Inferring the density matrix for a system of an unknown Hamiltonian

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An approximate inference approach is advanced in order to determine the density matrix in cases in which the pertinent Hamiltonian is unknown, and the available expectation values pertain to noncommuting observables. The inference of both pure and mixed states is addressed, and on an equal footing, without facing infinities in the pure state limit. Information-theoretical tools are employed. [S1050-2947(98)02604-3]

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I. INTRODUCTION

In order to attempt a quantum description of a system so as to obtain the concomitant wave function or density matrix, knowledge of the pertinent Hamiltonian is an all important requirement, as otherwise Schrödinger's equation (or Von Neumann's) cannot be written down. However, cases in which the Hamiltonian is unknown abound, and indeed much effort, from both theoretical and experimental viewpoints, has been expended in trying to determine, at the very least, appropriate *effective* Hamiltonians in order to remedy such informational failure.

Since in statistical mechanics (SM) *inference* is the overall purpose, because incomplete information is always presupposed, SM methods would seem to be called for in the case of an unknown Hamiltonian. Indeed, the main idea underlying statistical mechanics is that of describing the most salient characteristics of a given system by recourse to a small set of relevant expectation values (just $\langle H\rangle$ in the case of Gibb's canonical distribution) [1]. But once again, one is assumed to know the system's Hamiltonian in order to proceed to build up canonical, grand-canonical, or other types of ensembles. What is to be done if such energetic information is not available?

Several types of hardship are to be faced in numerically dealing with quantal problems by recourse to methods of statistical mechanics. Among them we can list the following: for pure states, the thermodynamical entropy is identically zero; the Hamiltonian may not be known; pure states and mixed states are often dealt with on an *unequal* footing, due to technical difficulties; some Lagrange multipliers may diverge; and the Kubo transform must be implemented in dealing with non-commuting observables [2], which is sometimes a rather difficult task.

Recourse to information theory (IT) [3], as employed by Jaynes [4] in his celebrated reformulation of SM (see also Refs. [4–8]), allows one to conveniently tackle the first two of the above problems, but subject to the following restrictions: (i) the pertinent methodology can be applied only in the case of *pure states*, and (ii) the *a priori* input information must refer only to commuting observables. For details, the reader is referred to Refs. [9–19]. The purpose of the present effort is that of addressing the last three of the hardships listed above, overcoming also the aforementioned limitations.

Concerning the fourth of the above-listed difficulties, if the associated scenario makes it possible to infer a statistical operator for *mixed* states *à la* Jaynes, as one approaches the pure state limit the associated Lagrange multipliers diverge, to either plus or minus infinity [20], which seems to erect a formidable barrier to the workings of numerical techniques. As for the last item in the lists of problems to be overcome, we mention that, if the available information refers to expectation values of *noncommuting* observables, recourse to the Kubo transform (KT) [2] becomes mandatory. Its beauty and elegance notwithstanding, the KT confronts one, in general, with involved integrals that are not always easy to deal with.

In what follows we show how to apply Jaynes' methodology in quantum-mechanical scenarios for which, the Hamiltonian not being available, just a small set of expectation values of *noncommuting operators* constitutes the only prior information. Both pure and mixed states will be tackled on an equal footing, without infinities in the Lagrange multipliers, and no recourse to the KT needs to be made.

One would envision utilizing this formalism in situations in which scarce information is available concerning the details of the interactions governing the physics of the system to be described. Inference would then be the name of the game. A number of such scenarios found, for example, in Refs. [21–47], is by no means an exhaustive list. The formalism is introduced in Sec. II, some illustrations are discussed in Sec. III, and conclusions are drawn in Sec. IV.

II. PRESENT FORMALISM

We assume that M expectation values are at our disposal,

$$\langle A_r\rangle = d_r, \quad r=1,\ldots,M, \tag{1}$$

and *we do not assume that* $\hat{A}_r$ *are commuting operators*.

In the (arbitrary) basis $|i\rangle$ the statistical operator is of the customary form

$$\hat{\rho} = \sum_{i,j}^{N} |i\rangle f_{ij}\langle j|, \tag{2}$$

and our input-information can be cast in the fashion

$$d_r = \langle \hat{A}_r \rangle = \mathrm{Tr}(\hat{\rho}\hat{A}); \tag{3}$$

with $|i\rangle$ an *arbitrary* basis, we can choose it (in principle, at least) as we please. Of course, practical considerations may make a given basis more attractive than others. Notice that, although N may be infinite, once more reasons of practicality will force us always to consider finite N values in actual numerical computations. N is, of course, chosen according to some appropriate criteria. It is clear, however, that, in general, we shall deal with scenarios in which N is larger (often considerably so) than M.

In order to make further progress, a change of notation will be necessary: we form, first of all, a vector $\vec{d}$ out of the M components d_r of Eq. (3). Next we rearrange (say, in lexicographic order) the subindices i and j of the matrix elements of the statistical operator $\hat{\rho}$ so as to obtain a vector $\vec{f}$ of N^2 components. Finally, using this rearrangement we will regard the matrix element $\langle i|\hat{A}_r|j\rangle$ as the element G_{rl} of a rectangular $(M \times N^2)$ matrix $\mathbf{G}$, where the row index r runs from one to M, while the columns are labeled by an index l $(1, \ldots, N^2)$ that combines in some fashion (lexicographic, for instance) the Hilbert space basis' indices i and j. In this matrix notation Eq. (3) adopt the appearance

$$\vec{d} = \mathbf{G}\vec{f}, \tag{4}$$

which clearly poses an underdetermined linear problem, as, usually, $M < N$. Very many, possibly infinite, distinct vectors $\vec{f}$ fulfill it.

Following Gibbs [48] we focus our attention not on Eq. (4) itself but on an *ensemble* of identical equations. More precisely, we consider an ensemble consisting of all its possible solutions. In the ensemble, every solution $\vec{f}_\alpha$ of Eq. (4) appears with a suitably normalized probability $P(\alpha)$

$$\int_{\mathcal{R}} P(\alpha)\, d\tau = 1, \tag{5}$$

where $\mathcal{R}$ is the space of ''realizations'' of the solutions $\vec{f}_\alpha$. If the coefficients f_{ij} in Eq. (2) are real, we write down the volume element $d\tau$ in the fashion

$$d\tau = df_1 df_2 \cdots df_{N^2}, \tag{6}$$

while, in the more general case, a slightly more complicated expression ensues, that is not needed for our present purposes.

Since it is *we* that ''build'' the ensemble, we take the liberty of designing it so that the vector $\vec{f}$, of mean ensemble value

$$\langle \vec{f} \rangle = \int d\tau P(\alpha) \vec{f}_\alpha, \tag{7}$$

is of such nature that (i) $\langle \vec{f} \rangle$ also fulfills Eq. (4), that can thus be written down in the guise

$$\vec{d} = \mathbf{G}\langle \vec{f} \rangle; \tag{8}$$

(ii) the expectation value of the norm $\mathcal{N}(\vec{f}) = \vec{f}^{\,\mathrm{tr}}\vec{f}$ is finite, i.e.,

$$\left\langle \sum_{i=1}^{N^2} f_i^2 \right\rangle = \mathcal{Z} = \text{finite real number}; \tag{9}$$

and (iii) $P(\alpha)$ maximizes the Shannon information measure

$$S = -\int d\tau\, P(\alpha) \ln P(\alpha), \tag{10}$$

which, of course, has nothing to do with thermodynamical entropy. The latter is of form (10), but involves the density operator. It describes quantum plus classical ignorance (the so-called double weighting [48]). With $P(\alpha)$ we go a step further, as Eq. (10) describes our ignorance about which is the suitable density matrix within an ensemble of such matrices. Here enters Jaynes' maximum entropy principle (MEP) [4], but applied, in this roundabout manner, to an appropriate Gibbs ensemble of different solutions of Eq. (4).

We do not claim that the requirements (i)–(iii) above are the only ones that can be made, neither that they are somehow superior in some sense to an alternative set of constraints that could be imposed. Remember that one has, in Gibbs' case, the canonical ensemble, the grand-canonical one, etc. We select (i)–(iii) merely on the basis that they are quite sensible requirements.

Obviously, we face a constrained extremization problem, which leads to the Lagrangian

$$\mathcal{L} = P(\alpha)\left[\ln P(\alpha) + (\lambda_0 - 1) + \gamma \sum_{i=1}^{N^2} f_i^2 + \sum_{\alpha=1}^{M} \lambda_\alpha \sum_{i=1}^{N^2} G_{\alpha i} f_i \right], \tag{11}$$

so that variations $\delta\mathcal{L}$ with respect to $P(\alpha)$ vanish;

$$\delta_{P(\alpha)} \int \mathcal{L}\, d\tau = 0. \tag{12}$$

A word of explanation is needed concerning condition (9). This should usually be construed as an inequality (and thus not amenable to the Lagrange multiplier treatment). However, the point is that we can *interpret* it as an equality, because we are not concerned with the exact value of the sum on the left-hand side ($\mathcal{Z}$). Any value would do, because, at the end, we will discover that our solution *does not depend upon the associated Lagrange multiplier γ, and thus neither upon any putative value of $\mathcal{Z}$.* We are allowed then to treat Eq. (9) as if it were an equality (any $\mathcal{Z}$ value goes).

Before discussing the solution to the MEP problem (12), we notice that the last term on the right-hand side of Eq. (11) can be recast as

$$\sum_{i=1}^{N^2} f_i \sum_{\alpha=1}^{M} G_{i\alpha}^{\mathrm{tr}} \lambda_\alpha = \sum_{i=1}^{N^2} f_i \Gamma_i = \vec{f}^{\,\mathrm{tr}}\vec{\Gamma}, \tag{13}$$

invoking transposition of the matrix $\mathbf{G}$, so that

$$\vec{\Gamma} = \mathbf{G}^{\mathrm{tr}}\vec{\lambda}. \tag{14}$$

The present MEP variational problem has an analytical solution

$$P(\alpha)=\exp(-\lambda_0)\exp[-\gamma(\vec{f})^2-\vec{\Gamma}\vec{f}], \tag{15}$$

where the partition function $Z=e^{\lambda_0}$ is given, on account of normalization, by

$$Z=\prod_{i=1}^{N^2}\left[\int df_i\exp(-\gamma f_i^2-\Gamma_i f_i)\right]. \tag{16}$$

The Gaussian integrals in Eq. (16) can be immediately performed so as to yield

$$Z=\prod_{i=1}^{N^2}[\sqrt{\pi/\gamma}\exp(\Gamma_i^2/4\gamma)], \tag{17}$$

so that Eq. (7) is translated into

$$\langle\vec{f}\rangle=-\vec{\Gamma}/2\gamma. \tag{18}$$

According to usual practice we are now in a position to claim that the components of $\langle\vec{f}\rangle$,

$$\langle f_i\rangle=-\Gamma_i/2\gamma, \tag{19}$$

are the best possible choice for the solutions of our problem. Out of the many possible solutions of Eq. (4), (19) is the ''best,'' in Gibbsian terms, in the same sense that the canonical statistical operator $\exp(\lambda_0-\beta\hat{H})$ is the best statistical operator one can infer when the *a priori* knowledge is just that of the expectation value of the Hamiltonian. But, of course, we are not through yet, as, thus far, $\vec{\Gamma}$ and γ are unknown quantities.

In order to make further progress let us focus our attention upon Eqs. (8), (14), and (18). By *formal* manipulation of Eq. (14), we find

$$\vec{\lambda}=(\mathbf{G}^{\mathrm{tr}})^{-1}\vec{\Gamma}, \tag{20}$$

while, from Eq. (18), we have

$$\vec{\Gamma}=-2\gamma\langle\vec{f}\rangle, \tag{21}$$

that, inserted into Eq. (20), gives

$$\vec{\lambda}=-2\gamma(\mathbf{G}^{\mathrm{tr}})^{-1}\langle\vec{f}\rangle, \tag{22}$$

that, on account of Eq. (8), yields

$$\vec{\lambda}=-2\gamma(\mathbf{G}^{\mathrm{tr}})^{-1}\mathbf{G}^{-1}\vec{d}, \tag{23}$$

which, reinserted into Eq. (22), leads finally to

$$\langle\vec{f}\rangle=\mathbf{G}^{\mathrm{tr}}(\mathbf{G}\mathbf{G}^{\mathrm{tr}})^{-1}\vec{d}, \tag{24}$$

which neatly expresses our inferred statistical operator *à la* Gibbs in terms of the input data $\vec{d}$ and the known matrix $\mathbf{G}$ (no dependence upon γ, as stated before).

The matrix

$$\mathbf{P}_G=\mathbf{G}^{\mathrm{tr}}(\mathbf{G}\mathbf{G}^{\mathrm{tr}})^{-1}, \tag{25}$$

is, of course, the celebrated Moore-Penrose pseudoinverse [49] of the matrix $\mathbf{G}$. The present treatment is seen to lead one to a most convenient tool of the numerical analysis weaponry.

In writing down Eq. (24) we accomplish our goal: the density matrix has been determined via a MEP approach. No Lagrange multipliers enter this equation. Everything is expressed in terms of the data input and of the matrix elements of the operators whose expectation values constitute our *a priori* information. Thus, everything should remain finite, even for pure states.

Notice that we actually *use* only the ensemble mean (19), not the whole distribution $P(\alpha)$. This should not be construed as an indication that our ensemble of density matrices is not necessary. Building it up is the price to pay for getting rid of the troublesome (within the present context) *original* Lagrange multipliers of Jaynes' treatment, and replacing them with our own multipliers. Thus, the essential difference between the present approach and the orthodox Jaynes' one, as employed in Refs. [9–19], lies in the fact that our Lagrange multipliers refer to the workings of our fictitious ensemble, i.e., to the collective of acceptable density matrices, and are thus not endowed with any obvious physical relevance. On the other hand, we have indeed overcome all the difficulties mentioned in Sec. I.

III. SIMPLE ILLUSTRATIONS

We shall illustrate the procedure advanced in Sec. II with reference to some simple examples. We consider only real density matrices.

A. Calculation in the oscillator basis

We assume now that we are expanding wave functions in a one-dimensional harmonic-oscillator basis. We choose $N=4$, so that we deal with 4×4 input matrices this time. Our *a priori* information is taken to be that of the expectation values of $\hat{x}^2$, $\hat{p}^2$, and $\hat{p}^4$, and, out of these three values, we intend to infer the ten independent elements of a 4×4 density matrix. We take it that the ''exact'' (in general, mixed) state is a linear admixture of two pure states, that in the oscillator-basis $|\textit{phonon number } n\rangle$, read

$$|A\rangle=\sqrt{(}0.3|n=0\rangle+\sqrt{(}0.2|n=2\rangle+\sqrt{(}0.2|n=4\rangle+\sqrt{(}0.3|n=6\rangle \tag{26}$$

and

$$|B\rangle=\sqrt{(}0.15|n=0\rangle+\sqrt{(}0.2|n=2\rangle+\sqrt{(}0.15|n=4\rangle+\sqrt{(}0.5|n=6, \tag{27}$$

respectively.

After determining our density matrix according to the considerations expounded in Sec. II, we perform the corresponding quality test with reference to its predictive power. To this end, we infer the expectation values of $\hat{x}^4$, $\hat{x}^6$, $\hat{x}^8$, and $\hat{p}^6$, and compare them to the ''exact'' ones for various values of the admixture proportion τ,

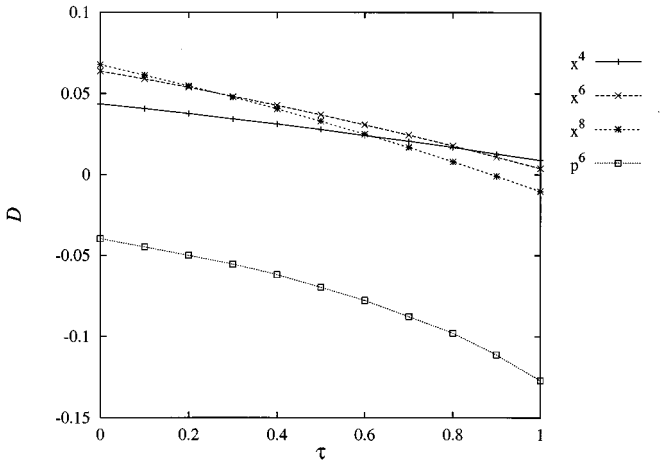

FIG. 1. Relative difference between exact and inferred expectation values vs the mixture parameter τ for a continuous one-dimensional problem.

$$\hat{\rho}_{\text{exact}}=(1-\tau)|A\rangle\langle A|+\tau|B\rangle\langle B|. \tag{28}$$

Figure 1, where τ labels the horizontal axis and the relative difference

$$D=\frac{\langle\hat{O}_{\text{test}}\rangle_{\text{exact}}-\langle\hat{O}_{\text{test}}\rangle_{\text{inferred}}}{\langle\hat{O}_{\text{test}}\rangle_{\text{exact}}}, \tag{29}$$

is represented in the vertical one, displays the corresponding results. It is seen that our predictive errors are smaller than 13%.

B. A discrete system

We assume that we confront a spin-2 system, and deal with 5×5 input matrices. Our *a priori* information is taken to be that of the expectation values of $\hat{J}_z$, $\hat{J}_y^4$, $\hat{J}_x^3$, and $\hat{J}_z^2\hat{J}_y^2+\hat{J}_y^2\hat{J}_z^2$, and, out of these four values, we intend to infer the 16 independent elements of a 5×5 density matrix. We take it that the ''exact'' (in general, mixed) state is a linear admixture of two pure states, that, in the J_z basis $|m\rangle$,

$$\hat{J}_z|m\rangle=m|m\rangle, \tag{30}$$

read

$$|A\rangle=\sqrt{(}0.25|2\rangle+\sqrt{(}0.20|1\rangle+\sqrt{(}0.25|0\rangle+\sqrt{(}0.15|-1\rangle+\sqrt{(}0.15|-2\rangle \tag{31}$$

and

$$|B\rangle=\sqrt{(}0.35|2\rangle+\sqrt{(}0.30|1\rangle+\sqrt{(}0.10|0\rangle+\sqrt{(}0.15|-1\rangle+\sqrt{(}0.10|-2\rangle, \tag{32}$$

respectively.

After determining our density matrix according to the considerations expounded in Sec. II, we perform the corresponding quality test with reference to its predictive power. To this end, we infer the expectation values of $\hat{J}_x$, $\hat{J}_x^2$, $\hat{J}_z^2$, $\hat{J}_z^3$, $\hat{J}_z^4$, and $\hat{J}_x^4$, and compare them to the ''exact'' ones for various values of the admixture proportion τ [see Eq. (28)].

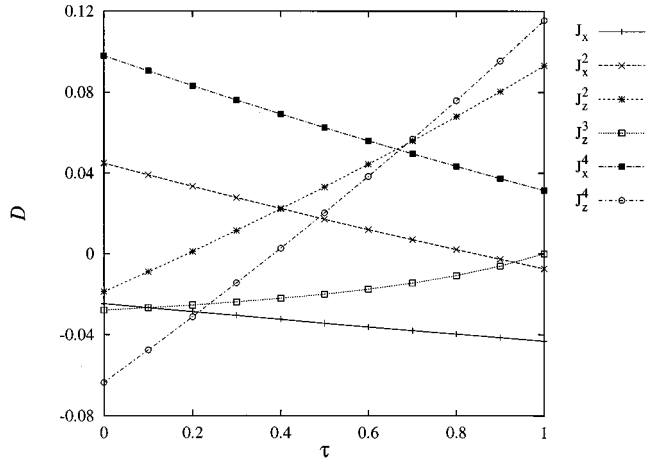

FIG. 2. Same as Fig. 1 for a spin-2 problem.

Figure 2, where τ labels the horizontal axis, and the relative difference [see Eq. (29)] is represented in the vertical one, displays the corresponding results. It is seen that our predictive errors are smaller than 10%.

In Fig. 3 we display the thermodynamical entropy

$$S_T=-\text{tr}[\rho\ln(\rho)] \tag{33}$$

as a function of the admixture coefficient τ. S_T should not be confused with the information measure (10). They are quite different entities. The solid line plots the ''exact'' entropy, while the dashed one corresponds to our inferred, approximate one. Obviously ours is larger, as our prior information is not abundant enough so as to be in a position to infer the exact solution in an errorless fashion. We clearly appreciate here the fact that the physical entropy is also an information measure, and thus is able to measure our ignorance, or lack of information. Indeed, the units on the vertical scale are bits (logarithms were evaluated in the basis 2). As expected, in the pure state limit the entropy vanishes. For mixed states ($0<\tau<1$), the entropy acquires finite values, and reflects

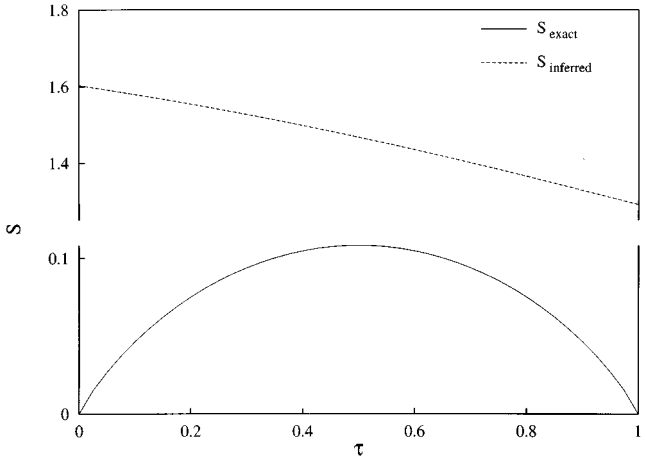

FIG. 3. Thermodynamical entropy for the problem of Fig. 2. Exact and inferred entropies are plotted against τ.

the lack of information associated with the fact that τ in our mixed state is not an amplitude, but a weight.

IV. CONCLUSIONS

Using rather well-known mathematical ideas [49], we have advanced a way of introducing complementary information into the Jaynes' maximum entropy machinery, so as to enable one to apply his philosophy to the inference of approximate density matrices *in cases in which the Hamiltonian of the system is unknown*. Both mixed and pure states are treated on equal footing, and no divergence of the pertinent Lagrange multipliers ensues in the pure state limit. Our approach was illustrated with reference to simple examples that illuminate the workings of our approach. It is shown that ours is a reasonably powerful inference technique.

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