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Concepts of Coarse Graining in Quantum Mechanics

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Various procedures of coarse graining in quantum mechanics and their relationships are reviewed. A recently developed notion of relative coarse graining is described which is based on a certain type of classical embedding of quantum states. The ensuing structure of the set of quantum observables is studied. As an application of the new concept an operational classical limit procedure is sketched out.

1. INTRODUCTION

In a recent work (Quadt and Busch, 1993) a general concept of (relative) coarse graining was presented and its meaning investigated in the context of quantum mechanics. While this work was concerned with developing the relevant notions and discussing various examples, the present contribution is devoted to a systematic comparison of different types of reduced descriptions and a more detailed elaboration of some structural aspects. Coarse graining shall be described as a reduced (statistical) description, obtained by the action of a stochastic map. Relative coarse graining is introduced as a (pre-)ordering of coarse graining procedures. Any observable can be interpreted as inducing a coarse-grained description, and relative coarse graining of observables affords a transition to unsharp and ultimately to macroscopic observables, both being needed for understanding the quantum–classical connection.

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2. COARSE GRAINING AS REDUCED DESCRIPTION

2.1. Probabilistic Framework

The common structure of classical and quantum theories is that of a statistical duality $\langle V, W \rangle$, where V is the state space and W the space of observables of the system under consideration (Ludwig, 1983; Stulpe, 1988). More explicitly, (V, S) is a base normed Banach space, with the convex set S of states being the base of the positive, convex, generating cone $V^+ \subset V$. The strictly positive linear charge, or trace functional, which assumes the value 1 on S, shall be denoted e. In the context of physical applications one may assume the existence of a minimal decomposition for $z \in V$, $z = z_+ - z_-$, where $z_\pm \in V^+$ and minimality is explained with reference to the base norm $\|\cdot\|_1$ via the condition $\|z\|_1 = e(z_+) + e(z_-)$. The triple (V, V^+, e) has been termed the measure cone in an axiomatization which is essentially equivalent to that of base normed spaces, but which emphasizes measure-theoretic aspects (Busch and Ruch, 1992).

The space W of observables is taken to be a σ-weakly dense, norm closed subset of V^* from which it is supposed to inherit the structure of an order unit space with order unit e. In the case of classical theories we shall consider statistical dualities with V being either $M(\Gamma, \Sigma)$, the space of bounded signed measures on phase space Γ (Σ being some σ-algebra of subsets), or as a subspace $M_\mu(\Gamma, \Sigma) \simeq L^1(\Gamma, \Sigma, \mu)$ of signed measures which are absolutely continuous with respect to a positive (σ-finite) reference measure μ. The corresponding spaces of observables may be taken to be the space $\mathscr{B}(\Gamma, \Sigma)$ of bounded measurable functions in the first case and $L^\infty(\Gamma, \Sigma, \mu)$ in the second case. The base norm and charge are identical to the total variation norm and the functional $m \mapsto e(m) := m(\Gamma)$, respectively. The quantum mechanical statistical duality shall be taken to be $V = \mathscr{T}_s(\mathscr{H})$, the space of self-adjoint trace class operators, and $W = \mathscr{L}_s(H)$, the space of self-adjoint bounded operators on a complex separable Hilbert space $\mathscr{H}$. Base norm and charge are here the trace norm and the trace $\rho \mapsto \mathrm{tr}[\rho]$, respectively. More generally, W can be the self-adjoint part of a von Neumann algebra of observables and V its space of states.

The positive part $\mathscr{E} = [o, e]$ of the order unit interval is of particular physical interest since its elements, the effects, represent the elementary events occurring as the outcomes of measurements. Therefore, according to the most general and most natural definition, an observable is an effect-valued measure on a measurable space $(\Omega, \mathscr{F})$, $E: \mathscr{F} \to \mathscr{E}$, that is, a device that assigns to any state $\rho \in S$ a probability measure on $(\Omega, \mathscr{F})$, $E_\rho: X \mapsto E_\rho(X) \equiv \langle \rho, E(X) \rangle$. The commonly used notion of observables as functions on phase space or as self-adjoint operators is contained in the present definition by virtue of the spectral theorem. We conclude that any observable E induces a linear "classical" embedding Φ_E of the given state space into a space of probability measures. With this we are facing our most prominent example of a reduced description.

2.2. Reduced Descriptions

A reduced (statistical) description of a physical system is obtained by means of the action of a mapping Φ: $V \to V'$ from the system's state space V into another state space V'. In general, a mapping of one set of objects into another one goes along with some loss of information, which may be due to the noninjectivity of the map or to some loss of structural features of the original set. In the present context, the mapping Φ must be a state transformation, so that $\Phi(S) \subseteq S'$. In addition, Φ should respect the convex constitution of states, that is, $\Phi|_S$ should be an affine map. Equivalently, Φ must be a linear, positive, charge-preserving map, in short, a stochastic map. A linear, charge-preserving map Φ is positive if and only if Φ is a contraction with respect to the base norm. Consequently, any stochastic map Φ generally leads to decreasing dissimilarity of state pairs unless Φ is an isometry. Interestingly, there are injective stochastic maps which are not isometric. The metric properties of stochastic maps furnish the basis for an information-theoretic characterization of reduced descsriptions (Ruch, 1992). The appropriate tool is given by the mixing distance from state ρ to state τ, $d[\rho/\tau]$, which induces a (pre-)ordering of state pairs characterizing the degree of their dissimilarity: $d[\rho/\tau] \succ d[\rho'/\tau']$ holds if and only if

$$\|\alpha\rho - \beta\tau\|_1 \geq \|\alpha\rho' - \beta\tau'\|_1 \qquad \text{for all} \quad \alpha, \beta \in \Re^+$$

This relation is satisfied whenever the pair ρ', τ' is obtained from the pair ρ, τ by means of the action of some stochastic map Φ: $V \to V'$. For a large class of classical state spaces $V = V'$ the converse statement holds true, thus ensuring the existence of some stochastic map Φ with $(\rho', \tau') = (\Phi\rho, \Phi\tau)$ whenever $d[\rho/\tau] \succ d[\rho'/\tau']$.[2] The common information-theoretic characterization of increasing similarity of state pairs is given in terms of some (relative) entropy functional. For example, for a certain class of suitably defined (positive, convex) relative entropy functions $f(\rho, \tau)$ of pairs of distributions one can show that $f(\rho, \tau) \geq f(\Phi\rho, \Phi\tau)$ for any stochastic map Φ. According to the theorem just quoted, the mixing distance affords a sufficient set of such functionals, thereby providing an exhaustive characterization of the (dis-)similarity phenomenon in question.

[2]This theorem, which is due to Ruch and co-workers, is reviewed in (Ruch, 1992); most recent extensions of its domain of validity were obtained by Ruch and Stulpe (1993).

Each single entropy function can only represent some aspect of the phenomenon.

Two coarse graining procedures $\Phi_k: V \to V_k$ $(k = 1, 2)$ can now be compared with each other in the following way. Φ_2 is (relatively) coarser than Φ_1, in short $\Phi_2 \prec \Phi_1$, whenever for all state pairs $\rho, \tau \in S \subset V$ the images under Φ_2 are more similar to each other than the corresponding images under Φ_1, that is, $d[\Phi_2\rho/\Phi_2\tau] \prec d[\Phi_1\rho/\Phi_1\tau]$. This relation will certainly hold whenever Φ_2 is operationally coarser than Φ_1, $\Phi_2 \sqsubseteq \Phi_1$, in the sense that there exists a stochastic map Ψ: $V_1 \to V_2$ such that $\Phi_2 = \Psi \circ \Phi_1$.

Rather than concentrating on the quality of the separation of different states that can be obtained by different reduced descriptions, one may alternatively refer to the mere ability of separating different states, irrespective of the resolution. Two stochastic maps $\Phi_k: V \to V_k$ $(k = 1, 2)$ are informationally equivalent if $\Phi_1^{-1}(\{\Phi_1\rho\}) = \Phi_2^{-1}(\{\Phi_2\rho\})$ for all states $\rho \in S \subset V$. If only an inclusion $\subseteq$ holds between these sets, then Φ_1 is more informative than Φ_2, $\Phi_2 \prec' \Phi_1$. In the extreme case where the first set is a singleton for any state ρ, the map Φ_1 is informationally complete. In other words, an injective state transformation induces an informationally complete reduced description.

The relation $\Phi_2 \prec' \Phi_1$ ensures the existence of a linear, positive, charge-preserving map Ψ from $\Phi_1(V)$ *onto* $\Phi_2(V)$ such that $\Psi(\Phi_1\rho) = \Phi_2(\rho)$. Due to the subsequent proposition, this map Ψ is a stochastic map. Conversely, the existence of such a map implies $\Phi_2 \prec' \Phi_1$. Obviously one has the implications $\sqsubseteq \Rightarrow \prec$ and $\sqsubseteq \Rightarrow \prec'$, but the relations $\prec$ and $\prec'$ are generally incomparable, corresponding to quite different metric characterizations of the coarse-graining procedures under consideration.

Stochastic maps are introduced so as to respect the essential structures of base norm spaces, or measure cones, such as positivity, the charges, and convex structures. They are structure preserving in a deeper sense described in the following proposition.

Proposition 1. Let Φ: $V \to V'$ be as stochastic map from a base normed space (V, S) into a base normed space (V', S'). Then $(\Phi(V), \Phi(S))$ is a base normed space with respect to the inherited norm

$$\|\Phi z\|_1^{(\Phi)} := \inf\{\|z + v\|_1 | v \in \mathrm{Ker}(\Phi)\} \equiv \|[z]_{\mathrm{Ker}(\Phi)}\|_1$$

[The last expression refers to the quotient norm on $V/\mathrm{Ker}(\Phi)$.] One has

$$\|\Phi z\|_1 \le \|\Phi z\|_1^{(\Phi)} \le \|z\|_1$$

Φ is injective if and only if $\|\Phi z\|_1^{(\Phi)} = \|z\|_1$ for all $z \in V$.

Proof. Using properties of Φ and the base norm space (V', S'), it is straightforward to verify that $\Phi(V^+)$ is a proper, generating, convex cone in $\Phi(V)$, with convex base $\Phi(S)$. The charge functional e' associated with S' is also strictly positive with respect to $\Phi(V^+)$. The map Φ induces a canonical bijection between the quotient space $V/\mathrm{Ker}(\Phi)$ and $\Phi(V)$, so that the quotient norm of the former is naturally inherited in the latter space. It remains to show that the norm $\|\cdot\|_1^{(\Phi)}$ is the Minkowski functional of the set $\mathrm{conv}(\Phi(S) \cup -\Phi(S))$, that is,

$$\|z\|_1^{(\Phi)} = \inf\{\lambda \geq 0 | z \in \lambda \ \mathrm{conv}(\Phi(S) \cup -\Phi(S))\}$$

Let $\epsilon > 0$. There exists $w \in \Phi^{-1}(\{z\})$ such that $0 < \|w\|_1 - \|z\|_1^{(\Phi)} < \epsilon/2$. Furthermore, there exist $\lambda \geq 0$, $x, y \in S$, and $\alpha \in [0, 1]$ such that $w = \lambda[\alpha x - (1-\alpha)y]$ and $0 \leq \lambda - \|w\|_1 < \epsilon/2$. It follows that

$$z = \Phi w = \lambda[\alpha \Phi x - (1-\alpha)\Phi y] \in \lambda \ \mathrm{conv}(\Phi(S) \cup -\Phi(S))$$

and $0 \leq \lambda - \|z\|_1^{(\Phi)} < \epsilon$. This completes the proof.

3. TYPES OF REDUCED DESCRIPTIONS

For a coarse-graining map Φ: $V \to V'$ the following cases are typically of interest in physical considerations:

(α) $V = M_\mu(\Gamma, \Sigma)$, $V' = M(\Omega, \mathscr{F})$.
(β) $V = \mathscr{T}_s(\mathscr{H})$, $V' = M(\Omega, \mathscr{F})$.
(γ) $V = M_\mu(\Gamma, \Sigma)$, $V' = \mathscr{T}_s(\mathscr{H})$.
(δ) $V = \mathscr{T}_s(\mathscr{H})$, $V' = \mathscr{T}_s(\mathscr{H})$.

The case (α) comprises coarse graining of classical theories. In the context of quantum mechanics it will be employed to perform procedures of *relative* coarse graining of observables. As we have seen above, any observable E in the sense of an effect-valued measure induces a classical embedding Φ_E, thus an instance of (β). Conversely, any stochastic map Φ: $\mathscr{T}_s(\mathscr{H}) \to M(\Omega, \mathscr{F})$ gives rise to an observable $E = E_\Phi$ on $(\Phi, \mathscr{F})$ such that $\Phi = \Phi_E$. The observable E is determined via the dual map Φ^*: $\mathscr{B}(\Omega, \mathscr{F}) \to \mathscr{L}_s(\mathscr{H})$ as follows: $E_\Phi(X) = \Phi^*(\chi_X)$ for $X \in \mathscr{F}$. Classical embeddings are extensively investigated in Bugajski *et al.* (1993) and Singer and Stulpe (1992).

The most familiar examples of classical coarse graining are phase space partitionings and convolutions. Letting $\Gamma = \bigcup \Gamma_i$ be a disjoint partitioning, define Φ_{part} on $M_\mu(\Gamma, \Sigma)$ such that

$$\Phi_{\mathrm{part}} m(X) = \sum_i \mu(X \cap \Gamma_i) m(\Gamma_i), \qquad X \in \Sigma$$

The induced (classical) effect-valued measure,

$$X \mapsto E_{\text{part}}(X) = \Phi^*_{\text{part}}\chi_X = \sum_i \chi_{\Gamma_i} \frac{\mu(X \cap \Gamma_i)}{\mu(\Gamma_i)}$$

is an unsharp observable in the sense that the effects are no projections (characteristic functions). However, in this case an equivalent description in terms of an ordinary observable is obtained in view of the one-to-one correspondence with the measures $\Phi_{\text{part}}m$ and the discrete measures $i \mapsto m_d(i) := m(\Gamma_i)$. Thus, one may consider instead the stochastic map $\tilde{\Phi}_{\text{part}}$ which sends the measures m to their discrete images m_d. Noting the dual relation $\langle m, \chi_{\Gamma_i}\rangle = \langle m_d, i\rangle$, the associated observable is now the discrete projection-valued measure $i \mapsto E_i := \chi_{\Gamma_i}$.

If the phase space Γ is endowed with the structure of an additive group, then one can perform convolutions. Let μ be the Haar measure on Γ, f a confidence distribution. The following is a stochastic map on $M_\mu(\Gamma, \Sigma) \simeq L^1(\Gamma, \Sigma, \mu)$:

$$\rho \mapsto \Psi_f \rho := f * \rho$$

These operations can be applied to produce relations of coarse grainings. The orderings $\prec$, $\prec'$, and $\sqsubseteq$ defined above for coarse-graining procedures can be transferred to pairs of observables via their associated classical embeddings. As an illustration we consider coarse grainings of phase space observables

$$a: \quad \mathscr{B}(\mathfrak{R}^2) \to \mathscr{E}(\mathscr{H}), \qquad \Delta \mapsto a(\Delta) := \int_\Delta T_{qp} \frac{dq\, dp}{2\pi\hbar}$$

[Here $T_{qp} := U_{qp} T_o U^+_{qp}$, $T_o \in \mathscr{T}_s(\mathscr{H})^+_1$, and $U_{qp} := \exp\{(i/\hbar)[pQ - qP]\}$ denotes a unitary irreducible (projective) representation (on $\mathscr{H}$) of the group of translations on phase space.] The associated classical embedding is

$$\Phi_a: \quad \rho \mapsto p_\rho, \qquad p_\rho(q, p) = \operatorname{tr}[\rho T_{qp}](2\pi\hbar)^{-1}$$

If a is an informationally complete observable, then Φ_a provides a phase space representation of quantum mechanics, which has been discussed by Ali and Prugovečki (1977), Singer and Stulpe (1992), and Schroeck (1982). [For an extensive account of quantum mechanics on phase space, see the monograph of Prugovečki (1986).] The condition for informational completeness is known to be $\operatorname{tr}[U_{qp}T_o] \neq 0$ (almost everywhere).

Let f be a confidence function on phase space. The stochastic map $\Psi_f \circ \Phi_a =: \Phi_{a_f}: \rho \mapsto p_\rho * f$ is another classical (phase space) embedding of the quantum mechanical state space, the associated observable a_f being

$$a_f: \quad \Delta \mapsto a_f(\Delta) := \int_\Delta T^f_{qp} \frac{dq\, dp}{2\pi\hbar}$$

This is again a phase space observable in view of the relation

$$T^f_{qp} = \int_{\Re^2} T_{q'p'} f(q' - q \cdot p' - p)\, dq'\, dp' = U_{qp} T^f_{oo} U^+_{qp}$$

Since Φ_{a_f} is a composition of Φ_a with another stochastic operator Ψ_f, we have the relation $\Phi_{a_f} \sqsubseteq \Phi_a$, or $a_f \sqsubseteq a$. The observable a_f is coarser than a. By choosing f with large variances one obtains macroscopically unsharp phase space observables for which it is possible to construct models of quasiclassical measurements (Quadt and Busch, 1993). Note that the condition of informational completeness will not be lost if f is taken to be a Gaussian distribution.

The stochastic maps of type (γ) appear to be, in the first instance, reduced descriptions of classical theories within a quantum mechanical frame. But a particular choice of the measurable space (Ω, $\mathscr{F}$) yields an interesting representation of the quantum mechanical statistical duality. In fact, let Ω be the set of extremals of the set of states $\mathscr{T}_s(\mathscr{H})_1^+$ endowed with the trace norm topology and the ensuing Borel structure $\mathscr{F}$. Then the map $\Phi_M: m \mapsto \int_\Omega p\, dm$ (Misra, 1974) is a stochastic map, and for any $A \in \mathscr{L}_s(\mathscr{H})$ one has

$$\operatorname{tr}[\Phi_M m \cdot A] = \int \operatorname{tr}[A \cdot p]\, dm = \langle m, \Phi^*_M A \rangle$$

The dual map $\Phi^*_M: A \mapsto \{\operatorname{tr}[A \cdot p]\}$ is an injective embedding of $\mathscr{L}_s(\mathscr{H})$ into the space of continuous functions on Ω. Clearly, $\Phi^*_M \mathscr{L}_s(\mathscr{H})$ does not separate $M(\Omega, \mathscr{F})$, so that many probability measures m are associated with a given mixed state ρ, thus representing the nonunique decomposability of nonpure quantum states. Generalizing this method, Bugajski (1991) presented an interesting framework for nonlinear extensions of quantum mechanics toward classical theories.

Finally, an example of type (δ) coarse graining is given by the analog of phase space partitioning, which has often been used for the description of macroscopic observables. Let $I = \sum_k P_k$ be a partitioning of the unit into finite-rank projections ($\operatorname{tr}[P_k] = n_k$), and define the stochastic map

$$\Phi^q_{\text{part}}: \quad \rho \mapsto \sum_k \operatorname{tr}[\rho P_k] \frac{1}{n_k} P_k$$

Since the state operators in the range Φ^q_{part} are mutually commutative, this map can be equivalently interpreted as a classical embedding $\rho \mapsto p_\rho(k) := \operatorname{tr}[\rho P_k]$.

Such an alternative interpretation is no longer possible in the case of a Lüders measurement operation,

$$\Phi_{\text{L}}: \quad \rho \mapsto \sum_k P_k \rho P_k \qquad \left(\sum_k P_k = I\right)$$

which describes the state change due to an ideal measurement. Φ_L coincides with the previous map exactly when the projections P_k are of rank one.

More generally, one may consider any completely positive stochastic map Φ: $\rho \mapsto \Phi\rho$. Any such map induces, by virtue of its dual Φ^*, a map on the set of observables, $E \mapsto \Phi^* \circ E := F$. In a measurement context these maps can be interpreted as follows. If a system is prepared in state ρ, it may suffer some external disturbance (noise), which changes its state into $\Phi\rho$. A subsequent measurement of E then is equivalent to measuring F directly on the state ρ, since $\mathrm{tr}[\rho \cdot F(X)] = \mathrm{tr}[\Phi\rho \cdot E(X)]$. Using Naimark's extension theorem, it is not hard to show that any effect-valued measure F can be obtained in this way from some projection-valued measure E, so that in any case a noise interpretation is possible in principle (Busch *et al.*, 1993). In some instances the maps Φ^* are seen to admit an interpretation in the sense of relative coarse graining (Quadt and Busch, 1993).

To conclude, we have surveyed a new conception of coarse graining, providing a unified formulation of various kinds of reduced descriptions of physical systems. The great flexibility achieved is due to the fact that the full set of observables is taken into account, including both ordinary (sharp) observables (spectral measures) as well as genuinely unsharp observables. The latter are exemplified by means of phase space observables which represent joint position and momentum measurements. The marginal observables are known to be obtained from ordinary position and momentum observables, to be obtained from ordinary position and momentum via convolution, hence relative coarse graining. Thus, classical features such as coexistence can be restored for noncommuting observables by performing suitable coarse grainings, which necessarily lead to unsharp observables. Moreover, macroscopic phase space observables display operational features which are characteristic of quasiclassical measurement situations, and these features emerge by themselves with increasing intrinsic inaccuracies, without any additional ad hoc assumptions. In this respect we expect that coarse graining as described here may ultimately lead to a representation of macroscopic, quasiclassical observables which is superior to the traditional description in terms of the quantum partitioning maps Φ^q_{part} (cf. also Ludwig, 1987). This view is reinforced by the fact that coarse graining yields a vast variety of classical representations of quantum mechanics, thereby providing a promising framework for further investigations into the quantum–classical connections.

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