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Quantum Mechanical State Preparation II—The Statistical Ensemble as a Thermostat

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Abstract

In this sequel to an earlier paper on quantal state preparation (Park & Band, 1972), the simple model used before is adapted and somewhat generalised to enable an exact treatment of the causal evolution of a system immersed in a statistical ensemble constituted of replicas of the system itself. The ensemble is initially in a state of statistical equilibrium, but the initial state of the system is arbitrary. It is established as a purely dynamical theorem that the system is eventually coerced into the same equilibrium state as that of the replicas in the ensemble. From this general result we obtain as a special case mechanical justification for the common assumption in statistical thermodynamics that an ensemble can function as a thermostat.

1. *The Dual Role of the Ensemble in Statistical Thermodynamics*

The statistical ensemble—an imaginary collection of replicas of an actual system of interest—has for decades played a basic role in most formulations of statistical physics, the only notable exceptions being kinetic theory and the modern information-theoretic version of statistics. Strictly speaking, the former in its pure form would not really be statistical at all since it would invoke no probabilistic assumptions; the latter, on the other hand, is deeply probabilistic, but the probabilities are interpreted subjectively so that the notion of ensemble becomes unnecessary (Jaynes, 1957; Hobson, 1971).

When the statistical ensemble is employed, its significance for the theory is always at least this: it permits an objective interpretation of the probability of an event as a quantity operationally defined as the relative frequency of occurrence of that event among the members of the ensemble. This type of ensemble is fundamental in every science that treats probability always as a measurable construct. It gives empirical meaning to abstract quantum theoretical derivations of collision cross-sections, and it is indispensable to the transformation

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into profit of the alluring design of a roulette wheel. In physics, such an ensemble–introduced in order to objectify probability–is properly termed Gibbsian, in recognition of its powerful entry into theoretical physics in Gibbs' now classic treatise (Gibbs, 1902; Tolman, 1938).

A Gibbsian ensemble is defined simply as a set of independent replicas of a system. Especially noteworthy is the qualifier 'independent': the elements of the set need not even exist simultaneously. Indeed the relative frequency definition of probability is normally considered to be valid only to the extent that the replicas do not interact. Thus an assembly of 10^{20} systems mutually interacting is not in general the statistical equivalent of an ensemble comprised of the same systems studied in isolation at the rate of one annually for 10^{20} years, but an assembly of 10^{20} non-interacting systems (like a perfect gas) may without contradiction be regarded also as a Gibbsian ensemble.

In statistical thermodynamics, the ensemble is often used in a manner which transcends these Gibbsian strictures by allowing, or rather demanding, that each system in the ensemble be in weak interaction with its replicas, the latter to be interpreted collectively as a heat reservoir, or thermostat. Such a construction, despite its transparently non-Gibbsian character, is nevertheless popularly termed a 'Gibbsian ensemble'. Now, at first it would appear that this is simply a misnomer for a rather strange model of a thermostat. However, in the ordinary practice of statistical thermodynamics, the 'ensemble' is in fact forced into an abashedly schizophrenic position; it functions as a thermostat, a role requiring mutual interactions and dynamical correlations imposed by conservation laws, and it is used to assign probabilities, via the relative frequency definition, to the states of its constituent systems, a role requiring mutual independence. We shall refer to the statistical ensemble interpreted in this dualistic fashion as *thermostatic* rather than Gibbsian.

The truly remarkable potency of the thermostatic ensemble as a predictive tool is abundantly illustrated in several treatises (Fowler & Guggenheim, 1939; Band, 1955) and this empirical success is often cited as an adequate foundation for the theory. But this view does not really alleviate the stigma of irrationality conveyed by the simultaneous necessity for distinct interpretations of the ensemble. Schrödinger clearly recognized the problem and offered the following concise justification of the thermostatic ensemble (Schrödinger, 1946):

> Here the N identical systems are mental copies of the one system under consideration–of the one macroscopic device that is actually erected on our laboratory table. Now what on earth could it mean, physically, to distribute a given amount of energy E over these N mental copies? The idea is, in my view, that you can, of course, imagine that you really had N copies of your system, that they really were in 'weak interaction' with each other, but isolated from the rest of the world. Fixing your attention on one of them, you find it in a peculiar kind of 'heat-bath' which consists of the N-1 others.

Even if this explanation is judged to be reasonable, there remains the striking dissimilarity between actual heat reservoirs and collections of replicas. This matter, often ignored, is disposed of by Schrödinger by appealing to empirical thermodynamics:

> Now you have, on the one hand, the experience that in thermodynamical equilibrium the behaviour of a physical system which you place in a heat-bath is always the same whatever be the nature of the heat-bath that keeps it a constant temperature, provided . . . that there is nothing else but heat exchange between them. On the other hand, the statistical calculations do not refer to the mechanism of interaction; they only assume that it is 'purely mechanical', that it . . . merely transfers energy from one [system] to the other.
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> These considerations suggest that we may regard the behaviour of any one of those N systems as describing the *one* actually existing system when placed in a heat-bath of given temperature. Moreover, since the N systems are alike and under similar conditions, we can then obviously, from their simultaneous statistics, judge of the probability of finding our system, when placed in a heat-bath of given temperature, in one or other of its private states.

Thus for theoretical purposes, an imaginary ensemble of replicas ought to be as efficacious as a real thermostat in maintaining a system in statistical equilibrium. In this paper we investigate the mechanical validity of this cornerstone of statistical thermodynamics. A simple quantum system will be placed in interaction with replicas of itself, the latter comprising an ensemble in statistical equilibrium. In an exact dynamical treatment it will be shown that the system, whatever its initial state, will indeed be coerced by this thermostatic ensemble into the same statistical equilibrium state which initially characterised the replicas. We have therefore a precise microphysical description of an ensemble of replicas functioning as a thermostat.

2. *A System in a Thermostatic Ensemble*

Consider a simple quantum system S, characterised by a two-dimensional Hilbert space $\mathscr{H}$ and a non-degenerate Hamiltonian H whose eigenvalues are E, F. Thus the eigenkets $|E\rangle$, $|F\rangle$ of H span $\mathscr{H}$, and the most general density matrix for statistical equilibrium is diagonal in H, with spectral expansion

$$\rho = \alpha|E\rangle\langle E| + (1-\alpha)|F\rangle\langle F|, \qquad 0 \leqslant \alpha \leqslant 1 \tag{2.1}$$

Quantum mechanically, ρ is already implicitly associated with a *Gibbsian* ensemble through which its inherent probability predictions become testable. However, to construct a *thermostatic* ensemble for the system S, we must provide a mechanism for interactions among the member systems and yet, at the same time, attempt to retain the original Gibbsian meaning for probability calculations.

To get the requisite mutual interactions, the implicit ensemble described by ρ must be replaced by an *assembly* of replicas of S: a composite physical system comprised of K subsystems $S_1, \ldots, S_K$, with Hilbert space

$$\mathscr{H}_T = \mathscr{H}_1 \otimes \ldots \otimes \mathscr{H}_K \tag{2.2}$$

To maintain the requirement that $\mathscr{H}_T$ be somehow identifiable with the Gibbsian ensemble characterized by (2.1), we adopt the postulate that for all applications of thermodynamic interest the density matrix for the thermostatic ensemble may be assigned the uncorrelated structure

$$\rho_T = \rho_1 \otimes \rho_2 \otimes \ldots \otimes \rho_k, \tag{2.3}$$

where each reduced density matrix ρ_k has the same statistical equilibrium form (2.1). Now, if we were considering a general assembly of K replicas, the form (2.3) would of course be quite unreasonable; but in the present context we face the powerful constraint that our assembly be capable of playing the dual role discussed earlier. Against that background, the form (2.3) seems essential.

There does emerge, however, a problem of internal consistency; for even if (2.3) holds initially, surely mutual interactions among the replicas will breed correlations and thereby destroy the form (2.3). We have already avoided this seeming dilemma by requiring not that ρ_T as expressed in (2.3) be the true density matrix forever but only that that uncorrelated form be *equivalent* to the true density matrix for *relevant thermodynamic calculations*. Since the purpose of even the thermostatic ensemble is to describe statistically only one of its members—the actual system which was replicated—it suffices to demand only that the reduced density matrix ρ_k for each system S_k always have the form (2.1); with respect to observables associated with each S_k alone, this is entirely equivalent to using (2.3) as the global density matrix. That this is dynamically possible will be explicitly demonstrated below.

Having noted that only the motion of one (typical) S_k is of interest, we next convert the intractable many-body problem represented by the thermostatic ensemble into a soluble problem involving only pair interactions. If we envisage a thermostat whose parts chaotically interchange energy as equilibrium is maintained, we are led to describe the mingling of S_k amongst its replicas as a sequence of 'collisions'; i.e., S_k interacts for a time with S_l alone, then with S_m alone, etc.

To complete our model of a thermostatic ensemble, we recall several theorems established in an earlier paper on quantum state preparation (Park & Band, 1972), hereinafter designated I. In the latter a system S_0 interacted sequentially with the constituents of an assembly $\{S_1, \ldots, S_K\}$ having an initial density matrix of uncorrelated structure like (2.3). It was established that for the sake of tracing the time development of S_0 alone the following procedure gives the appropriate reduced density matrix:

(a) Find the unitary evolution of $S_0 + S_1$ from $t = 0$ to $t = t_1$; then obtain $\rho_0(t_1)$ by using the partial trace technique (von Neumann, 1955) to reduce the $S_0 + S_1$ density matrix.

(b) Take $\rho_0(t_1)$ as the initial state of S_0 and find the unitary evolution of $S_0 + S_2$ until $t = t_2$; obtain $\rho_0(t_2)$ by reduction of the $S_0 + S_2$ density matrix.

(c) Repeat the procedure until $\rho_0(t_K)$ is determined.

In I the assembly with which S_0 interacted did not consist of replicas of S_0, but it is easily transformed to such an assembly by setting the degeneracy index N employed in I equal to unity. Moreover, in I the initial reduced density matrix of each S_k was not of the general statistical equilibrium form to be considered here, but corresponded only to the $\alpha = 0$ case of (2.1), a microcanonical ensemble. By paying attention to these differences and similarities, we can readily adapt to the present problem several expressions tediously derived in I.

As in I, we choose as the interaction potential energy between S_0 and S_k the simple operator V_{0k} defined by the matrix

$$\langle m|V_{0k}|n\rangle = \left\{\begin{matrix} v(1-\delta_{mn}), & 1 < m,\, n \leqslant 3 \\ 0, & \text{otherwise} \end{matrix}\right\} \tag{2.4}$$

where the representation is that given by this basis for $\mathscr{H}_0 \otimes \mathscr{H}_k$:

$$\begin{matrix} |E\rangle_0|E\rangle_k \equiv |1\rangle & |E\rangle_0|F\rangle_k \equiv |3\rangle \\ |F\rangle_0|E\rangle_k \equiv |2\rangle & |F\rangle_0|F\rangle_k \equiv |4\rangle \end{matrix} \tag{2.5}$$

The motivation for selecting (2.4) is thoroughly discussed in I, but we would like to reiterate that V merely promotes energy exchange between S_0 and S_k without net transfer. Thus $H_0 + H_k$ is separately conserved even while V_{0k} is operative. We believe therefore that this model mimics rather faithfully the dualistic conception of a thermostatic ensemble as an assembly which must in a sense exhibit both mutual interaction and mutual independence of its constituents.

Let S_0 be characterised initially ($t = 0$) by the arbitrary density matrix

$$\begin{aligned}\rho_0(0) &= a|E\rangle_{0\,0}\langle E + c|E\rangle_{0\,0}\langle F| \\ &\quad + c^*|F\rangle_{0\,0}\langle E| + (1-a)|F\rangle_{0\,0}\langle F|, \qquad 0 \leqslant a \leqslant 1\end{aligned} \tag{2.6}$$

and let the thermostatic ensemble be in the statistical equilibrium state (2.3). If the ensemble of replicas can indeed function as a thermostat, then in the course of serial interactions of S_0 with the various S_k, S_0 should ultimately be coerced into the state (2.1) common to all the replicas in equilibrium. We shall prove that this is in fact the case.

From I we know immediately that the proposed evolution occurs for the special case $\alpha = 1$, and hence by simple relabeling for the case $\alpha = 0$. And it might seem at first glance that this observation is sufficient to render obvious the proposition that S_0 can also be coerced into the form (2.1) which is, after all, just an incoherent superposition, or mixture, of $|E\rangle$ and $|F\rangle$. Such an argument would be admissible if but one interaction, say between S_0 and S_1 were required to accomplish the coercion; for then it could be said that the initial mixed state (2.1) for S_1 describes an imaginary quantal ensemble divisible into two sub-ensembles, one characterised by $|E\rangle_1$, the other by $|F\rangle_1$, to each of which the result in I could be separately applied. This reasoning is spurious, however, for a *sequence* of interactions between S_0 and *different* S_k, since S_0 would have to be regarded as interacting sometimes with an S_k in state $|E\rangle_k$, sometimes with an S_k in state $|F\rangle_k$. We would therefore not be secure in any *a priori* declaration that the desired result is just an 'obvious' consequence of I.

3. *Coercion of the System to Equilibrium*

To prove mechanically that an ensemble of replicas can function as a thermostat, we first apply the general method reviewed above to determine the reduced density matrix for S_0 after a sequence of interactions with the replicas S_1, S_2, . . ., S_K. Let τ_k denote the duration of the time interval during which S_0 interacts with S_k. The mathematical manipulations required involve three stages: (i) time evolution of $S_0 + S_1$ from $\rho_0(0) \otimes \rho_1(0)$, as defined in (2.1), (2.3), (2.6), through the interval τ_1; (ii) reduction of the final density matrix in (i) to obtain $\rho_0(t_1 = \tau_1)$; (iii) iteration to find $\rho_0(t_2)$, $t_2 = \tau_1 + \tau_2, \ldots, \rho_0(t_K)$, $t_K = \sum_{k=1}^{K} \tau_k$. Since at any given step only $S_0 + S_k$ is involved, it is convenient to display the matrix representation of operators using the representation given by (2.5):

(i) $S_0 + S_1$ *Dynamics*

$$\rho_{01}(0) \equiv (\rho_0(0) \otimes \rho_1(0)) = \begin{bmatrix} a\alpha & c\alpha & 0 & 0 \\ c^*\alpha & b\alpha & 0 & 0 \\ 0 & 0 & a\beta & c\beta \\ 0 & 0 & c^*\beta & b\beta \end{bmatrix} \tag{3.1}$$

where

$$\beta \equiv 1 - \alpha, \qquad b = 1 - a \tag{3.2}$$

The Hamiltonian matches that studied in I, provided we set $N = 1$. Therefore the evolution operator may be copied directly from I (with $\hbar = 1$):

$$\exp\left[-i\tau(H_0 + H_1 + V_{01})\right] = \begin{pmatrix} e & 0 & 0 & 0 \\ 0 & y(X+1) & yX & 0 \\ 0 & yX & y(X+1) & 0 \\ 0 & 0 & 0 & f \end{pmatrix} \tag{3.3}$$

where

$$\begin{aligned} e &\equiv e^{-i\tau 2E}, & f &\equiv e^{-i\tau 2F}, \\ y &\equiv e^{-i\tau(E+F-v)}, & X &\equiv 1/2(e^{-i\tau 2v} - 1) \end{aligned} \tag{3.4}$$

By matrix multiplication we obtain the $S_0 + S_1$ state for time t_1:

$$\rho_{01}(t_1) = (\exp[-i\tau_1(H_0 + H_1 + V_{01})])(\rho_{01}(0))(\exp[-i\tau_1(H_0 + H_1 + V_{01})])$$

$$= \begin{pmatrix} a\alpha & ec\alpha y^*(X^*+1) & ec\alpha y^* X^* & 0 \\ y(X+1)c^*\alpha e^* & \begin{array}{l} b\alpha(X+1)(X^*+1) + \\ \quad a\beta XX^* \end{array} & \begin{array}{l} b\alpha X^*(X+1) + \\ \quad a\beta X(X^*+1) \end{array} & yXc\beta f^* \\ yXc^*\alpha e^* & \begin{array}{l} b\alpha X(X^*+1) + \\ \quad a\beta X^*(X+1) \end{array} & \begin{array}{l} b\alpha XX^* + \\ \quad a\beta(X+1)(X^*+1) \end{array} & y(X+1)c\beta f^* \\ 0 & fc^*\beta y^* X^* & fc^*\beta y^*(X^*+1) & b\beta \end{pmatrix} \tag{3.5}$$

(ii) *Reduced Density Matrix* $(\rho_0(t_1))$

$$(\rho_0(t_1)) = (Tr_1 \rho_{01}(t_1))$$
$$= \begin{pmatrix} a\alpha + b\alpha XX^* + a\beta(X+1)(X^*+1) & ec\alpha y^*(X^*+1) + y(X+1)c\beta f^* \\ y(X+1)c^*\alpha e^* + fc^*\beta y^*(X^*+1) & b\alpha(X+1)(X^*+1) + a\beta XX^* + b\beta \end{pmatrix} \tag{3.6}$$

By substitution from (3.2), (3.4) and application of trigonometrical half angle formulae, (3.6) finally simplifies to

$$(\rho_0(t_1)) = \begin{pmatrix} a(t_1) & c(t_1) \\ c^*(t_1) & 1 - a(t_1) \end{pmatrix} \tag{3.7}$$

where

$$\begin{aligned} a(t_1) &= \alpha(1 - \epsilon_1) + a\epsilon_1 \\ c(t_1) &= \lambda(\tau_1)c \\ \epsilon_1 &\equiv \cos^2 v\tau_1 \\ \lambda(\tau) &\equiv \alpha e y^*(X^*+1) + \beta f^* y(X+1) \end{aligned} \tag{3.8}$$

(iii) *Iterative Determination of* $\rho_0(t_k)$

Let $a(t)$, $c(t)$ be defined for all t by

$$(\rho_0(t)) = \begin{pmatrix} a(t) & c(t) \\ c^*(t) & 1 - a(t) \end{pmatrix} \tag{3.9}$$

Note that $a(0) = a$, $c(0) = c$.

Now, by the same reasoning that produced (3.7) and (3.8) we immediately obtain a recurrence relation describing the evolution of $a(t)$ and $c(t)$ in the interval $[t_{k-1}$ to $t_k]$:

$$\left.\begin{aligned} a(t_k) &= \alpha(1 - \epsilon_k) + a(t_{k-1})\epsilon_k \\ c(t_k) &= c(t_{k-1})\lambda(\tau_k) \end{aligned}\right\} \tag{3.10}$$

Repeated application of (3.10) yields

$$\begin{aligned} a(t_K) &= \alpha(1-\epsilon_K) + a(\tau_{K-1})\epsilon_K \\ &= \alpha(1-\epsilon_K) + [\alpha(1-\epsilon_{K-1}) + a_{K-2}\epsilon_{K-1}]\epsilon_K \\ &= \alpha(1-\epsilon_{K-1}\epsilon_K) + a(t_{K-2})\epsilon_{K-1}\epsilon_K \\ &= \ldots = \alpha\left(1-\prod_{k=1}^{K}\epsilon_k\right) + a\prod_{k=1}^{K}\epsilon_k \end{aligned} \tag{3.11}$$

and

$$\begin{aligned} c(t_K) &= c(t_{K-1})\lambda(\tau_K) = c(t_{K-2})\lambda(\tau_{K-1})\lambda(\tau_K) = \ldots \\ &= c\prod_{k=1}^{K}\lambda(\tau_k) \end{aligned} \tag{3.12}$$

We now have only to show that when the number of systems in the thermostatic ensemble is large, S_0—whatever its initial state—will be coerced into the common statistical equilibrium state (2.1) of the replicas. We are interested therefore in these limits:

$$a(t_\infty) = \operatorname*{Lim}_{K\to\infty} a(t_K) \tag{3.13}$$

$$c(t_\infty) = \operatorname*{Lim}_{K\to\infty} c(t_K) \tag{3.14}$$

To evaluate (3.13), note that $\epsilon_k = \cos^2 v\tau_k$; hence

$$0 \leqslant \epsilon_k \leqslant 1 \tag{3.15}$$

It follows that

$$\prod_{k=0}^{\infty}\epsilon_k = 0 \tag{3.16}$$

unless *only a finite* number of the $\{\epsilon_k\}$ differ from unity. But $\epsilon_k = 1$ only for certain discrete points in the continuum of possible interaction times τ_k; thus (3.16) will 'almost never' be incorrect. From (3.16) we immediately obtain

$$a(t_\infty) = \alpha \tag{3.17}$$

The evolution of (3.14) is a bit more involved since $\lambda(\tau)$ defined in (3.8) and (3.4) is complex. By straightforward algebraic manipulation we first find that

$$|\lambda(\tau)|^2 = \lambda^*\lambda = \cos^2 v\tau \tag{3.18}$$

Hence

$$0 \leqslant \lambda(\tau) \leqslant 1 \tag{3.19}$$

Now from (3.12) and (3.14) we have, taking absolute values,

$$|c(t_\infty)| = \left| c \prod_{k=1}^{\infty} \lambda(\tau_k) \right| = |c| \prod_{k=1}^{\infty} |\lambda(\tau_k)| \tag{3.20}$$

Finally (3.19) and (3.20) together imply

$$c(t_\infty) = 0 \tag{3.21}$$

Combining (3.9), (3.17), (3.21) we now have the desired result:

$$(\rho_0(t_\infty)) = \begin{pmatrix} \alpha & 0 \\ 0 & 1-\alpha \end{pmatrix} \tag{3.22}$$

i.e.

$$\rho_0(t_\infty) = \alpha|E\rangle_{00}\langle E| + (1-\alpha)|F\rangle_{00}\langle F| \tag{3.23}$$

which is identical to (2.1), the statistical equilibrium state shared by members of the thermostatic ensemble.

4. *Conclusion*

We are now in a position to validate the claim made in Section 2, that each system in a thermostatic ensemble can, despite the mutual interactions, remain at all times in a statistical equilibrium state described by a reduced density matrix of the form (2.1). This behavior is an immediate consequence of (3.7), (3.8); for if we place into the thermostatic ensemble a system S_0 already in the same equilibrium (2.1) as the ensemble members, then, the coercive process being complete *ab initio*, no state transformation occurs. We set $a = \alpha$, $c = 0$, and find

$$\begin{aligned} a(t_1) &= \alpha(1-\epsilon_1) + \alpha\epsilon_1 = \alpha \\ c(t_1) &= \lambda(\tau_1)(0) = 0 \end{aligned} \tag{4.1}$$

Hence

$$(\rho_0(t_1)) = \begin{pmatrix} \alpha & 0 \\ 0 & 1-\alpha \end{pmatrix} = (\rho_0(0)) \tag{4.2}$$

Our specific, exactly soluble, illustration has shown therefore that the concept of a thermostatic ensemble is entirely rational so far as its dynamical realisability is concerned. Left to itself, the thermostatic ensemble is *stable*: the reduced density matrices, any one of which would characterise the entire ensemble in the Gibbsian sense, remain stationary in spite of the mutual interactions which were required in order to justify the thermostat interpretation. In interaction with an arbitrarily prepared system S_0, the thermostatic ensemble (constituted of replicas of S_0) coerces S_0 ultimately into the same statistical equilibrium state that originally characterised each replica. Finally it should be noted that after the interaction of S_0 and S_k, the latter system is no longer described by the density matrix (2.1); hence every replica that actually participates in the coercion of S_0 towards equilibrium is itself thrown out of equilibrium. However if the thermostatic ensemble is infinitely populous, and so chaotic that systems which lose equilibrium are unlikely to be exposed to each other, then each participating S_k just begins, after interacting with S_0, its own forced march back towards equilibrium.

To see the reasonableness of this mathematical model, consider a physical parallel: when a tiny meteor falls into an ocean, the final temperature of the meteoroid-plus-ocean assembly will be, for all practical purposes, the original oceanic temperature. It is precisely this extreme kind of thermostatic process—involving a small system and an extremely large reservoir—for which the present work has provided a simple yet exact quantum mechanical explanation. Larger questions, mentioned at the end of I, concerning irreversibility and approach to equilibrium in general cases remain unanswered. Nevertheless we are hopeful that obvious generalisations of the foregoing analysis, coupled with suitable approximations, may prove fruitful in the study of more complex systems engaged in irreversible processes.

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