} \frac{y^{n}}{n!}$$

$$U(a,b,y) = \frac{\pi}{\sin(\pi b)} \left(\frac{M(a,b,y)}{\Gamma(1+a-b)\Gamma(b)} - y^{1-b} \frac{M(1+a-b,2-b,y)}{\Gamma(a)\Gamma(2-b)} \right)$$

where (a_n) denotes $(a_n) = a(a+1)\cdots(a+n-1)$, with $(a_0) = 1$.

The general solution $\psi(s)$ can be written as

$$\psi(s) = e^{-m\omega L^2/2\hbar} \left[\left(A + B \frac{\sqrt{\pi}}{\Gamma((1-\nu)/2)} \right) M \left(-\frac{\nu}{2}, \frac{1}{2}, \frac{m_0 \omega s^2}{\hbar} \right) - 2B \frac{\sqrt{\pi}}{\Gamma(-\nu/2)} \sqrt{\frac{m_0 \omega}{\hbar}} s M \left(\frac{1-\nu}{2}, \frac{3}{2}, \frac{m_0 \omega s^2}{\hbar} \right) \right].$$

The first term on the right-hand side is an even function and the second one is odd. Therefore, the conditions on the parameter ν for $\psi(s)$ to be an eigenfunction are

$$\begin{split} \left(A + B \frac{\sqrt{\pi}}{\Gamma((1-\nu)/2)}\right) M \left(-\frac{\nu}{2}, \frac{1}{2}, \frac{m_0 \omega L^2}{\hbar}\right) &= 0 \quad \text{for even functions} \\ \frac{\sqrt{\pi}}{\Gamma(-\nu/2)} \sqrt{\frac{m_0 \omega}{\hbar}} M \left(\frac{1-\nu}{2}, \frac{3}{2}, \frac{m_0 \omega L^2}{\hbar}\right) &= 0 \quad \quad \text{for odd functions} \end{split}$$

These equations should be used to determine the energy eigenvalues.

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