

# On the Control of Quantum Statistical Systems

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The problem of preparing a system in some initial configuration is discussed for quantum statistical systems whose dynamics are generated by Markovian semigroups. The system is regulated by a set of controls and the central problem is to determine how the controls should be varied in order to bring the system as close as possible to the desired configuration in a fixed finite time. General equations are derived which allow one to determine how the controls should be regulated. The application of the result to a simple system is outlined.

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**KEY WORDS:** Control theory; quantum statistical dynamics; semigroups.

## 1. INTRODUCTION

An experiment usually begins with the preparation of the system being studied in some initial, often nonequilibrium, configuration. Determining how to generate such an initial configuration is a problem that experiment designers must deal with all the time. This problem is usually dealt with on a case-by-case basis by optimizing design in order to bring the system as close as possible to the desired configuration. The optimum design will generally have a stationary and a time-dependent part. It is the latter that we wish to address here.

In order to manipulate the system the experimenter has controls which can be used to apply various forces to the system and to transfer heat into or out of the system. In this paper we provide a general mathematical framework which mimics the experimental procedure. To do this we present a formalism which includes both controls and relaxation processes and allows us to formulate the optimization problem in general terms. In

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particular, we provide a finite-time formalism in the sense that the system does not evolve either infinitely slowly or instantaneously (although we allow controls to be changed instantaneously).

For systems which can be treated classically, there exists a general mathematical procedure for carrying through the required optimization calculation<sup>(1)</sup>; therefore, we limit our considerations to a class of quantum statistical systems. In particular, we treat Markovian systems and derive necessary conditions for driving them from an initial equilibrium state to a final configuration in a fixed, finite time. We have used the term configuration, as distinct from state, because experimentalists often do not require that their systems be in definite states but only that a certain set of measurements yield specific results.

In the next section we present the general mathematical formulation of the problem we wish to analyze, and discuss some of its features. In the third section we derive necessary conditions for the existence of an optimal solution. We then consider two special cases which make the actual solution of the problem tractable. The first of these, discussed in Section 4 treats finite-dimensional systems. The second, which reduces to the finite-dimensional case, considers the case in which the state of the system is required to be a maximum entropy state.<sup>2</sup> Finally in the last section we state our results and conclusions.

## 2. MATHEMATICAL FORMULATION

We shall first formally present the system we wish to analyze and then discuss some of its properties. We consider a system specified by a separable, complex Hilbert space,  $H$ . The states of the system are density matrices, which are defined, as usual, to be elements  $\rho$  of the set of linear operators on  $H$  such that

- (i)  $\rho$  is self-adjoint:  $\rho = \rho^\dagger$
- (ii)  $\rho$  is non-negative:  $(\psi, \rho\psi) \geq 0$  for all  $\psi \in H$
- (iii)  $\rho$  has unit trace:  $\text{tr } \rho = 1$

An observable is a linear, self-adjoint operator defined on some suitable domain in  $H$ .

The dynamics of the system is assumed to be generated by a quantum dynamical semigroup<sup>(3-5)</sup>:

$$\frac{\partial \rho(t)}{\partial t} = -iL(t)\rho(t) \quad (2.1)$$

<sup>2</sup> See Ref. 2; this book contains an extensive set of references, as well as several interesting papers.

where for any density matrix  $\rho$ , the generator of the semigroup is given by

$$\begin{aligned}
 -iL\rho &= x\rho + \rho x^\dagger + \sum_{n=1}^N B_n^\dagger \rho B_n \\
 x &= -iH - R, \quad R = \frac{1}{2} \sum_{n=1}^N B_n B_n^\dagger, \quad \text{and} \quad H = H^\dagger \quad (2.2)
 \end{aligned}$$

We shall further assume that

$$L = L_0 + L'(t) = L_0 + \sum_{j=1}^c g_j(t)L_j \quad (2.3)$$

where  $\{L_0, L_j\}$  are time-independent operators and the  $\{g_j(t)\}$  are piecewise continuous, real, scalar functions. These functions will be the means of controlling the system. We shall refer to the vector  $\mathbf{g}(t) = (g_1(t), \dots, g_c(t))$  as the control vector, and require that it lie within a closed bounded region  $G$  of a  $c$ -dimensional, Euclidean vector space.

We are finally ready to state the problem we wish to study. Let  $\{A_j, j = 1, \dots, n\}$  be a set of linearly independent observables and let the system be in the state  $\rho_0$  at  $t = 0$ . We wish to find the control vector  $\mathbf{g}(t) \in G$  such that at  $t = t_f > 0$  the system is close to a configuration defined by a set of real numbers  $\{a_j\}$  in the sense that

$$J = \frac{1}{2} \sum_{j=1}^n \langle (A_j - a_j 1)^2 \rangle_f \quad (2.4)$$

is a minimum. Where for any bounded operator  $O$ ,

$$\langle O \rangle_f = \text{tr } \rho(t_f) O \quad (2.5)$$

with  $\rho(t_f)$  the solution to Eq. (2.1) with  $\rho(0) = \rho_0$ .

We now wish to discuss the restrictions implied by the assumptions made above. The dynamics of the system is the quantum analog of a Markovian system.<sup>(3-6)</sup> If  $R$  and, therefore, all the  $B_n$  vanish, the dynamics becomes Hamiltonian. If  $R$  is not zero the system is dissipative. This means that the Gibbs entropy of the system,

$$S(\rho) = -\text{tr } \rho \ln \rho \quad (2.6)$$

may change, and consequently, as  $\mathbf{g}$  varies over  $G$ , we have a greater range of density matrices accessible from a given initial state than in the purely Hamiltonian case.

As mentioned in the Introduction, we have specified the final configuration of the system. That is, we have not asked for a specific density matrix but only that the average value of some operators be suitably well-approximated in the sense that Eq. (2.4) be minimized. It is well known that once a set  $\{\langle A_j \rangle_f\}$  is determined, except in the case that the

$\{A_j\}$  are a complete set of observables, there are many density matrices that will give the same average values.<sup>(2,4)</sup> It has been suggested<sup>(4)</sup> that the set of all these density matrices be called the macrostate of the system with respect to the set  $\{\langle A_j \rangle_f\}$ . Furthermore this macrostate may be uniquely represented by the element that has the maximum Gibbs entropy. Thus we may wish to replace the minimization condition (2.4) by a condition such as

$$J' = \min[\text{tr}(\rho(t_f) - \hat{\rho})^2] \quad (2.7)$$

here  $\hat{\rho}$  is the maximum entropy representative of the macrostate in which we wish to prepare our system. Since this is a different condition, unlike Eq. (2.4) it is not linear in  $\rho(t_f)$ , it will lead to a different final configuration.

Although the condition at the end of the preparation is specified in terms of a configuration, the condition at  $t = 0$  has been given in terms of a density matrix. This is justified for the case of most interest when  $\rho_0$  is an equilibrium state of the system. Of course, nothing prevents us from taking a configuration as our initial condition. Even in this case, where only some average values are given and nothing else is specified, as has been argued by Jaynes,<sup>(2)</sup> the initial state is most likely to be the maximum entropy representative of the macrostate.

The choice of  $J$  in Eq. (2.4) as a figure of merit for the preparation of the final configuration is arbitrary. As we stated above we could replace  $J$  by a quantity such as  $J'$  defined in Eq. (2.7). Alternatively, one might seek to minimize a quantity such as the value of the Gibbs entropy at  $t_f$ , that is, loosely speaking, find the most ordered state of the system that can be reached in a time  $t_f$  from a given initial state using the controls in  $G$ . Alternatively we might replace  $J$  by  $\sum_j \langle A_j \rangle_f - a_j$  which is quadratic in  $\rho(t_f)$ . Finally it should be noted that multiplying each term in the sum in Eq. (2.4) by a positive weighting factor does not change the problem since these factors can be absorbed into the  $\{A_j\}$  and  $\{a_j\}$ .

### 3. NECESSARY CONDITIONS FOR THE OPTIMAL SOLUTION

We now turn to the task of obtaining the necessary conditions for solving Eqs. (2.1)–(2.5). We follow the procedure used in the analogous classical problems<sup>(1)</sup> by introducing a time-dependent Lagrange multiplier  $\psi(t)$  in order to treat the equation of motion (2.1) as a constraint. In contrast to the classical case,  $\psi(t)$  must be an operator on the Hilbert space of the system. We now define

$$M = J + \int_0^{t_f} dt [K - \text{Tr} \psi \dot{\rho}] \quad (3.1)$$

where

$$K = \text{Tr} \psi (-iL\rho)$$

$J$  is given by Eqs. (2.4) and (2.5), and  $L$  is given by Eqs. (2.1)–(2.3). We require that  $\psi$  be self-adjoint to ensure that  $M$  and  $K$  are real. As we shall see, the dynamics of  $\psi$  as given by Eqs. (3.8) and (3.9) are consistent with this requirement. In the literature of optimal control theory the quantity  $K$  is called the Hamiltonian; we shall reserve this name for the  $H$  in Eq. (2.2).

To perform the variational calculation, it is necessary to consider the variation of  $\rho$  and the controls about the optimal solution. We shall do these two calculations separately.

### 3.1. The State Variation

To derive the equation of motion for  $\psi$  we consider a variation of  $\rho$  around the optimal solution  $\hat{\rho}$ :  $\hat{\rho} \rightarrow \rho' = \hat{\rho} + \eta$ . Since  $\rho'$  must be a state of the system, the conditions (i) and (iii) of Section 2 imply that  $\eta$  is self-adjoint and has vanishing trace. The positivity condition is more difficult to handle. In control theory, it is usually difficult to deal with systems whose dynamical variables are constrained.<sup>(1,7)</sup> We shall see that the positivity condition presents a serious problem.

Introducing  $\rho'$  into  $M$  and performing the usual integration-by-parts we obtain

$$M[\rho'] = M[\hat{\rho}] + M'[\hat{\rho}, \eta] \tag{3.2a}$$

$$M'[\hat{\rho}, \eta] = \sum_{j=1}^N \text{tr} \eta(t_j) \{ (A_j - a_j \mathbb{1})^2 - \psi(t_j) \} + \int_0^{t_f} dt \text{tr} \eta [ (-i\hat{L}^\dagger \psi) + \psi ] \tag{3.2b}$$

where  $\hat{L}^\dagger$  is the adjoint of  $\hat{L}$ , the generator of the optimal solution. We now assume that  $\eta$  is small<sup>3</sup> and require that  $M[\hat{\rho}]$  be a (local) minimum. This requires that  $M' \geq 0$ .

There is an analytic and an algebraic part to the calculation. The analytic part is the standard procedure of requiring that  $\eta$  be nonvanishing on a small subinterval of  $[0, t_f]$  so that the condition on  $M'$  can be applied to the integrand in Eq. (3.2b). The end point variation then allows us to require that the first term on the right-hand side of Eq. (3.2b) be nonnegative. Thus we are left with conditions of the form

$$\text{tr} \eta O \geq 0 \tag{3.3}$$

where  $O$  is one of the self-adjoint operators multiplying  $\eta$  in Eq. (3.2b). The

<sup>3</sup>The requirement that  $\eta$  be small means that  $\|\eta\| = \text{tr}|\eta| \ll 1$ , where  $|\eta|$  is the positive square root of  $\eta^2$ . See, for example, Ref. 8.

algebraic part of the problem entails removing the trace in order to obtain an equation for  $O$ .

Since  $\eta$  has a vanishing trace, if  $O$  is a multiple of the identity operator Eq. (3.3) is automatically satisfied. In order to consider Eq. (3.3) for a general  $\eta$  we shall write

$$\eta = -i\epsilon L' \hat{\rho} \quad (3.4)$$

where  $-iL'$  is an arbitrary operator of the form (2.2) and  $0 < \epsilon \ll 1$ . Then for  $\epsilon$  sufficiently small  $\rho' = (1 - i\epsilon L')\hat{\rho}$  is a state,<sup>(5,9)</sup> so  $\eta$  satisfies the required constraints.

We carry out the calculation in two steps. First, we take an arbitrary Hamiltonian variation,  $\eta = -i\epsilon[H, \hat{\rho}]$ ,  $H = H^\dagger$ . Equation (3.3) becomes  $-i\epsilon \text{tr} H[\hat{\rho}, O] \geq 0$ . Since  $O$  is self-adjoint, we may choose  $H = -i[\hat{\rho}, O]$ , which gives  $-\epsilon \text{tr}[\hat{\rho}, O]^2 \geq 0$  so that  $[\hat{\rho}, O] = 0$ .

Next we consider a purely dissipative variation,  $\eta = -(\epsilon/2)[BB^\dagger \hat{\rho} + \hat{\rho}BB^\dagger - 2B^\dagger \hat{\rho}B]$ . Let  $\{|\alpha\rangle\}$  be a basis in which  $\hat{\rho}$  and  $O$  are diagonal; then Eq. (3.3) becomes

$$\epsilon \sum_{\alpha} \hat{\rho}_{\alpha} \left\{ \sum_{\alpha'} O_{\alpha'} |\langle \alpha|B|\alpha'\rangle|^2 - O_{\alpha} \langle \alpha|BB^\dagger|\alpha\rangle \right\} \geq 0 \quad (3.5)$$

Let  $V = \{\alpha : \hat{\rho}_{\alpha} > 0\}$  and  $V'$  be the complement of  $V$ . Then we choose  $\langle \alpha|B|\alpha'\rangle = b\delta_{\alpha\beta}\delta_{\alpha'\gamma}$  for  $\beta, \gamma \in V$ ,  $\beta \neq \gamma$  so that Eq. (3.5) becomes  $\epsilon \hat{\rho}_{\beta}(O_{\gamma} - O_{\beta}) \geq 0$ . Reversing the role of  $\beta$  and  $\gamma$  we conclude that  $O_{\beta} = c$  for all  $\beta \in V$ .

Now let  $\langle \alpha|B|\alpha'\rangle = b\delta_{\alpha\beta}\delta_{\alpha'\gamma}$ , where  $\beta \in V$  and  $\gamma \in V'$ . Equation (3.5) now becomes  $\epsilon \hat{\rho}_{\beta}(O_{\gamma} - c) \geq 0$ , which requires that  $O_{\gamma} \geq c$  for all  $\gamma \in V'$ . Unfortunately we learn nothing new if we reverse the roles of  $\beta$  and  $\gamma$  because  $\hat{\rho}_{\gamma} = 0$ . This means that the  $\psi$  equation of motion has a term in it that depends on  $\hat{\rho}$  in a complicated way. This type of difficulty is typical of control problems in which the state variables are constrained.<sup>(7)</sup>

We can avoid the difficulty mentioned above if we restrict our considerations to systems in which  $\hat{\rho}$  is strictly positive. This means that  $V'$  is empty and we may conclude that  $O = c1$ , where  $c$  is a scalar function of time. Thus from Eq. (3.26) we obtain

$$\dot{\psi} = -i\hat{L}^\dagger \psi + c(t)1 \quad (3.6)$$

$$\psi(t_f) = \sum_{j=1}^N (A_j - a_j 1)^2 + k1 \quad (3.7)$$

Since a simple calculation shows that  $\hat{L}^\dagger(1) = 0$ , we can redefine  $\psi$  so that  $\psi \rightarrow \psi + k' + \int_0^t c(t) dt 1$  and eliminate the last terms from Eq. (3.6). By a suitable choice of  $k'$  we can also eliminate the constant in Eq. (3.7).

We have

$$\dot{\psi} = -i\hat{L}^\dagger\psi \tag{3.8}$$

$$\psi(t_f) = \sum_{j=1}^N (A_j - a_j\mathbb{1})^2 \tag{3.9}$$

It should be noted that  $\psi$  does not satisfy the equation of motion of a Heisenberg operator because of the minus sign in Eq. (3.8). This is characteristic of control problems. The natural evolution of  $\psi$  is backwards in time in the sense that Eq. (3.9) determines  $\psi(t_f)$ .

Before ending this long section we should make a comment about the requirement  $\hat{\rho} > 0$ . This implies that  $\hat{\rho}$  can never be a pure state; in particular, it cannot be a pure state at  $t_f$ . It might plausibly be argued that  $\hat{\rho} > 0$  is a physically reasonable condition since one can never eliminate “infinitesimal” admixtures of arbitrary states. This is clearly an evasion and may even be false. However, for the example worked out in Section 5,  $\hat{\rho}$  is in fact strictly positive. In any particular problem the question of whether  $\hat{\rho}$  is strictly positive will depend on the initial condition,  $\hat{\rho}(0)$  and the form of  $\hat{L}$ .

### 3.2. The Control Variation

The effect of the variation with respect to the controls is most simply studied using the Pontryagin minimum principle<sup>(1,10)</sup>:

$$\text{Tr} \psi [ -i(L_t - \hat{L})\hat{\rho} ] \geq 0 \tag{3.10}$$

where  $\psi$  is the solution to Eqs. (3.8) and (3.9) and  $L_t$  is the operator of Eq. (2.2) with the optimal controls replaced by an arbitrary, allowed control. Using Eq. (2.3) this becomes

$$\sum_{j=1}^c [ g_j(t) - \hat{g}_j(t) ] \text{tr} [ \psi(-iL_j\hat{\rho}) ] \geq 0 \tag{3.11}$$

where  $\mathbf{g}(t)$ , the trial control, and  $\hat{\mathbf{g}}(t)$ , the optimal control, both lie on  $G$ .

The analysis of Eq. (3.11) is standard.<sup>(1)</sup> For example, suppose  $G = \{ \mathbf{g}; |\mathbf{g}| \leq g_0 \}$ ,  $\Lambda_j = -i \text{tr} \psi L_j \hat{\rho}$  and denote by  $\Lambda$  the  $c$ -dimensional Cartesian vector with components  $\Lambda_j$ . Then if  $|\Lambda| \neq 0$ ,  $\hat{\mathbf{g}}$  lies on the boundary of  $G$  and  $\Lambda$  must point along the radius of  $G$ , i.e.,  $\hat{\mathbf{g}} = -G\Lambda/|\Lambda|$ . If  $|\Lambda| = 0$ , then Eq. (3.11) does not determine  $\hat{\mathbf{g}}$  directly and further analysis is required. In the next section we outline such an analysis for the example presented there.

This concludes our general discussion. For the dynamical system defined by Eqs. (2.1)–(2.3) we have derived the necessary conditions Eqs.

(3.8), (3.9), and (3.11) for a local minimum of  $J$  defined by Eq. (2.4). The fact that we have a local minimum rather than just an extremum follows from the use of an inequality in studying Eq. (3.2b).

#### 4. CONTROL OF A TWO-LEVEL SYSTEM

Any finite-dimensional system may be handled more simply than the general case treated in Sections 2 and 3. The control problem can be reduced to a standard problem by expanding all the operators in terms of a complete set of matrices. For example,  $\rho = (1/N)(1 - \mathbf{P} \cdot \boldsymbol{\Sigma})$  where the elements of the vector  $\boldsymbol{\Sigma}$  are  $N^2 - 1$  independent self-adjoint matrices with vanishing trace normalized so  $\text{tr} \Sigma_i \Sigma_j = \delta_{ij}$  and  $\mathbf{P}$  is an  $(N^2 - 1)$ -dimensional real vector such that  $|\mathbf{P}|^2 \leq N(N - 1)$ . From the equation of motion for  $\rho$ , an equation for  $\mathbf{P}$  may be derived and the problem now becomes one involving  $N^2 - 1$  coupled ordinary differential equations which may be treated as a control problem with a state variable constraint  $|\mathbf{P}|^2 \leq N(N - 1)$ . In fact any practical treatment will involve such a reduction at some point in order to make the computation tractable.

We now consider the example of a spin-1/2 particle in an axisymmetric environment, interacting with a thermal bath.<sup>(6,11)</sup> The spin will be controlled by means of a weak magnetic field. As stated at the beginning of this paper, we are concerned with the Markovian limit in which the system has no memory.

We shall take the dynamics of the system to be such that we obtain the Bloch equation.<sup>(6)</sup> Thus we take

$$\begin{aligned} B_1 &= (\alpha\gamma_1)^{1/2} \sigma_-, & B_2 &= (\alpha\gamma_2)^{1/2} \sigma_+, \\ B_3 &= [(\gamma_1 + \gamma_2)/2]^{1/2} \sigma_3, & H_0 &= 0 \end{aligned} \quad (4.1)$$

for  $L_0$  in Eq. (2.3). The  $\sigma$ 's are the Pauli matrices,  $[\sigma_i, \sigma_j] = i\epsilon_{ijk} \sigma_k$  and  $\sigma_{\pm} = \frac{1}{2}(\sigma_i \pm i\sigma_2)$ . The controls are taken to be Hamiltonian:

$$H'(t) = \mathbf{g}(t) \cdot \boldsymbol{\sigma}, \quad |\mathbf{g}| \leq g_0 \quad (4.2)$$

so that the domain  $G$  is the closed sphere of radius  $g_0$  centered at the origin.  $J$  will be chosen to be

$$J = \frac{1}{2} \langle (\boldsymbol{\sigma} - \mathbf{S}_f)^2 \rangle_f \quad (4.3)$$

The Liouville operator  $L_0$  has a stationary state solution

$$L_0 \rho_0 = 0, \quad \rho_0 = \frac{1}{2} \left( 1 - \frac{\gamma_1 - \gamma_2}{\gamma_1 + \gamma_2} \sigma_3 \right) \quad (4.4)$$

which will be taken as the initial state:  $\hat{\rho}(0) = \rho_0$ . We shall drop the circumflex over the  $\rho$  from now on since we only will be concerned with the optimal solution.



Assuming that  $\rho$  is strictly positive, we may write the equation for  $\psi(t)$ :

$$\begin{aligned} \dot{\psi}(t) = & -iL^\dagger(t)\psi(t) = -i[H'(t), \psi(t)] \\ & + \gamma_1(\sigma_+[\sigma_-, \psi(t)] + [\psi(t), \sigma_-]\sigma_+) \\ & + \gamma_2(\sigma_-[\sigma_+, \psi(t)] + [\psi(t), \sigma_+]\sigma_-) \\ & + \frac{1}{4}(\gamma_1 + \gamma_2)(\sigma_3[\sigma_3, \psi(t)] + [\psi(t), \sigma_3]\sigma_3) \end{aligned} \quad (4.5)$$

$$\psi(t_f) = \frac{1}{2}(\sigma - \mathbf{S}_f \mathbb{1})^2 = \frac{1}{2}(3 + \mathbf{S}_f^2)\mathbb{1} - \sigma \cdot \mathbf{S}_f \quad (4.6)$$

We now reduce the operator equations for  $\rho$  and  $\psi$  to ordinary differential equations by setting  $\rho = \frac{1}{2}(1 - \mathbf{p} \cdot \sigma)$  and  $\psi = \frac{1}{2}[\psi_0 \mathbb{1} + \psi \cdot \sigma]$ . We obtain

$$\dot{\mathbf{p}} = 2(\mathbf{g} \times \mathbf{p}) - \Gamma(\mathbf{p} - \eta \hat{e}_3) \quad (4.7)$$

$$\dot{\psi} = 2(\mathbf{g} \times \psi) + \Gamma \psi \quad (4.8)$$

$$\dot{\psi}_0 = \eta \Gamma \psi_3 \quad (4.9)$$

$$\mathbf{p}(0) = \eta \hat{e}_3, \quad \psi(t_f) = -2\mathbf{S}_f, \quad \psi_0(t_f) = 3 + \mathbf{S}_f^2 \quad (4.10)$$

where  $\Gamma = 2(\gamma_1 + \gamma_2)$  and  $\eta = (\gamma_1 - \gamma_2)/(\gamma_1 + \gamma_2)$ .

These equations cannot be solved until  $\mathbf{g}(t)$  is determined. Equation (3.11) becomes

$$(\mathbf{g}_t - \mathbf{g}) \cdot (\psi \times \mathbf{p}) \geq 0 \quad (4.11)$$

where  $\mathbf{g}$  is the optimal control and the trial control,  $\mathbf{g}_t$ , is any element of the set  $G$ . If  $|\psi \times \mathbf{p}| \neq 0$ ,  $\mathbf{g}$  must lie on the boundary of  $G$ ,  $\mathbf{g} = g_0 \hat{e}$ , where  $\hat{e}$  is a unit vector, and  $\psi \times \mathbf{p}$  must be antiparallel to  $\hat{e}$ . If  $|\psi \times \mathbf{p}| = 0$ , Eq. (4.11) does not immediately determine  $\mathbf{g}$ .

Before continuing, we note that  $\psi_0$ , the coefficient of the identity matrix, does not play a role in the determination of the optimal solution. This is an explicit justification for our treatment of the terms  $c(t)$  and  $k$  in Eqs. (3.6) and (3.7).

We now consider the case  $|\psi \times \mathbf{p}| = 0$ . If this condition can only be fulfilled at discrete points, then all the solutions correspond to  $\mathbf{g}$  lying on the boundary of  $G$ . The points at which  $|\psi \times \mathbf{p}| = 0$  allow for the possibility of discontinuous shifts in the direction of  $\hat{e}$ . If  $|\psi \times \mathbf{p}| = 0$  on a finite time interval, then the optimal solution may have branches along which  $\mathbf{g}$  may lie inside of  $G$ .

We now examine the possibility that  $|\psi \times \mathbf{p}| = 0$  on a finite interval.  $|\psi \times \mathbf{p}| = 0$  implies that either  $\psi = 0$ ,  $\mathbf{p} = 0$  or  $\psi$  and  $\mathbf{p}$  are colinear. From Eq. (4.8) and the fact that  $\psi(t_f) \neq 0$ , it follows that  $\psi$  never vanishes.

Equation (4.7) implies that if  $\mathbf{p} = 0$ ,  $\dot{\mathbf{p}} = +\Gamma\eta\hat{e}_3$ . Thus  $\mathbf{p}$  cannot vanish on a finite time interval, and we are left with the case that  $\psi$  and  $\mathbf{p}$  are colinear.

If  $|\psi \times \mathbf{p}| = 0$  on a finite time interval, then inside this interval  $(d/dt)(\psi \times \mathbf{p})$  also vanishes. From this and Eqs. (4.7) and (4.8) we find that the possible solutions are

$$\begin{aligned}\psi &= \psi(t_0)\hat{e}_3 e^{\Gamma(t-t_0)}, & \mathbf{p} &= \hat{e}_3\{\eta + [p(t_0) - \eta]e^{-\Gamma(t-t_0)}\} \\ \mathbf{g} &= g(t)\hat{e}_3\end{aligned}\quad (4.12)$$

where  $g(t)$  is an arbitrary, piecewise continuous function in  $G$ . This corresponds to a solution in which the value of  $g$  is irrelevant and  $\mathbf{p}$  simply relaxes towards its equilibrium value. It seems intuitively clear that such a branch is not really useful except to waste time. For example if  $t_0 = 0$ , then  $p(t_0) = \eta$  and the system is unchanged. Therefore we obtain the not surprising result that we wish to use as large a magnetic field as we can.

To determine the solution for  $\mathbf{g}(t) = g_0\hat{e}(t)$  is tedious and must be done numerically. Since we are not interested in the numerical results we merely outline the procedure. We introduce a rotating set of orthonormal vectors  $\{\hat{e}, \hat{f}, \hat{k}\}$  where  $\hat{f}$  is defined by the equation  $d\hat{e}/dt = \gamma\hat{f}$  and  $\hat{k}$  by  $d\hat{f}/dt = -\gamma\hat{e} + \alpha\hat{k}$ . Each unit vector satisfies the equation  $d/dt = (\Omega \times)$  where  $\Omega = \alpha\hat{e} + \gamma\hat{k}$ . The fact that  $\psi \times \mathbf{p}$  must be colinear with  $\hat{e}$  then implies that  $\psi \cdot \hat{e} = \mathbf{p} \cdot \hat{e} = 0$ . It also turns out that either  $\psi$  is colinear with  $\hat{k}$  and  $\alpha = 2g_0$  or  $\gamma = 0$ .

If  $\gamma = 0$ , then along this branch  $\hat{e}$  is independent of time and Eq. (4.7) has as one of its consequences that  $\hat{e} \cdot \hat{e}_3 = 0$ . In this case the solution may be written in terms of the fixed orthonormal basis  $\{\hat{e}, \hat{e}_2, \hat{e}_3\}$ :

$$\begin{aligned}\psi &= \psi(t_0)e^{\Gamma(t-t_0)}[\hat{e}_2 \cos(2g_0t + \phi) + \hat{e}_3 \sin(2g_0t + \phi)] \\ \mathbf{p} &= \mathbf{p}_s + Be^{-\Gamma(t-t_0)}[\hat{e}_2 \cos(2g_0t + \chi) + \hat{e}_3 \sin(2g_0t + \chi)] \\ \mathbf{p}_s &= (\eta\Gamma/\Omega^2)[-2g_0\hat{e}_2 + \Gamma\hat{e}], & \Omega &= (4g_0^2 + \Gamma^2)^{1/2}\end{aligned}$$

where  $B = |\mathbf{p}(t_0) - \mathbf{p}_s|$  and  $\mathbf{p}_s$  is the steady solution to Eq. (4.7) for the given  $\mathbf{g} = g_0\hat{e}$ . Finally, the duration of a branch is determined by the condition  $(\psi \times \mathbf{p}) \cdot \hat{e} \leq 0$ . The beginning and end of the branch occur when the equality holds.

This solution has the property that for the initial condition  $\mathbf{p}(0) = \eta\hat{e}_3$ ,  $\mathbf{p}$  lies inside the cone swept out by  $\mathbf{p}_s$  as  $\hat{e}$  rotates through  $2\pi$  in the  $x$ - $y$  plane. Thus if  $\mathbf{S}_f$  lies inside this cone, this solution is adequate and if  $t_f$  is long enough,  $J$  may attain the minimum value of zero. If  $\mathbf{S}_f$  lies outside this cone, or if our initial condition were such that  $\hat{e}_3$ ,  $\mathbf{S}_f$ , and  $p(0)$  were not coplanar, the control becomes more complicated. In this case,  $\hat{e}$  rotates around  $\Omega$  which itself is time dependent since  $\gamma$  is in general not constant.

In order to reduce this problem farther it is necessary to use the equation for  $\mathbf{p}$  to obtain a set of equations for the rotating coordinate system in terms of the fixed, laboratory frame.

To put together a solution one starts with  $\psi(t_f)$  given by Eq. (4.10) and guesses a final  $\mathbf{p}(t_f)$ . These will determine the direction of  $\hat{e}(t_f)$  and then one must integrate back to  $t = 0$  to determine if  $\mathbf{p}(0) = \eta\hat{e}_3$ . It seems clear that the optimal solution has  $|\mathbf{g}| = g_0$  and  $\hat{e}(t)$  varies smoothly remaining orthogonal to the  $\mathbf{p} - \psi$  plane, although I have not proved this. Suffice it to say that one can obtain an optimal solution to this quantum statistical problem.

Finally we note that it is not difficult to include thermal control into this problem. The temperature of the environment is related to the value of  $\eta^6$  and one could treat  $\eta$  as a control parameter.

### 5. THE MAXIMUM ENTROPY FORMALISM

In the general discussion of the variational calculation in Section 3, we considered variations with respect to arbitrary density matrices. In this section we consider a more restricted set of variations which makes solving the equations of motion simpler.

We consider  $\{C_j\}$  to be the linearly independent set of self-adjoint operators that appear in Eq. (2.4). Thus the  $\{C_j\}$  spans the same space as  $\{1, A_j, A_j^2, j = 1, \dots, n\}$  (we shall set  $C_0 = 1$ ). Then we have

$$J = \sum_{j=0}^M k_j \langle C_j \rangle_f \tag{5.1}$$

We now restrict our states to those of the form  $\ln \rho = -\sum_{j=0}^M \lambda_j C_j$ . It is assumed that  $\rho(0)$  may be written in this form, so that if  $\rho(0) = e^{-(\mu + \beta H_0)}$  then there is a linear combination of the  $C_j$  which equals  $H_0$ .

The condition that  $\rho$  remains in the restricted subspace imposes constraints on the form of  $L(t)$ , the generator of the dynamical semigroup. The maximum entropy formalism provides a natural way to obtain an appropriate  $L$  from any given generator.<sup>(4,12)</sup> In this case, one obtains a set of ordinary, nonlinear, differential equations for the  $\{\lambda_j(t), j = 1, \dots, M\}$  or alternatively for the averages of the  $C_j$  with respect to the optimal density matrix. The density matrix itself now vanishes from the problem, which is reduced to a standard control theory problem.

### 6. SUMMARY AND CONCLUSIONS

We have presented a general formulation of the control problem for a class of quantum statistical systems. We have also shown how in some cases the problem can be reduced to the analog of a classical control

problem. It should be emphasized that the control problem of preparing an initial configuration is a finite time problem. This is in contrast to the theoretical extremes of the infinite-time, adiabatic preparation of an initial state familiar in scattering theory, and the instantaneous preparation of a state by means of a projection operator.

Although we have confined our discussion to Markovian systems, more general systems present "only" technical difficulties. Finally, we also note that the problem analyzed in this paper has application to the study of finite time measurements. In that case the properties of the initial state are to be determined by controlling a measuring device.

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