Relevant spaces in quantum dynamics and statistical physics

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A systematic method for the decoupling of a relevant subspace of the Hilbert space from the rest of it is developed, on the basis of the dynamical properties of the observables one is interested in.

I. INTRODUCTION

Recent developments concerning applications of information theory (IT) to physical problems[1–7] deal with the time evolution of the Lagrange parameters entering the definition of the density operator $\rho(t)$.[8] The basic feature of this approach is that a set of coupled equations of motion for these multipliers is obtained, which is equivalent to the time-dependent Schrödinger equation, provided that one includes in ρ all those operators O_m that close an algebra under commutation with the Hamiltonian H of the system.[6–8]

In this work we wish to place this closure (of a partial Lie algebra[6–8]) within a much more general context, by relating it to some characteristic aspects of the many-body problem. In this way, the corresponding closure relations arise in a natural fashion, without any *a priori* reference to information theory.

Let us consider then the following situation. Given H and its corresponding Hilbert space Ξ, any basis spanning Ξ, even if it is finite, is so large that a diagonalization is out of the question. Physical intuition, which takes into account the most salient aspects of the problem at hand, is often the only guide at our disposal in order to truncate Ξ so as to render the concomitant problem a manageable one.

We wish here to propose a systematic way of decoupling some relevant portion of Ξ from the rest of it, where the term "relevant" will be understood as follows. Assume our knowledge of the corresponding system stems from the experimental determination (say, at the time $t=t_0$) of the expectation values of M (linearly independent) operators G_i,

$$\langle G_i \rangle = g_i \quad i=1,\ldots,M \;. \tag{1.1}$$

We call *relevant* the set of operators G_i, $i=1,\ldots,M,\ldots$ such that knowing $\langle G_i \rangle_{t_0}$ enables one to build up a density operator ρ that is a solution of the Liouville equation

$$\frac{d}{dt}=[H,\rho]=\hat{L}\rho \tag{1.2}$$

with

$$\hat{L}=[H,\;],$$

for all $t>t_0$. Another (and related) way of defining *our* version of the term relevance would run as follows: if $\langle G_i \rangle$, $i=1,\ldots,M$, are the observables we are interested in, we would like to find that subspace Ξ_R of Ξ that wholly encompasses the time evolution of these quantities.

II. FORMALISM

A. The vector space of the operators on Ξ

We shall focus our attention upon the vector space Γ spanned by the set of (linearly independent) operators G_i that are (at least in principle) accessible to measurement in connection with the physical system one is interested in. For the sake of definiteness let us call μ the number (in general infinite) of such operators. The density matrix is an operator belonging to Γ, although one usually expresses it in terms of vectors belonging to the Hilbert space Ξ, where it adopts the familiar appearance

$$\rho=\sum_{l,m} |\,l\,\rangle \rho_{ml} \langle\, m\,| \;, \tag{2.1}$$

in terms of a given basis $|\,l\,\rangle$ of Ξ. The scalars ρ_{lm} are members of the field of the complex numbers. Notice that, within the framework of Schrödinger's representation (the one to be employed throughout), ρ depends upon the time because the vectors $|\,l\,\rangle$ possess such a dependence. Now, the Liouville operator $\hat{L}$ *is a linear operator on* Γ, as for any two scalars a,b and two arbitrary vectors G_1,G_2

$$\hat{L}(aG_1+bG_2)=a\hat{L}G_1+b\hat{L}G_2 \,, \tag{2.2}$$

and we may consider that the physics of the system is to be derived from the action of $\hat{L}$ upon the vectors belonging to Γ. Our aim is to decompose it into a direct sum

$$\Gamma=\Gamma_R+\Gamma_{NR}, \tag{2.3}$$

$$0=\Gamma_R\cap\Gamma_{NR}\,, \tag{2.4}$$

in which Γ_R is the (physically) relevant portion of Γ and Γ_{NR} the "nonrelevant" one. Assuming that N is the dimension of Γ_R we have

$$\mu = N + \dim(\Gamma_{NR}), \tag{2.5}$$

and we may say that Γ_R and Γ_{NR} *reduce* Γ.[9]

Among the set of linear operators on Γ (which from now on, and in order to avoid misunderstandings) we shall call superoperators, we will look for a projection superoperator $\hat{P}$ such that, for all $T \in \Gamma$ [that can uniquely be written as $T_R + T_{NR}$, with $T_R \in \Gamma_R$ and $T_{NR} \in \Gamma_{NR}$ (Ref. 9)]

$$T = T_R + T_{NR}, \quad T_R \in \Gamma_R, \quad T_{NR} \in \Gamma_{NR}, \tag{2.6}$$

$$\hat{P} T = T_R, \tag{2.7}$$

$$\hat{P} T_{NR} = 0, \tag{2.8}$$

$$\hat{P}^2 = \hat{P}, \tag{2.9}$$

so that finding the structure of $\hat{P}$ neatly solves the problem posed in Sec. I, as we can confidently assert now that there exists a unique decomposition

$$\rho = \rho_R + \rho_{NR}, \tag{2.10}$$

$$\hat{P}\rho = \rho_R, \tag{2.11}$$

$$(\hat{1} - \hat{P})\rho = \rho_{NR}, \tag{2.12}$$

where $\hat{1}$ is the identity superoperator.

Enter now the dynamics of the problem, embedded in Eq. (1.2), which we recast as

$$i\hbar \frac{d}{dt}(\rho_R + \rho_{NR}) = \hat{L}(\rho_R + \rho_{NR}) \,. \tag{2.13}$$

Our goal must be that of decoupling the time evolution of ρ_R from that of ρ_{NR}. To this end let us operate twice on (2.13), by applying in one case, $\hat{P}$ on the left, and in the other case, $\hat{1} - \hat{P}$ in a similar fashion. We obtain

$$i\hbar \frac{d\rho_R}{dt} = \hat{P}\hat{L}\rho_R + \hat{P}\hat{L}\rho_{NR} \tag{2.14}$$

and

$$i\hbar \frac{d\rho_{NR}}{dt} = (\hat{1} - \hat{P})\hat{L}\rho_R + (\hat{1} - \hat{P})\hat{L}\hat{\rho}_{NR} \tag{2.15}$$

a set of *coupled* equations, which is immediately seen to transform itself into a set of *decoupled* equations if

$$\hat{P}\hat{L} = \hat{L}\hat{P} \tag{2.16}$$

[cf. Eqs. (2.11) and (2.12)]. In other words, if we find a superoperator P that complies with (2.7)—(2.9) and with (2.16), we can recast the dynamical problem in the fashion

$$i\hbar \frac{d\rho_R}{dt} = \hat{L}\rho_R, \tag{2.17}$$

$$i\hbar \frac{d\rho_{NR}}{dt} = \hat{L}\rho_{NR}, \tag{2.18}$$

and forget henceforth about (2.18), concentrating all efforts upon (2.17).

B. The structure of the projection operator

In order to make further progress we must provide Γ with a richer structure by considering it as an inner-product vector space.[10] The inner product of any two vectors Q,T (a_1 and a_2 are scalars) is a scalar (Q,T) such that

$$\begin{aligned} &(Q,T) = (T,Q)^*, \\ &(a_1 Q_1 + a_2 Q_2, T) = a_1^*(Q_1,T) + a_2^*(Q_2,T), \\ &(T,(a_1 Q_1 + a_2 Q_2)) = a_1(T,Q_1) + a_2(T,Q_2), \\ &(Q,Q) \geq 0, \end{aligned} \tag{2.19}$$

where

$$(Q,Q) = 0 \tag{2.20}$$

if and only if $Q = 0$.

Let $\{A_i\}$ be a complete orthonormal basis of Γ,[9] which obeys

$$(A_i, A_j) = \delta_{i,j}, \quad j \leq N \tag{2.21a}$$

$$(A_i, A_j) = 0, \quad j > N \tag{2.21b}$$

such that the subset $\{A_i,\ i \leq N\}$ spans Γ_R. Consequently, a general expression for any $Q_m \in \Gamma$ is of the form (remember, μ is the dimension of Γ)

$$Q_m = \sum_i^{\mu} w_{im} A_i \tag{2.22}$$

with

$$w_{im} = (A_i, Q_m) \,. \tag{2.23}$$

We propose the following expression for $\hat{P}$,

$$\hat{P} = \sum_j^N A_j(A_j, \ ), \tag{2.24}$$

so that, if $Q_m \in \Gamma$,

$$\begin{aligned} PQ_m &= \sum_j^N A_j(A_j, Q_m) \\ &= \sum_j^N w_{jm} A_j = Q_{m,R} \in \Gamma_R \end{aligned} \tag{2.25}$$

and proceed to demonstrate both that $\hat{P}$ is an idempotent superoperator and that (under certain conditions) it commutes with the Liouville superoperator $\hat{L}$.

(i) Idempotency. We have

$$\begin{aligned} \hat{P}^2 Q_m &= \hat{P} \sum_i^N w_{im} A_i \\ &= \sum_k^N \sum_i^N A_k(A_k, w_{im} A_i) \\ &= \sum_i^N w_{im} A_i = Q_{m,R} \end{aligned} \tag{2.26}$$

which is the result of Eq. (2.25).

(ii) Commutativity (with $\hat{L}$). We start with

$$\hat{P}\hat{L}Q_m = \sum_j^N A_j(A_j,[H,Q_m]) \tag{2.27}$$

and expand Q_m according to (2.22), which leads to

$$\hat{P}\hat{L}Q_m = \sum_j^N f_{jm} A_j , \tag{2.28}$$

where f_{jm} stands for the scalar product. Using Eq. (2.21b)

$$f_{jm} = \left[A_j, \left[H, \sum_i^{\mu} w_{im} A_i \right] \right] . \tag{2.29}$$

On the other hand,

$$\hat{L}\hat{P}Q_m = \sum_i^N [H, A_i(A_i,Q_m)]$$
$$= \sum_i^N w_{im}[H,A_i] . \tag{2.30}$$

The right-hand sides of Eqs. (2.28) and (2.30) are easily seen to coincide if the following set of conditions is fulfilled:

$$[H,A_i] = \sum_l^N c_{li} A_l, \quad i=1,\ldots,N . \tag{2.31}$$

Under these conditions the f_{jm} become

$$f_{jm} = \sum_i^N c_{ji} w_{im} , \tag{2.32}$$

so that

$$\hat{L}\hat{P}Q_m = \sum_j^N \sum_i^N c_{ji} w_{im} A_j , \tag{2.33}$$

which guarantees that, for any Q_m

$$\hat{L}\hat{P}Q_m = \hat{P}\hat{L}Q_m . \tag{2.34}$$

An important point to be stressed here is the following one: our projection operator $\hat{P}$ commutes with $\hat{L}$ and hence with the Hamiltonian. As $\hat{P}$ does not explicitly depend upon the time, $\hat{P}$ is thus seen to be a constant of the motion, and its expectation value is a constant. The projected relevant space Γ_R is, consequently, invariant and remains the same as time evolves.

III. APPLICATION TO INFORMATION THEORY

A. Generalities

In this section we shall apply the results of the preceding paragraphs to the density operator defined within the information theory framework.[1–8,10] This formalism yields a definite prescription that allows one to construct the density operator (or matrix) starting from the knowledge of the measured expectation values of, say, M operators

$$\langle Q_m \rangle = q_m = \langle Q_m / \rho \rangle, \quad 0 \le m \le M \tag{3.1}$$

with $M \le N$ ($Q_0 = 1$, identity). Maximization of the entropy[1–8,10] leads to an expression for $\ln\rho$

$$-\ln\rho = \sum_m \lambda_m Q_m \tag{3.2}$$

in terms of a set of $M+1$ Lagrange multipliers λ_m which are determined so as to fulfill the set of relations (3.1).

The statistical operator is, then, given by

$$\rho(t) = \exp\left[-\sum_m \lambda_m Q_m \right] . \tag{3.3}$$

Let us introduce into this formalism our equation (2.31) which decouples the general ρ into two portions, the relevant and the nonrelevant ones. Equation (2.31) was first employed by Levine *et al.*[8] with reference to this particular and specific context. Then, using (2.22) and (2.31), we obtain

$$[H,Q_m] = \sum_{r=1}^N d_{mr} Q_r , \tag{3.4a}$$

where the d_{mr} and the c_{ij} are related by (using an underbar to denote a matrix)

$$\underline{d} = \underline{w}\,\underline{c}\,\underline{w}^{-1} . \tag{3.4b}$$

Using now the $\hat{P}$ superoperator we obtain

$$\hat{P}\rho = \rho_R = \sum_i^N A_i \left[A_i, \exp\left[-\sum_m \lambda_m Q_m \right] \right], \tag{3.5a}$$

$$\hat{P}\ \ln\rho = (\ln\rho)_R = -\sum_i^N A_i \left[A_i, \left[\sum_m^m \lambda_m Q_m \right] \right], \tag{3.5b}$$

and if we define the scalar product operation in Γ [see Eqs. (2.19)–(2.21)] in the following fashion, namely

$$(Q_m, Q_j) = \mathrm{Tr}(Q_m^\dagger Q_j), \tag{3.6}$$

Eq. (3.5) can be rewritten as

$$\rho_R(t) = \sum_{i=0}^N A_i \langle A_i / \rho \rangle_t , \tag{3.7a}$$

$$(\ln\rho)_R = \sum_{i=0}^N A_i \lambda_i(t) w_{im} , \tag{3.7b}$$

where in general A_i is not Hermitian and, consequently, $\langle A_i \rangle_t$ can be a complex scalar.

B. A simple example

In order to exemplify the above formalism let us apply it to the Larmor precession Hamiltonian,

$$H = \omega_L s_Z, \quad \omega_L = -eB/2mc \tag{3.8}$$

for an electron with charge e and mass m, bound in an s state in the presence of a magnetic field of strength B in the Z direction, whose Larmor precession frequency is denoted by ω_L. In this situation we deal with a set $\{Q\}$ of four operators

$$Q_0 = \mathbf{1}\ \text{(identity)}, \quad Q_1 = S_x, \quad Q_2 = S_y, \quad Q_3 = S_z, \tag{3.9}$$

where the S_i are the spin angular momentum operators. Our interest here revolves around the time evolution of their expectation values

$$\begin{aligned}\mathscr{S}_x(t)&=\mathrm{Tr}[\rho(t)S_x],\\ \mathscr{S}_y(t)&=\mathrm{Tr}[\rho(t)S_y],\\ \mathscr{S}_z(t)&=\mathrm{Tr}[\rho(t)S_z],\\ 1&=\mathrm{Tr}(\rho),\end{aligned} \tag{3.10}$$

and the statistical operator ρ is of the general form

$$\rho=\exp(-\lambda_0-\lambda_1 S_x-\lambda_2 S_y-\lambda_3 S_z)\ . \tag{3.11}$$

This $\{Q\}$ set can be expanded, as prescribed in Eq. (2.22), by the following $\{A\}$ set:

$$A_0=1/\sqrt{2},\quad A_1=S_-,\quad A_2=S_+,\quad A_3=2S_z \tag{3.12}$$

as

$$\begin{aligned}&Q_0=\sqrt{2}A_0,\quad Q_3=\tfrac{1}{2}A_3,\\ &Q_1=\tfrac{1}{2}(A_1+A_2),\quad Q_2=(i/2)(A_1-A_2)\ .\end{aligned} \tag{3.13}$$

Since

$$\mathrm{Tr}A_iA_j=\langle \tfrac{1}{2}\tfrac{1}{2}\,|\,A_iA_j\,|\,\tfrac{1}{2}\tfrac{1}{2}\rangle+\langle \tfrac{1}{2}\,-\tfrac{1}{2}\,|\,A_iA_j\,|\,\tfrac{1}{2}\,-\tfrac{1}{2}\rangle \tag{3.14}$$

we immediately verify (2.21), using

$$\begin{aligned}(S_+,S_+)&=\mathrm{Tr}S_+^\dagger S_+=\mathrm{Tr}S_-S_+\\ &=\mathrm{Tr}(S^2-S_z^2-S_z)=1\ ,\end{aligned} \tag{3.15a}$$

$$(S_-,S_+)=\mathrm{Tr}S_-^\dagger S_+=\mathrm{Tr}S_+^2=0\ , \tag{3.15b}$$

$$(S_z,S_z)=\mathrm{Tr}S_z^2=\tfrac{1}{4}\ , \tag{3.15c}$$

and so on. The action of the superoperator $\hat{P}$ upon, say, S_x, reads

$$\begin{aligned}\hat{P}S_x=\tfrac{1}{2}\mathrm{Tr}(S_x)&+S_+\mathrm{Tr}(S_-S_x)+S_-\mathrm{Tr}(S_+S_x)\\ &+4S_z\mathrm{Tr}(S_zS_x)\ ,\end{aligned} \tag{3.16}$$

while for ρ_R we find

$$\rho_R(t)=\tfrac{1}{2}+a_1(t)S_++a_2(t)S_-+a_3(t)S_z\ , \tag{3.17}$$

with

$$\begin{aligned}a_1(t)&=[\mathscr{S}_x(t)-i\mathscr{S}_y(t)],\\ a_2(t)&=[\mathscr{S}_x(t)+i\mathscr{S}_y(t)],\\ a_3(t)&=2\mathscr{S}_z(t)\ .\end{aligned} \tag{3.18}$$

The matrix $\underset{\sim}{d}$ [cf. Eq. (3.4b)]

$$\underset{\sim}{d}=\begin{bmatrix}0&0&0&0\\0&\omega_L&0&0\\-\omega_L&0&0&0\\0&0&0&0\end{bmatrix} \tag{3.19}$$

while

$$\underset{\sim}{w}=\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&2\end{bmatrix} \tag{3.20}$$

so that [cf. Eq. (3.4b)]

$$\underset{\sim}{c}=\underset{\sim}{d} \tag{3.21}$$

in this particular instance.

This ρ_R [cf. Eq. (3.17)] is easily seen to lead to the well-known Larmor results.[6] Thus the whole dynamical problem can be solved via the $\langle A_i\rangle_t$ expectation values, whose temporal evolution is completely determined by recourse to the information theory formalism.[6–8,10,11] Due to the relationship (2.22), the $\{\langle A_i\rangle\}$ set can be expressed as a linear combination of the (measured) $\{\langle Q_i\rangle\}$ which, of course, are *real* scalars. In particular, $\mathscr{S}_x$, $\mathscr{S}_y$ and $\mathscr{S}_z$ were evaluated, using information theory tools, in Ref. 6.

IV. CONCLUSIONS

Our goal has thus been achieved, and we have [cf. Eq. (2.24)] a superoperator $\hat{P}$ that decouples the relevant portion Γ_R of Γ from the rest. The set of conditions (2.31) that must be fulfilled in order that $\hat{P}$ commute with $\hat{L}$ provides us with some fresh insight into the physics underlying our procedure.

The subset $\{A_i\}$ of orthogonal dimension N employed in the definition of $\hat{P}$, closes a partial Lie algebra under commutation with the Hamiltonian. This is clearly a dynamical requirement that selects the relevant operators [cf. the paragraph following Eq. (1.1)] according to their behavior under commutation with H.

The procedure is then quite simple. Starting with the initial set (the "data" set) of Eq. (1.1), one must add to that set a certain number of (linearly independent) operators that arise as one commutes the original G_i with H, and this process is to be continued until an algebra is closed. We can then guarantee that the time evolution of the N primitive observables is totally decoupled from the rest of the universe.

We have thus justified the closure condition that is the basic ingredient of the work performed in Refs. 6–8 and 10, and that in particular guarantees the conservation of the entropy,[6–8,10,12] from a rather general and even more natural point of view, that is not *a priori* related to information theory.

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