Dynamics of Statistical Quantum System in Terms of Bosonic Occupation Numbers

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Abstract

The second-order approach of entropy gradient maximization, applied to the problem of a quantum bosonic system, results in an integro-differential dynamic equation. Its local approximation provides the conventional diffusion and the wave equation

1 Introduction

The *entropy gradient maximization* approach recently proposed in [1] and extended to the second-order formalism [2] is reconsidered below in the context of a simple quantum system. This formalism is applied to the system with many degrees of freedom (DoF's) of arbitrary nature, and on this point it should be noted, that *degrees of freedom do not mean* necessary the three-dimensional *spatial coordinates*. For instance, in the case of a quantum system with a large number of undistinguished units (e.g. particles), the state *occupation number* is the more appropriate measure.

Especially, for a quantum many-particle system of identical units, the key object of the *entropy gradient maximization* -the entropy function- in terms of these variables is a simple and well-defined combinatorial expression. It has been demonstrated on the example of a system with large number of quantum states occupied by infinitely many bosonic units.

The approach is shown to provide a meaningful relation for dynamics of this system, having the form of integro-differential equation. Its local

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interpretation leads to constructions which are well recognizable as usual equations for diffusion and wave propagation.

In opposition to to the probabilistic approach, conventional in the statistical physics, the formalism is based on the deterministic postulation of the entropy function, defined on the space of all possible states. The application of the *entropy gradient maximization* formalism is outlined in detail in the mathematical appendix.

Started initially with the discrete set of states occupied by discrete quantum numbers (ensemble), it arrives at the discrete system of equations, describing the collective dynamics of this ensemble.

A generalization of the discrete system to the continuum provides the integro-differential equation for the time-dependent space distribution of quantum occupation numbers in the state space.

Subsequently, a local behavior of a compact perturbation of a distribution is shown to obey the diffusion-like and wave-like propagation as well, which can be interpreted as 'statistically driven', since both equations result from the same global integro-differential dynamical law and entirely only from the entropy construction by the local application of the second law of thermodynamics [1]

2 Application of the *entropy gradient maximization* in terms of occupation numbers

2.1 Formulation of the Problem

Consider a system of $\mathcal{N}$ units, which are distributed in a discrete set of $2N+1$ different states numbered as $-N, -N+1, ..., i-1, \ ... \ i, \ i+1, ..., N-1, N$ occupied by numbers ..., n_{i-1} n_i, n_{i+1}, n_{i+2}, ...

It is noted again, that the 'units' generally do not mean 'particles'. It could be rather any conserved quantity, like electric charge in units of e or action (distance $\times$ momentum, energy $\times$ time interval) in units of $\hbar$.

Suppose, any state of the system is completely determined by the quantum occupation numbers n_i and the state τ of a time-reference subsystem ('clock'). Thus, the system $\{n_i, \tau\}$ is closed and the *entropy gradient maximization* can be applied.

The second-order entropy variation, as outlined in [1, 4], is given by

$$\begin{aligned}\delta S[n_i,\tau] &= \sum_i \left[S_{n_i} dn_i + \frac{1}{2} S_{n_i n_i} dn_i^2 + + S_{n_i \tau} dn_i d\tau \right] \\ &+ \sum_{i \neq k} S_{n_i n_k} dn_i dn_k + S_\tau d\tau + \frac{1}{2} S_{\tau\tau} d\tau^2 + \frac{1}{3!}(\text{third order}) + ...\end{aligned} \tag{1}$$

The condition of conservation for the total occupation number (e.g. number of particles) $\mathcal{N}$ is considered as the additional global *ergodicity condition*

$$\sum_{i=-N}^{N} n_i = \mathcal{N}. \tag{2}$$

The total differentiation of this equation gives the local *ergodicity condition* ϵ :

$$\epsilon := \left\{ \sum_{i=-N}^{N} dn_i = 0 \right\} \tag{3}$$

The maximization of the ergodic entropy variation regarding the (3)

$$\delta S^\epsilon = \delta S + \lambda \sum_{i=-N}^{N} dn_i \tag{4}$$

in the case of *discoupled clock* τ [3]

$$S_{n_i \tau} = 0, \tag{5}$$

results in the set of dynamical equations:

$$\begin{aligned}\frac{\partial}{\partial n_i} \delta S^\epsilon[n_i] &= S_{n_i} + S_{n_i n_i} dn_i + \sum_{i \neq k} S_{n_i n_k} dn_i + \lambda = 0 \\ \frac{\partial}{\partial \tau} \delta S^\epsilon[n_i] &= S_\tau + S_{\tau\tau} d\tau = 0\end{aligned} \tag{6}$$

Now consider the given system of $2N+1$ states $-N, -N+1, ..., -1, 0, 1, 2, ..., N$, each of them can be occupied arbitrarily many times by $n_{-N}, n_{-N+1}, ..., n_{-1}, n_0, n_1, n_2, ..., n_N$ units (particles), which are not distinguished from each other. It corresponds statistically to the *bosonic* case.

The statistical weight of the state vector of occupation numbers n_i is given combinatorially by

$$W_{n_i} = \frac{(n_1 + n_2 + ... + n_N)!}{n_1! n_2! ... n_N!} = \frac{\left(\sum\limits_{i=-N}^{N} n_i\right)!}{\prod\limits_{i=-N}^{N} n_i!}$$

and the related additive entropy is the logarithm of W - the *discrete bosonic entropy* :

$$S[n_i] = \ln W_{n_i} = \ln \left(\sum_{i=-N}^{N} n_i\right)! - \sum_{i=-N}^{N} \ln n_i! \tag{7}$$

In the continuum limit at very large numbers n_i factorials are replaced by Gamma-functions:

$$S[n(i)] = \ln W_{n(i)} = \ln\ \Gamma\left[\sum_{i=-N}^{N} n(i)\right] - \sum_{i=-N}^{N} \ln\ \Gamma[n(i)] \tag{8}$$

For the both cases (7 - 8) one obtains for partial derivatives (Sec. Appendix):

$$S_{n_i} = \sum_i n_i - n_i;\ \ S_{n_i n_k} = 1; S_{n_i n_i} = 0$$

Thus, for the dynamical equations we have:

$$\sum_i n_i - n_i + \sum_{i \neq k} dn_k + \lambda = 0 \quad \Rightarrow dn_i = \sum_{k=-N}^{N} -n_i + \lambda \tag{9}$$

$$S_\tau + S_{\tau\tau} d\tau = 0 \quad \Rightarrow d\tau = -\frac{S_\tau}{S_{\tau\tau}} = -1/(\ln S_\tau)_\tau \tag{10}$$

Further we obtain from (9) using (3):

$$\sum_{i=-N}^{N} dn_i = (2N+1) \sum_{k=-N}^{N} n_k - \sum_{i=-N}^{N} n_i + (2N+1)\lambda = 0 \tag{11}$$

Finally (Appendix):

$$dn_i = \sum_{k=-N}^{N} n_k - n_i - \frac{N-1}{N} \sum_{k=1}^{N} n_k = \frac{1}{N} \sum_{k=1}^{N} n_k - n_i$$

and the dynamical equation for the state vector n_i reads

$$\frac{dn_I}{d\tau} = -\frac{S_\tau}{S_{\tau\tau}}\left[\frac{1}{2N+1}\sum_{i=-N}^{N} n_i - n(i)\right] \tag{12}$$

In a continuum limit for very large $N \to \infty$ the index i can be considered as a continuous coordinate in a one-dimensional state space. Without restriction of generality let the values i belong to the symmetric interval $i \in [-N, N]$, the length of the interval is $2N+1$.

Thus the dynamical equation is an integro-differential equation, which reads now:

$$\frac{dn(i)}{d\tau} = -\frac{S_\tau}{S_{\tau\tau}}\left[\frac{1}{2N+1}\int_{-N}^{N} n(i)di - n(i)\right] \tag{13}$$

Especially, recalling that $2N+1$ - number of states, $\mathcal{N}$ - number of units

$$\frac{1}{2N+1}\int_{-N}^{N} n(k)dk = \frac{\mathcal{N}}{2N+1} = \overline{n}$$

is the expectation value of n, the equation becomes

$$\frac{dn(i)}{d\tau} = -\frac{S_{\tau\tau}}{S_\tau}\left(\overline{n} - n(i)\right) \tag{14}$$

The integro-differential relations (12-13) describes a set of states $-N, ..., i, i+1, ...N$ occupied by number of quantum units n_i, which change with the increasing time-reference τ by changing of each occupation number $n(i)$ towards the global averaging occupation number - expectation value of the distribution $n(i)$ independently of each other (Fig.1), that maximizes the entropy. The rate of change for n_i is proportional to the difference $n_i - \overline{n}$.

In this sense, two different degrees of freedom $n(i), n(k)$ 'does not see' a *near-far order*. It means that no relations like a pairwise interaction potential $U(i,k)$ appear in the dynamics, since n_i is not an ordered set and the numerations i is absolutely discretionary.

Instead of that, a collective interaction potential $\overline{n} - n(i)$ occurs within the *correlation subset* $-N, N$, where the occupation untis are identical. It corresponds to the quantum-mechanical phenomena of *exchange interaction.*

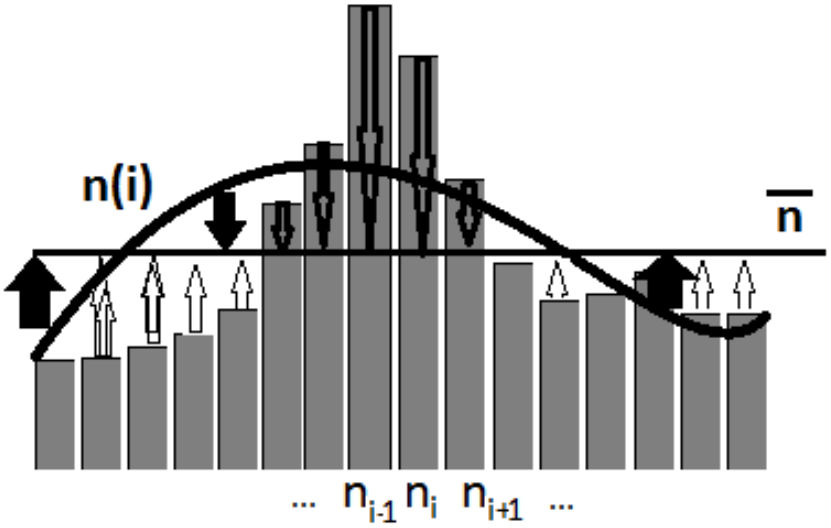

Figure 1

2.2 Local interpretations

Consider a perturbation $\tilde{n}(i)$ of a solution n_0, for instance the trivial constant solution $n(i) = n_0$ =const, which is localized inside of the *correlation subset* $-N, N$. Then the integral of obeys the condition of *global translational invariance*, that for a finite i

$$\int_{-N}^{+N} \tilde{n}(k+i)dk = \int_{-N}^{+N} \tilde{n}(k)dk$$

as long as the displaced distribution $\tilde{n}(i)$ still lies inside of the *correlation subset*.

2.2.1 Diffusion equation

For a perturbation $\tilde{n}(i)$ defined above, at $|k| << |i|$ the expansion

$$\int_{-N}^{+N} \tilde{n}(k+i)dk \approx \tilde{n}(i) \int_{-N}^{+N} dk + \tilde{n}'(i) \int_{-N}^{+N} kdk + \frac{\tilde{n}''(i)}{2!} \int_{-N}^{+N} k^2 dk + \frac{\tilde{n}'''(i)}{3!} \int_{-N}^{+N} k^3 dk + ...$$

$$\frac{dn(i)}{d\tau} = -\frac{S_\tau}{S_{\tau\tau}}\left[\frac{1}{2N+1}\int_{-N}^{N} n(i)di - n(i)\right] \approx -\frac{S_\tau}{S_{\tau\tau}}\left[\frac{N^3}{6(2N+1)}\tilde{n}''(i) + \frac{N^5}{(120(N+1)}\tilde{n}''''(i)\right] \tag{15}$$

which reproduces in the first leading order the local diffusion equation (Fick's law), where the factor at the second derivative should be interpreted as the diffusion constant.

Without further restrictions on the perturbation $\tilde{n}(i)$ the diffusion rate and especially the diffusion constant diverge for a large correlation interval ($N \to \infty$), as the expectation value of a localized finite distribution on the infinite interval vanishes. To avoid this artificial fact, we restrict the class of considered perturbations which are localized on a finite correlation interval.

2.2.2 Wave equation

Before proceeding with this class of local perturbations it should be pointed out, that the dynamic equations (12-13) possess a remarkable property:

$$\frac{d^2}{d\tau^2}n(i) = -\frac{S_{\tau\tau\tau}}{S_\tau}\left(\overline{n} - n(i)\right) \tag{16}$$

(see Appendix for derivation).

Therefore, the procedure like the outlined above for the diffusion equation, provides now:

$$\frac{d^2}{d\tau^2}\tilde{n}(i) = -\frac{S_{\tau\tau\tau}}{S_\tau}\frac{N^3}{6(2N+1)}\tilde{n}''(i) \tag{17}$$

which looks locally as a conventional wave propagation of the perturbation $\tilde{n}(i)$, provided i is interpreted as a space coordinate.

2.3 Causality problem

Since the *causality condition* [1] for the system (7, 2) is not satisfied. Namely, for a time-discoupled system $S_{n_i\tau} = 0$ the dependence of clock-reference is required by causality to obey

$$S_\tau > 0 \text{ time eligibility and } S_{\tau\tau} < 0 \text{ time concavity,}$$

while the Sylvester-Jacobi criterion for sub-determinants of $S_{n_i n_k}$ gives $-1, 2, -3, ...$ It means, the system (**??**) describes a set n_i, where a (half-)part of degrees

of freedom for the increasing τ with $S_\tau > 0$ maximizes the entropy, while the another one minimizes, that suggests a splitting of the system in two equations related to $\pm\frac{\partial}{\partial\tau}$. This realizes the scenario of Schrödinger equation with two-component (complex) state function.

On the other hand, a physical interpretation of the equation (**??**) can be first possible, if some function $x_m(n_i)$ is given, which maps the infinitely-dimensional state-space n_i of occupation numbers in the physical finite-dimensional (e.g. three-dimensional) configuration space x_m of coordinates. The form of (15, 17) should be also retained in terms of x_m.

2.4 Conclusion

The simple quantum-statistical model outlined above has been used to demonstrate, that the *entropy gradient maximization* formalism applied to the infinite-dimensional system, provides finally local PDE's of construction typical for field theories and continuous media.

Namely, the key equation governing the dynamics of a statistical system with many degrees of freedom is an integro-differential equation, global on the entire state space. Its local approximation of the first order in time-reference reproduces a form of the the diffusion (also Schrödinger) and wave equations.

Alternatively to a usual probabilistic approach [**?**] for deriving of diffusion equation, the formalism outlined above is pure deterministic, based on the straightforwardly constructed combinatoric expression for the entropy function.

It is worth remarking in contrary to the conventional probabilistic derivation, that there are no additional requirements needed, like special conditions for entropy, probability distributions, transition amplitude between two occupied states etc. [5]

Likewise, the construction of the wave equation for propagation of a localized perturbation results from the same key dynamical equation directly, without introducing the potential between two degrees of freedom with special properties (linear approximation).

The model formulated above does not admit a direct physical interpretation, since the general causality condition is not satisfied. This that indicates,that the resulted system of dynamical equations describes a dynamics of two components for opposite directions evolutions ('time directions'), which could be gathered together e.g. as a complex component.

The causality and splitting problem should be considered together in a context of the construction for a coordinate space. This discussion is postponed for the forthcoming investigation.

3 Appendix

3.1 Partial derivatives of entropy

Using the continuation of

$$\frac{d}{dn}n! = \lim_{n\to\infty}\frac{(n+1)! - n!}{1} = n!n$$

we can generalize it for Gamma-function as

$$\frac{d}{dn}\Gamma(n) = n\Gamma(n),$$

and

$$\frac{d}{dn}\ln n! = n, \quad \frac{d}{dn}\ln\Gamma(n) = n$$

respectively.

Then we obtain for $S(n_i)$:

$$\frac{\partial}{\partial n_i}S[n(i)] = \frac{\partial}{\partial n_i}\left\{\ln\ \Gamma\left[\sum_{i=-N}^{N} n(i)\right] - \sum_{i=-N}^{N}\ln\ \Gamma[n(i)]\right\} = \sum_{k=-N}^{N} n(k) - n(i) \tag{18}$$

and

$$S[n(i)]_{n_i n_i} = \frac{\partial^2}{\partial n_i \partial n_i}\sum_{k=-N}^{N} n(k) - n(i) = 0; \tag{19}$$

$$S[n(i)]_{n_i n_l} = \frac{\partial^2}{\partial n_i \partial n_l}\sum_{k=-N}^{N} n(k) - n(i) = 1,\ i \neq l; \tag{20}$$

3.2 Derivation of dynamical equation

Adding dn_i to the both sides of

$$\sum_{k=-N}^{N} n(k) - n(i) + \sum_{k\neq i} dn_k + \lambda = 0$$

(in order to use the ergodicity condition $\sum_k dn_k = 0$), and summing subsequently

$$dn_i = \sum_{k=-N}^{N} n(k) - n(i) + \lambda$$

once again over i

$$\sum_{i=-N}^{N} dn_i = (2N+1)\sum_{k=-N}^{N} n(k) - \sum_{i=-N}^{N} n(i) + (2N+1)\lambda = 0$$

we eliminate the λ by

$$\lambda = -\frac{2N}{2N+1}\sum_{k=-N}^{N} n(k)$$

and obtain finally:

$$dn_i = \sum_{k=-N}^{N} n(k) - n(i) - \frac{2N}{2N+1}\sum_{k=-N}^{N} n(k) = \frac{1}{2N+1}\sum_{k=-N}^{N} n(k) - n_i$$

3.3 Second time derivative

$$\ddot{n}_i := \frac{d}{d\tau}\frac{dn}{d\tau} = \frac{d}{d\tau}\left[-\frac{S_{\tau\tau}}{S_\tau}\left(\frac{1}{N}\sum_{k=1}^{N} n_k - n_i\right)\right]$$

$$= -\frac{d}{d\tau}\frac{S_{\tau\tau}}{S_\tau}\left(\frac{1}{N}\sum_{k=1}^{N} n_k - n_i\right) - \frac{S_\tau}{S_{\tau\tau}}\left(\frac{1}{N}\sum_{k=1}^{N}\frac{d}{d\tau}n_k - \frac{d}{d\tau}n_i\right)$$

(substituting again the original first-order relation)

$$= -\frac{S_{\tau\tau\tau}S_\tau - S_{\tau\tau}^2}{S_\tau^2}\left(\frac{1}{N}\sum_{k=1}^{N} n_k - n_i\right) -$$

$$-\frac{S_\tau}{S_{\tau\tau}}\left[\frac{1}{N}\sum_{k=1}^{N} -\frac{S_{\tau\tau}}{S_\tau}\left(\frac{1}{N}\sum_{l=1}^{N} n_l - n_k\right) - \frac{-S_{\tau\tau}}{S_\tau}\left(\frac{1}{N}\sum_{k=1}^{N} n_k - n_i\right)\right] =$$

$$= \left[-\frac{S_{\tau\tau\tau}}{S_\tau} + \frac{S_{\tau\tau}^2}{S_{\tau^2}}\right](\overline{n} - n_i) + \left(\frac{S_\tau}{S_{\tau\tau}}\right)^2\left(\frac{1}{N^2}\sum_{k=1}^{N}\sum_{l=1}^{N} n_l - \frac{1}{N}\sum_{k=1}^{N} n_k - \frac{1}{N}\sum_{l=1}^{N} n_l + n_i\right)$$

$$= \left[-\frac{S_{\tau\tau\tau}}{S_\tau} + \frac{S_{\tau\tau}^2}{S_{\tau^2}} \right] (\overline{n} - n_i) + \left(\frac{S_\tau}{S_{\tau\tau}} \right)^2 (\overline{n} - 2\overline{n} + n_i)$$

$$= -\frac{S_{\tau\tau\tau}}{S_\tau} (\overline{n} - n_i)$$

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