Quantum Central Limit Theorems, Emergence of Classicality and Time-dependent Differential Entropy

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Summary of Results

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- We derive some quantum mechanical versions of CLTs for expectation values of observable coarse-grained observables, which are functions of coarse-grained hermitean operators
- With hermicity constraints, we obtain positive-definite distributions for the expectation values
- Those probability distributions enable a path way for emergence of classical coarse-graining behaviours, which is due to neither environmental decoherence nor interactions among the constituents
- The probability distributions of the quantum CLT further enable us to evaluate some differential entropies, which are symmetric with respect to time reversal, as is the underlying quantum dynamics. Nevertheless, they could have some interesting and non-trivial temporal dependence

Overview

Central Limit Theorem and Renormalisation Blocking

- Renormalisation group blocking plays a central role in understanding emerging bulk behaviours and collective phenomena.
- We start with a path integral or partition function in some set of fundamental microscopic variables / operators.
  Let us take the path integral expression for a quantum system having the action $\mathcal{S}[\xi]$ in the fundamental field variable ξ,

$$\mathcal{Z} = \int \exp\{i\mathcal{S}[\xi]\}\mathcal{D}\xi. \tag{1}$$

  We introduce the coarse-grained field variable Ξ as a function of the fundamental variables ξ in some chosen blocking scheme $\Xi_j = h(\xi)$, as in an averaging scheme, for example,

$$\Xi_j = \frac{1}{V_j} \sum_{\xi_i \in \text{block } j} \xi_i, \tag{2}$$

  where V_j is a measure of the "volume" of each block.

Central Limit Theorem and Renormalisation Blocking

The expectation value of a quantum operator $\langle F(\Xi)\rangle$ of the coarse-grained variables could then be expressed as

$$\langle F(\Xi(\xi))\rangle = \frac{1}{\mathcal{Z}}\int F(\Xi(\xi))\exp\{i\mathcal{S}[\xi]\}\mathcal{D}\xi. \tag{3}$$

To convert the last path integral in $\mathcal{D}\xi$ to that in $\mathcal{D}\Xi$, we insert the resolution of unity

$$1 = \int \delta(\Xi - h(\xi))\mathcal{D}\Xi \tag{4}$$

into (3) then interchange the order of integration to obtain

$$\langle F(\Xi)\rangle = \frac{1}{\mathcal{Z}}\int F(\Xi)\exp\{i\mathcal{S}'[\Xi]\}\mathcal{D}\Xi, \tag{5}$$

where

$$\exp\{i\mathcal{S}'[\Xi]\} = \int \delta(\Xi - h(\xi))\exp\{i\mathcal{S}[\xi]\}\mathcal{D}\xi. \tag{6}$$

Successive repeating of the last expression defines a renormalisation group flow.

Central Limit Theorem and Renormalisation Blocking

- We will phrase the quantum central limit theorems in this paper as a restricted renormalisation blocking in the sense that we consider only the expectation values of hermitean operators and not functions for arbitrary operators.
- Our restricted consideration results in positive-definite measures which can be interpreted as probability measures, from which the fixed-point distributions of the renormalisation blocking emerge.

Quamtum CLT for Single Hermitean Variable

The centre of mass, or intensive variables in general, of a composite systems of N components can be expressed as

$$\hat{X} = \frac{1}{N}\left(\hat{x}_1 \otimes \hat{1}_2 \cdots \otimes \hat{1}_N + \hat{1}_1 \otimes \hat{x}_2 \cdots \otimes \hat{1}_N + \cdots + \hat{1}_1 \otimes \hat{1}_2 \cdots \otimes \hat{x}_N\right)$$
$$\equiv \frac{1}{N}\sum_{i=1}^{N} \hat{x}_i \qquad (7)$$

We now consider a system with identical and non-interacting components (such as the case of an ideal gas)

$$|\Phi\rangle = \otimes_i^N |\phi_i\rangle,$$

where $|\phi_i\rangle = |\phi\rangle$, for all i.

With some general function f, we obtain the following result for $N \gg 1$

$$\left\langle \Phi \left| f\left(\frac{1}{N}\sum_i^N \hat{x}_i\right) \right| \Phi \right\rangle \xrightarrow{N\to\infty} \frac{1}{(\sigma_x/\sqrt{N})2\pi\sqrt{2\pi}} \int dX f(X) \exp\left\{-\frac{(X-\langle x\rangle)^2}{2(\sigma_x/\sqrt{N})^2}\right\}, \quad (8)$$

where

$$\langle x\rangle \equiv \int x|\langle x|\phi\rangle|^2 = \langle\phi|\hat{x}|\phi\rangle, \quad (9)$$

$$\sigma_x^2 \equiv \langle x^2\rangle - \langle x\rangle^2. \quad (10)$$

We can also easily generalise the result to the case when the initial state is a mixed state instead of being pure.

In the limit of $N \to \infty$ the gaussian distribution in (8) converges to a delta distribution,

$$\frac{1}{(\sigma_x/\sqrt{N})2\pi\sqrt{2\pi}} \exp\left\{-\frac{(X-\langle x\rangle)^2}{2(\sigma_x/\sqrt{N})^2}\right\} \quad \overset{N\to\infty}{\longrightarrow} \quad \delta(X-\langle x\rangle). \tag{11}$$

We thus have from (8), for arbitrarily finite integer m,

$$\left\langle \Phi \middle| \hat{X}^m \middle| \Phi \right\rangle \quad \overset{N\to\infty}{\longrightarrow} \quad \int dX\, X^m \delta(X-\langle x\rangle) = \langle x\rangle^m. \tag{12}$$

This is an indication of an emergence of classical behaviours for macroscopically blocked variable X, as the right hand side of the last expression contains $\langle x\rangle^m$ rather than $\langle x^m\rangle$.
In order to verify such emergence we will need to further consider quantum mechanically non-commuting variables.

Quantum CLT for Non-commuting Variables

The centre of mass, or intensive variables in general, of a composite systems of N components can be expressed as

$$\begin{aligned}\hat{X} &= \frac{1}{N}\left(\hat{x}_1 \otimes \hat{1}_2 \cdots \otimes \hat{1}_N + \hat{1}_1 \otimes \hat{x}_2 \cdots \otimes \hat{1}_N + \cdots + \hat{1}_1 \otimes \hat{1}_2 \cdots \otimes \hat{x}_N\right) \\ &\equiv \frac{1}{N}\sum_{i=1}^{N} \hat{x}_i. \qquad (13)\end{aligned}$$

We also introduce the blocked variable $\hat{P}$ of the momentum $\hat{p}_i$

$$\begin{aligned}\hat{P} &= \frac{1}{N}\left(\hat{p}_1 \otimes \hat{1}_2 \cdots \otimes \hat{1}_N + \hat{1}_1 \otimes \hat{p}_2 \cdots \otimes \hat{1}_N + \cdots + \hat{1}_1 \otimes \hat{1}_2 \cdots \otimes \hat{p}_N\right) \\ &\equiv \frac{1}{N}\sum_{i=1}^{N} \hat{p}_i, \qquad (14)\end{aligned}$$

this blocked variable $\hat{P}$ corresponds to a measure of the velocity of the centre of mass.

In the Heisenberg picture

$$\begin{aligned} \frac{d}{dt}X &= \frac{i}{\hbar}[H, X], \\ &= \frac{i}{\hbar}\left[\sum_{i}^{N}\frac{p_i^2}{2m} + V_i(x_i), \frac{1}{N}\sum_{j}^{N}x_j\right], \\ &= P/m. \end{aligned} \tag{15}$$

We now consider a system with identical and non-interacting components (such as the case of an ideal gas)

$$|\Phi\rangle = \otimes_i^N |\phi_i\rangle,$$

where $|\phi_i\rangle = |\phi\rangle$, for all i.
We also only consider a *hermitian* combination of some finite sum of products of $\hat{X}$ and $\hat{P}$, which can be expressed in general as, by constraint of hermiticity,

$$c_{mn}(\hat{X})^m(\hat{P})^n + c_{mn}^*(\hat{P})^n(\hat{X})^m, \tag{16}$$

where c_{mn} are c-numbers.

For $N \gg 1$, we obtain the following result,

$$\left\langle \Phi \left| \sum_{mn} (c_{mn} X^m P^n + c^*_{mn} P^n X^m) \right| \Phi \right\rangle =$$
$$\int dXdP \, \left(2 \sum_{mn} \Re(c_{mn}) X^m P^n \right) \mathcal{P}_{re}(X, P)$$
$$+ \int dXdP \, \left(\sum_{mn} \Im(c_{mn}) X^m P^n \right) \mathcal{P}_{im}(X, P), \qquad (17)$$

where the probability distribution for the real parts $\Re(c_{mn})$ is

$$
\begin{aligned}
&\mathcal{P}_{re}(X,P) \sim \\
&\exp\left\{-\frac{[(X-\langle x\rangle)\cos\theta_+ + (P-\langle p\rangle)\sin\theta_+]^2}{(\sigma_x^2+\sigma_p^2+\Delta_+)/N}\right\} \\
&\times\exp\left\{-\frac{[(P-\langle p\rangle)\cos\theta_+ - (X-\langle x\rangle)\sin\theta_+]^2}{(\sigma_x^2+\sigma_p^2-\Delta_+)/N}\right\}, \quad (18)
\end{aligned}
$$

where

$$
\begin{aligned}
\langle xp\rangle_c &= \frac{1}{2}\langle \hat{x}\hat{p}+\hat{p}\hat{x}\rangle - \langle\hat{x}\rangle\langle\hat{p}\rangle, && (19)\\
\theta_+ &= \frac{1}{2}\arctan\left(\frac{2\langle xp\rangle_c}{\sigma_x^2-\sigma_p^2}\right), && (20)\\
\Delta_+ &= \sqrt{(\sigma_x^2-\sigma_p^2)^2+4\langle xp\rangle_c^2}, && (21)
\end{aligned}
$$

While the probability distribution for the imaginary parts $\Im(c_{mn})$ is

$$\mathcal{P}_{im}(X,P) = \mathcal{N}_1 \exp\left\{-\frac{[(X-\langle x\rangle)\cos\theta_- + (P-\langle p\rangle)\sin\theta_-]^2}{(\sigma_x^2+\sigma_p^2+\Delta_-)/N}\right\} \times \exp\left\{-\frac{[(P-\langle p\rangle)\cos\theta_- - (X-\langle x\rangle)\sin\theta_-]^2}{(\sigma_x^2+\sigma_p^2-\Delta_-)/N}\right\} - \mathcal{N}_2 \exp\left\{-\frac{(P-\langle p\rangle)^2}{2\sigma_p^2/N} - \frac{(X-\langle x\rangle)^2}{2\sigma_x^2/N}\right\}. \tag{22}$$

In the above, $\mathcal{N}_1$ and $\mathcal{N}_2$ are normalising factors, and

$$\langle xp\rangle_- = i\langle \hat{x}\hat{p} - \hat{p}\hat{x}\rangle, \tag{23}$$

$$\theta_- = \frac{1}{2}\arctan\left(\frac{2\langle xp\rangle_-}{\sigma_x^2-\sigma_p^2}\right), \tag{24}$$

$$\Delta_- = \sqrt{(\sigma_x^2-\sigma_p^2)^2 + 4\langle xp\rangle_-^2}. \tag{25}$$

An Emergence of Classicality

It can be shown that the correlation between the coarse-grained/renormalisation block variables $\hat{X}$ and $\hat{P}$

$$\begin{aligned}
\frac{1}{2}\left\langle \Phi \left| \hat{X}\hat{P} + \hat{P}\hat{X} \right| \Phi \right\rangle \quad &\overset{N\to\infty}{\sim} \quad \int dXdP\, XP\, \mathcal{P}_{re}(X,P), \\
&\overset{N\to\infty}{\sim} \quad \langle x\rangle\langle p\rangle + \langle xp\rangle_c/N, \\
&\overset{N\to\infty}{\sim} \quad \left\langle \Phi \left| \hat{X} \right| \Phi \right\rangle \left\langle \Phi \left| \hat{P} \right| \Phi \right\rangle + O(1/N),
\end{aligned} \tag{26}$$

indicating that, in this limit, the coarse-grained/renormalisation block variables are uncorrelated and behaving as classically independent variables.

We further observe that, in the limit of infinitely many identical and non-interacting quantum subsystems, $N \to \infty$,

$$
\begin{aligned}
\mathcal{P}_{re}(X,P) \overset{N\to\infty}{\longrightarrow} \quad & \delta\left((X-\langle x\rangle)\cos\theta_{+}+(P-\langle p\rangle)\sin\theta_{+}\right) \\
& \times\delta\left((P-\langle p\rangle)\cos\theta_{+}-(X-\langle x\rangle)\sin\theta_{+}\right), \\
\overset{N\to\infty}{\longrightarrow} \quad & \delta\left((X-\langle x\rangle)/\cos\theta_{+}\right)\delta\left((P-\langle p\rangle)\cos\theta_{+}\right), \\
\overset{N\to\infty}{\longrightarrow} \quad & \delta(X-\langle x\rangle)\delta(P-\langle p\rangle). \qquad (27)
\end{aligned}
$$

And

$$
\begin{aligned}
\mathcal{P}_{im}(X,P) \overset{N\to\infty}{\longrightarrow} \quad & \delta\left((X-\langle x\rangle)\cos\theta_{-}+(P-\langle p\rangle)\sin\theta_{-}\right) \\
& \times\delta\left((P-\langle p\rangle)\cos\theta_{-}-(X-\langle x\rangle)\sin\theta_{-}\right) \\
& -\delta(X-\langle x\rangle)\delta(P-\langle p\rangle), \\
\overset{N\to\infty}{\longrightarrow} \quad & 0. \qquad (28)
\end{aligned}
$$

Thus,

$$\left\langle \Phi \left| \sum_{mn} (c_{mn} X^m P^n + c^*_{mn} P^n X^m) \right| \Phi \right\rangle \xrightarrow{N \to \infty} 2 \sum_{mn} \Re(c_{mn}) \langle x \rangle^m \langle p \rangle^n. \tag{29}$$

- The right hand side above now involves only $\langle x \rangle^i$ and $\langle p \rangle^j$, and contains neither $\langle x^i \rangle$ nor $\langle p^j \rangle$, nor the quantum correlations $\langle x^i p^j \rangle$
- Implied also in this last expression, which does not include the imaginary parts $\Im(c_{mn})$, is that the expectation value of the commutator of the coarse-grained variables $\hat{X}$ and $\hat{P}$ is vanishingly small with sufficiently large N
- As a consequence, a regime of classicality could be emerging due to the fact that quantum correlations and all traces of quantum behaviours are now suppressed, except those inherent in the quantum expectation values $\langle x \rangle$ and $\langle p \rangle$

Time-dependent Differential Entropies

A direct generalisation of information Shannon entropy for discrete probabilities

$$S_d = -k_B \sum_i p_d^{(i)} \ln p_d^{(i)} \tag{30}$$

to the case of continuous probability distributions might be

$$DEnt_1 = -k_B \int Pr(X,P) \ln Pr(X,P) \, dXdP. \tag{31}$$

This is normally called the differential entropy.

- This definition of differential entropy, however, does not share all properties of discrete entropy. For example, the differential entropy above can be negative; more importantly, it is not invariant under continuous coordinate transformations. In fact, Jaynes showed that the expression above is NOT the correct limit of the expression for a finite set of probabilities
- It is TIME-INDPENDENT due to the unitary nature of quantum evolution
- Following Janes, we introduced a modification of differential entropy to address defects in the initial definition of differential entropy by adding an invariant measure factor to correct these

From hereon we adopt, following Jaynes, a modified differential entropy

$$DEnt = k_B \int Pr(X,P) \ln \left(\frac{Pr(X,P)}{\int Pr(X,P)dP \int Pr(X,P)dX} \right) dXdP. \quad (32)$$

- This entropy notion is a special instance of the relative entropy in information theory, also known as the Kullback–Leibler divergence or relative entropy
- It is a statistical distance to measure how one probability distribution is different from a second reference probability distribution
- A simple interpretation of this divergence is the expected excess surprise from using the latter as a model when the actual distribution is the reference distribution

Restricting ourselves to observables in general, it suffices to consider only the particular case whereby c_{mn} in (17) are real. Substituting the probability distribution for the real component (18) (which suffices for classical observables) into our adopted entropy (32), we arrive at

$$DEnt = -k_B \ln \left[(\sigma_x^2 \sigma_p^2 - \langle xp \rangle_c) / \sigma_x^2 \sigma_p^2 \right] . \tag{33}$$

We see from this explicit expression that the non vanishing of $\langle xp \rangle_c$ in general, due to quantum correlations, that enables some non-trivial time dependence for the differential entropy.

Free Particles

For free particles in one dimension, we have in the Heisenberg picture,

$$\begin{aligned} \hat{H} &= \frac{\hat{p}^2}{2m}, \\ \hat{x}(t) &= \hat{x}(0) + \frac{\hat{p}(0)}{m} t, \\ \hat{p}(t) &= \hat{p}(0) = \hat{p}. \end{aligned} \tag{34}$$

It then follows that the coarse-grained entropy, for sufficiently large time, is behaving as

$$DEnt(t) \stackrel{t \to \infty}{\longrightarrow} \mathcal{O}(\ln |t|). \tag{35}$$

- which is increasing irreversibly with time (unless the individual subsystem is initially in a momentum eigenstate) – *cf* Sackur-Tetrode equation
- although invariant with time-reversal, $t \to -t$ and $\hat{p} \to -\hat{p}$, as is the symmetry of the underlying dynamics

Uniform and Constant Force

For a system under an uniform and constant external force, we have in the Heisenberg picture

$$\begin{aligned} \hat{H} &= \frac{\hat{p}^2}{2m} - a\hat{x}, \\ \hat{x}(t) &= \hat{x}(0) + \hat{p}(0)t/m + at^2/2m, \\ \hat{p}(t) &= \hat{p}(0) + at. \end{aligned} \tag{36}$$

Upon which, the coarse-grained entropy is, for large time, also increasing irreversibly,

$$DEnt \xrightarrow{t\to\infty} \mathcal{O}(\ln|t|), \tag{37}$$

unless $\sigma_p^2(0) = 0$ and $\langle x(0)p(0)\rangle_c = 0$, that is, unless when the individual subsystem is in a momentum eigenstate initially.

Oscillatory Particles

On the other hand, an example in which the differential entropy is not monotonic in time is that of the quantum simple harmonic oscillator,

$$\begin{aligned} \hat{H} &= \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2, \\ \hat{x}(t) &= \hat{x}(0)\cos(\omega t) + \frac{\hat{p}(0)}{m\omega}\sin(\omega t), \\ \hat{p}(t) &= \hat{p}(0)\cos(\omega t) - m\omega\hat{x}(0)\sin(\omega t). \end{aligned} \tag{38}$$

- In this case, the differential entropy is not, even for large time, a monotonic function of the time
- Not surprising for a driven system

Concluding Remarks

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- Those probability distributions enable a path way for emergence of classical coarse-graining behaviours, which is due to neither environmental decoherence nor interactions among the constituents
- The probability distributions of the quantum CLT further enable us to evaluate some differential entropies, which are symmetric with respect to time reversal, as is the underlying quantum dynamics. Nevertheless, they could have some interesting and non-trivial temporal dependence