Coarse-grained quantum systems and symmetries

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Abstract. Constrained Hamiltonian dynamics is exploited to provide the mathematical framework of a coarse-grained description of the quantum system of two interacting qubits and of nonlinear interacting oscillators. The coarse-graining is treated as an equivalence relation on the set of quantum states resulting in the emergence of the classical phase-space. The equivalence relation imposes constraints on the Hamiltonian dynamics of the quantum system. It is seen that the evolution of the coarse-grained system preserves constant and minimal quantum fluctuations of the fundamental observables. This leads to the emergence of typical classical properties, like the relation between symmetry and integrability, and in the case of oscillators in the macro-limit implies the emergence of the classical system.

1. Introduction
It has been realized many times that some sort of coarse-graining is necessary in order that typically quantum features of a system (with finite number of degrees of freedom) do not dominate its appearance. The coarse-graining enters differently in different theories of quantum to classical relation (QCR), and is not always equally strongly emphasized. In the theories of decoherences [1] the emphasis is on the influence of the environment, but the description of the environment must be coarse-grained to fulfill the desired decoherence effects. On the other hand, authors like [2] and [3, 4] emphasize the primary role of the coarse-graining, associated with limited precision of the devices used to observe the quantum system.

In this paper we shall study the emergence of classical properties in two typical examples of quantum systems: a) a pair of qubits and b) a system of nonlinear oscillators. We shall clearly distinguish two independent steps that are necessary for the emergence of classical properties of a quantum system: a) system specific coarse graining and b) the macroscopic limit. Implementations of the two steps are analogous for different systems but the details of the implementations depend on the system. First we shall analyze the particular coarse-graining which is necessary for the classical behavior of the basic observables and then analyze the macroscopic limit of these observables if such limit is appropriate like in the case of oscillators. The classical model will be constructed using formalization of the coarse-grained description via an equivalence relation imposed on the quantum states and the corresponding constrained dynamics.

2. Geometric formulation of coarse-grained quantum systems
2.1. Hamiltonian form of quantum dynamics with constraints
It is well known (please see [5] or [6] and references therein) that the evolution of a quantum pure state in an $n$ dimensional Hilbert space $\mathcal{H}$ (where $n$ is finite or infinite) as given by the
Schroedinger equation can be equivalently described by a Hamiltonian dynamical system on the real manifold $\mathcal{M}$ with Riemanienn and symplectic structure. If $\mathcal{H}$ is finite n-dimensional then $\mathcal{M} \equiv \mathbb{R}^{2n}$, but in general $\mathcal{M}$ is an infinite dimensional Euclidean manifold. The evolution equations on $\mathcal{M}$ are in the Hamiltonian form:

$$\dot{X} = \Omega(\nabla X, \nabla H), \quad (1)$$

where $X$ is the vector of coordinates $q_i$ and momenta $p_i$. The Hamilton’s function $H(x)$ is given by the quantum expectation of the Hamiltonian $\hat{H}$ in the state $|\psi>: H = <\psi|\hat{H}|\psi>$, the symplectic form $\Omega$ is given by the imaginary part of the scalar product in $\mathcal{M}$, and $\nabla$ is the gradient on $\mathcal{M}$.

The Hamiltonian framework for quantum dynamics enables one to describe the evolution of a dynamical system generated by the Schroedinger equation with quite general additional constraints [6, 7, 8]. Suppose that the evolution given by the Hamiltonian $H$ is further constrained onto a submanifold $\Gamma$ of $\mathcal{M}$ given by a set of $k$ independent functional equations $f_l(X) = 0, \ l = 1, 2, \ldots, k. \quad (2)$

Equations of motion of the constrained system are in general obtained using the method of Lagrange multipliers. In the Hamiltonian form, developed by Dirac [9], the method assumes that the dynamics on $\Gamma$ is determined by the following set of differential equations

$$\dot{X} = \Omega(\nabla X, \nabla H_{tot}), \quad H_{tot} = H + \sum_{l=1}^{k} \lambda_l f_l, \quad (3)$$

that should be solved together with the equations of the constraints (2). The Lagrange multipliers $\lambda_l$ are functions on $\mathcal{M}$ that are to be determined from the following, so called compatibility, conditions

$$0 = \dot{f}_l = \Omega(\nabla f_l, \nabla H_{tot}) \quad (4)$$

$$= \Omega(\nabla f_l, \nabla H) + \sum_{m=1}^{k} \lambda_m \Omega(\nabla f_l, \nabla f_m) \quad (5)$$

on the constrained manifold $\Gamma$. We shall not go into the details of the standard Dirac’s procedure that stress on the distinction between the first and the second class constraints. In order to apply the standard procedure, the constraints have to be regular. A set of constraints is irregular if there is et least one such that the derivative of the constraint with respect to at least one of the coordinates is zero in at least one point on the constrained manifold. Otherwise the constraints are regular. If the constraint (2) is irregular the Dirac’s classification into the first and the second class is blurred and the straightforward application of Dirac’s recipe is not possible. It will turn out that the cases of interest here involve precisely irregular constraints that must be described in the most convenient way.

2.2. Constraints as a coarse-graining of the quantum system

Consider a system with the dynamical algebra $g$. The manifold $\Gamma$ of $g$-coherent states $\alpha \in \Gamma$ is determined by the condition that $\Delta_g(\psi)$ is minimal on $\Gamma$:

$$\Delta_g(\psi) \equiv \sum_l <L_l^2> - <L_l>^2 \equiv \sum_l (\Delta L_l)^2 = \text{min.} \quad (6)$$
where \( L_l \) are the generators of the algebra. Expressions for the minimal value of \( \Delta_g(\psi) \) in terms of the simple roots of \( g \) are known [10] and read

\[
\Delta_g(\psi) \geq \sum_k k_l < \alpha_l, \alpha_l > \equiv \min,
\]

where the highest weight vector \( \lambda = \sum k_l \alpha_l \) in terms of simple roots \( \alpha_l \).

The generators of the algebra can be used to define an equivalence relation on \( M \): \( \psi_1 \) and \( \psi_2 \) are equivalent iff:

\[
< L_l > \psi_1 = < L_l > \psi_2 \quad \text{for all} \quad L_l.
\]

The two examples considered in this paper are such that there is a single coherent state in each equivalence class.

The Hamiltonian system with the additional constraints equivalent to (6) that constrain the evolution on \( \Gamma \) preserves the equivalence classes, i.e. the classes evolve like single units and could be considered as states of the coarse-grained i.e. constrained system. This is the coarse-grained description. Such constrained Hamiltonian systems also preserve minimal the quantum fluctuations (6). However, the constraint (6) is not regular and needs to be replaced by more convenient equivalent constraints.

3. Examples

3.1. Two qubits

Consider the dynamical algebra of local observables \( g = su(2) \otimes su(2) \). The quantum phase space is the projective space \( M = S^7/S^1 \).

As for the Hamiltonian we consider two typical examples

\[
H_s = \sigma_z^1 + \sigma_z^2 + \mu \sigma_z^1 \sigma_z^2
\]

\[
H_{ns} = \sigma_z^1 + \sigma_z^2 + \mu \sigma_x^1 \sigma_x^2.
\]

The constraint (6) is equivalent to \( c_1 c_4 = c_2 c_3 \) where \( c_1, c_2, c_3, c_4 \) are coefficients of \(|\psi\rangle\) in the computational basis, and the equation of this constraint is equivalent to two real equations

\[
\sqrt{2} p_3 = p_2 q_1 + p_1 q_2,
\]

\[
\sqrt{2} q_3 = q_1 q_2 - p_1 p_2.
\]

These are regular and of second class.

The constrained manifold is \( \Gamma = S^2 \times S^2 \), and there are the corresponding (constrained) Hamilton equations on \( \Gamma \) [6].

Constrained dynamics of the symmetric Hamiltonian \( H_s \) is regular, while that of the Hamiltonian \( H_{ns} \) with no such symmetry displays typical properties of the Hamiltonian chaos [6]. Thus appropriately coarse-grained description of the quantum system has the typical classical relation between integrability and symmetry.

3.2. System of oscillators [11]

The Hilbert space of the system is \( \mathcal{H} = L_2(R^n) \). The fundamental observables are represented by \( 2n \) operators \( (\hat{Q}_i, \hat{P}_i) \), \( i = 1, 2, \ldots n \), satisfying \([\hat{Q}_i, \hat{P}_j] = i\delta_{i,j}\). The Hamiltonian is of the form

\[
\hat{H} = \sum_{i=1}^{n} \frac{1}{2m_i} \hat{P}_i^2 + V(\hat{Q}_1, \hat{Q}_2, \ldots, \hat{Q}_n)
\]

\[
= \sum_{i=1}^{n} \frac{1}{2m_i} \hat{P}_i^2 + \frac{m_i \omega_i^2}{2} \hat{Q}_i^2 + \ldots,
\]
The symplectic phase space $\mathcal{M}$ of the Hamiltonian formulation of the quantum oscillators system is given as the product of $n$ infinite dimensional symplectic spaces. The canonical coordinates of this infinite dimensional symplectic space can be written using the continuous index as: $\phi(q_1, \ldots, q_n), \pi(q_1, \ldots, q_n)$ ($q_i \in \mathbb{R}$)

The constrained system defined by the Hamiltonian (11) and the following set of $2n$ constraints

$$f_q^i(X) = (\Delta \hat{Q}_i)^2 - \frac{\hbar}{2m\omega_i} = 0,$$

$$f_p^i(X) = (\Delta \hat{P}_i)^2 - \frac{m\omega_i\hbar}{2} = 0,$$

should preserve the dispersions of all fundamental quantum observables. However, the constraints (12) are irregular. The conservation of minimal dispersions is achieved by a more suitable set of constraints.

To formulate the primary constraints in the alternative procedure, we associate with each point from $\mathcal{M}$ denoted $X$ a point $\alpha(\psi)$ on the coherent state manifold $\Gamma$ such that

$$\alpha(\psi) = (\langle \hat{Q} \rangle_\psi, \langle \hat{P} \rangle_\psi).$$

We formulate the following two constraints

$$\Phi_q = \langle V(\hat{Q}) \rangle_\psi - \langle V(\hat{Q}) \rangle_{\alpha(\psi)} = 0,$$

$$\Phi_p = \langle \hat{P}^2 \rangle_\psi - \langle \hat{P}^2 \rangle_{\alpha(\psi)} = 0.$$

The role of the constraints is to preserve during the evolution the association of the set of points $\psi(t)$ with the corresponding single coherent state $\alpha(\psi(t))$.

The total Hamiltonian assumes the standard form

$$H_{tot} = \langle \hat{H} \rangle_\psi + \lambda_q \Phi_q + \lambda_p \Phi_p,$$

and the compatibility condition

$$\{\Delta(f(\hat{Q}), \hat{P}), H_{tot}\} = 0,$$

yields the values of Lagrange multipliers

$$\lambda_q = -1, \quad \lambda_p = -\frac{1}{2m},$$

independently of the function $f(\hat{Q})$, leading to

$$H_{tot} = \frac{1}{2m} \langle \hat{P}^2 \rangle_{\alpha(\psi)} + \langle V(\hat{Q}) \rangle_{\alpha(\psi)} \equiv \langle \hat{H} \rangle_{\alpha(\psi)}.$$ 

Noting that $\langle \hat{P}^2 \rangle_{\alpha(\psi)} = \langle \hat{P}^2 \rangle_{\alpha(\psi)} + m\omega_i\hbar/2$ and dropping irrelevant constant we finally obtain the total constrained Hamiltonian

$$H_{tot} = \frac{1}{2m} \langle \hat{P}^2 \rangle_{\alpha(\psi)} + \langle V(\hat{Q}) \rangle_{\alpha(\psi)},$$

that preserves the evolution on the manifold of the coherent states $\Gamma$.

The total Hamiltonian (21) is up to additive constant equal to the initial Hamiltonian $H \equiv \langle \hat{H} \rangle_\psi$ on the constrained manifold $\Gamma$. However, $H_{tot}$ preserves constant and minimal quantum fluctuations of fundamental observables, while the evolution with $H$ can in general make them quite large.
3.3. Macro-limit of the oscillators system

The total Hamiltonian in a point \( \alpha \equiv (q, p) \) on the constrained manifold is

\[
H_{\text{tot}} = \frac{p^2}{2m} + V(q) + \sum_{k=1}^{\infty} \frac{\hbar^k V^{(2k)}(q)}{2^k k! (2m\omega)^k}.
\]

\[\equiv h_{\text{cl}} + \sum_{k=1}^{\infty} \frac{\hbar^k V^{(2k)}(q)}{2^k k! (2m\omega)^k}.\]  \hspace{1cm} (22)

In the macroscopic limit, represented as \( \hbar \to 0 \) the terms in the sum in (22) tend to zero yielding

\[H_{\text{tot}} \to h_{\text{cl}}, \quad \hbar \to 0.\]  \hspace{1cm} (23)

To summarize: We see that the classical system emerges because of: a) the coarse-grained description of the quantum system and then b) the macroscopic limit. It is important to note that the two factors, i.e. the coarse-graining and the macro-limit, are independent and both are necessary.

For the system with more than one oscillators, that might be nonlinear and interacting, the condition that \( \Delta \hat{Q}_i \) and \( \Delta \hat{P}_i \) are simultaneously minimal implies that each of the oscillators is always in some pure \( H_4 \) coherent state \( |\alpha_i(t)\rangle \). Thus, the total state \( |\psi(t)\rangle \) is always given by the tensor product of the single oscillator’s pure coherent states \( |\psi(t)\rangle = \otimes_i |\alpha_i(t)\rangle \), implying for example

\[\langle \psi(t) | \hat{Q}_1 \otimes \hat{Q}_2 | \psi(t) \rangle = \langle \hat{Q}_1 \rangle_{\alpha_1(t)} \times \langle \hat{Q}_2 \rangle_{\alpha_2(t)} = q_1(t) \times q_2(t).\]  \hspace{1cm} (24)

4. Summary

We have used the formulation of quantum dynamics in the form of a Hamiltonian dynamical system to study the relation between a quantum system and its coarse-grained description. The type of coarse-graining is dictated by the systems dynamical algebra and determines the classical model of the quantum system. Kinematical and dynamical properties of the classical model are obtained from the quantum one via the two step procedure consisting of: a) coarse-graining and b) macroscopic limit if appropriate. The coarse-graining is mathematically treated as an equivalence relation on the set of quantum states, and as a result emerges the classical phase-space. The equivalence relation imposes a constraint on the Hamiltonian dynamics of the quantum system. The effect of the constraints is to preserve constant and minimal quantum fluctuations of the canonical observables. The formulation of the most appropriate finite set of constraints that fulfil the goal is not straightforward, and involves the nonlinear potential. Resulting constrained Hamiltonian system on the constrained manifold represents the coarse-grained description of the quantum system. In the case of the quantum system obtained by quantization of classical oscillators systems the emergent coarse-grained system differs from the classical one with the same potential only in the terms that are arbitrary small in the macroscopic limit.

The procedure can be generalized to obtain other classical systems from the coarse-grained quantum systems in the corresponding macroscopic limit.

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