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Hamiltonian statistical mechanics

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Abstract
A framework for statistical-mechanical analysis of quantum Hamiltonians is introduced. The approach is based upon a gradient flow equation in the space of Hamiltonians such that the eigenvectors of the initial Hamiltonian evolve towards those of the reference Hamiltonian. The nonlinear double-bracket equation governing the flow is such that the eigenvalues of the initial Hamiltonian remain unperturbed. The space of Hamiltonians is foliated by compact invariant subspaces, which permits the construction of statistical distributions over the Hamiltonians. In two dimensions, an explicit dynamical model is introduced, wherein the density function on the space of Hamiltonians approaches an equilibrium state characterized by the canonical ensemble. This is used to compute quenched and annealed averages of quantum observables.

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(Some figures in this article are in colour only in the electronic version)

In the conventional approach to statistical mechanics the Hamiltonian of the system under consideration is held fixed. If the system is in equilibrium with a heat bath, then uncertainties in the state of the system arise from 'thermal noise' due to random interactions with the bath. The equilibrium distribution over the state space of the system (configuration space of a classical spin system, classical phase space or the space of pure quantum states) is then established. However, in some cases—as in amorphous alloys—the Hamiltonian need not be fixed, and may even fluctuate owing to thermal or other intrinsic sources. Observable effects arising from such Hamiltonians may even be significant in the quantum domain.

The purpose of the present communication is to introduce a theoretical framework for an equilibrium theory of Hamiltonians. The fact that parameters or matrix elements of the Hamiltonian themselves are subject to random fluctuations for some systems has long been recognized in the literature of spin glass [1] or random matrix theory [2]. The novel idea introduced here, as distinguished from that considered in the theory of spin glass or random matrices, is the construction of equilibrium distributions over *invariant subspaces of the space of quantum Hamiltonians* by using a gradient flow equation on the space of Hermitian matrices.

In classical statistical mechanics the notion of a gradient flow plays an important role in describing the approach to equilibrium: a system immersed in a heat bath naturally tends to

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release its energy into the environment and thus approach its minimum energy state, and this tendency is characterized by a Hamiltonian gradient flow. An equilibrium state is attained when this flow is on the average counterbalanced by thermal noise, where the magnitude of the noise is determined by the temperature of the bath. Accordingly, we shall introduce a *gradient flow equation* on the space of Hamiltonians such that the eigenstates of an arbitrary initial Hamiltonian H_0 at time $t = 0$ tend towards alignment with those of a reference Hamiltonian, denoted by G. Thus, G plays the role of the 'fixed' Hamiltonian in conventional quantum statistical mechanics. The eigenstates of H_t thus evolve towards those of G under the flow. By introducing of a suitable noise term, we then characterize the approach to an equilibrium distribution.

This communication is organized as follows. The key results concerning the properties of the double-bracket equation that generates the gradient flow are summarized first in the proposition. The notion of a double-bracket flow was first introduced by Landau and Lifshitz in the context of characterizing dispersions in magnetism [3]. In its 'modern form' it was introduced by Brockett [4] and has been successfully applied to many areas, such as optimal control, linear programming, sorting algorithms and dissipative systems. Although some assertions of the proposition are valid in all dimensions, we shall analyse only the two-dimensional case in full detail. We subsequently construct an explicit model for the 'equilibrization' of 2×2 quantum Hamiltonians, such that the stationary state is given by the canonical distribution. The resulting statistical theory of quantum Hamiltonians can be extended to a modification of quantum statistical mechanics. In particular, we work out the quenched and annealed averages of quantum observables. We conclude by indicating how the analysis can be extended to higher dimensions.

Proposition. *Let H_t and G be arbitrary 2×2 Hermitian matrices, where H_t is time dependent and G is fixed. Let H_t satisfy the double-bracket evolution equation*

$$\frac{\mathrm{d}H_t}{\mathrm{d}t} = -\lambda\,[H_t, [H_t, G]] \qquad (\lambda \in \mathbb{R}_+), \tag{1}$$

with initial condition H_0. Then the evolution (1) is isospectral, i.e. the eigenvalues of H_0 are preserved under (1), and $\lim_{t\to\infty}[H_t, G] = 0$. Furthermore, the space of Hermitian Hamiltonians is foliated by a family of invariant 2-spheres $\mathcal{L}$, and (1) induces a gradient flow on each $\mathcal{L}$.

We remark that in terms of the Hermitian operator $X = \mathrm{i}[H, G]$ the double-bracket evolution (1) can be rewritten as $\mathrm{d}H = \mathrm{i}\lambda[H, X]\,\mathrm{d}t$, which formally is just the Heisenberg equation of motion. However, owing to the H-dependence of X the evolution is nonunitary. We also note that in units $\hbar = 1$ the parameter λ has dimension [Energy]$^{-1}$. The Hamiltonians H_0 and G are both assumed nondegenerate; otherwise, if at least one of the Hamiltonians is degenerate, then H_0 is a fixed point of the flow. We now proceed to establish the proposition.

The fact that equation (1) asymptotically drives H_t towards $[H_t, G] = 0$, *irrespective of the dimensionality of the matrices*, follows from the relation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{tr}(H_t - G)^2 = -2\lambda\,\mathrm{tr}([G, H_t]^\dagger[G, H_t]) \leqslant 0, \tag{2}$$

where the equality is attained if and only if $[H_t, G] = 0$. To see that (1) defines an isospectral flow (which is also valid irrespective of the dimensionality of the matrices) we note that the right-hand side of (1) can be written in the form $\lambda\mathrm{d}(\mathrm{e}^{-\mathrm{i}sX}H_t\,\mathrm{e}^{\mathrm{i}sX})/\mathrm{d}s|_{s=0}$. The isospectral property then follows from the relation $\det(\mathrm{e}^{-\mathrm{i}sX}H_t\,\mathrm{e}^{\mathrm{i}sX} - E\mathbb{1}) = \det(H_t - E\mathbb{1})$. To prove that the orbit of the flow for a given initial value H_0 lies on a 2-sphere $\mathcal{L}$ (which is isomorphic to the space of pure states for a two-level system), and that (1) defines a gradient flow on $\mathcal{L}$, we shall solve (1) explicitly for the case of 2×2 Hermitian matrices.

Let the 2×2 Hamiltonian H_t be represented in terms of the Pauli matrices as

$$H_t = \tfrac{1}{2}u_t \mathbb{1} + \tfrac{1}{2}\nu \boldsymbol{\sigma} \cdot \mathbf{n}_t, \tag{3}$$

where $\mathbf{n}_t = (\mathrm{x}_t, \mathrm{y}_t, \mathrm{z}_t)$. Similarly for the reference Hamiltonian G we write

$$G = \tfrac{1}{2}\upsilon \mathbb{1} + \tfrac{1}{2}\mu \boldsymbol{\sigma} \cdot \mathbf{g} \tag{4}$$

for a unit vector $\mathbf{g}$. Bearing in mind the relations

$$\dot{u} \propto \mathrm{tr}[H_t, X] = 0 \qquad \text{and} \qquad [H_t, G] = \tfrac{1}{2}\mathrm{i}\nu\mu \boldsymbol{\sigma} \cdot (\mathbf{n}_t \times \mathbf{g}) \tag{5}$$

we find that (1) reduces to

$$\frac{\mathrm{d}\mathbf{n}_t}{\mathrm{d}t} = \omega \mathbf{n}_t \times (\mathbf{n}_t \times \mathbf{g}), \tag{6}$$

where $\omega = \lambda\nu\mu$. From

$$\frac{\mathrm{d}(\mathbf{n}_t \cdot \mathbf{n}_t)}{\mathrm{d}t} \propto \mathbf{n}_t \cdot (\mathbf{n}_t \times (\mathbf{n}_t \times \mathbf{g})) = 0 \tag{7}$$

we see that the norm of $\mathbf{n}_t$ remains constant under (6). Without loss of generality we work with the basis in which G is diagonal, and choose $\mathbf{g} = (0, 0, 1)$. In terms of the usual spherical parametrization in the G-basis we have $\mathbf{n}_t = (\sin\theta_t \cos\phi_t, \sin\theta_t \sin\phi_t, \cos\theta_t)$. Therefore, (6) reduces to

$$\dot{\theta}_t = \omega \sin\theta_t \qquad \text{and} \qquad \dot{\phi}_t = 0. \tag{8}$$

Solving these, we obtain

$$\cos\theta_t = \tanh(c_0 - \omega t) \qquad \text{and} \qquad \phi_t = \phi_0, \tag{9}$$

where $c_0 = \tanh^{-1}(\cos\theta_0)$ and ϕ_0 are initial values. The solution H_t to (1) is thus

$$H_t = \frac{1}{2}\begin{pmatrix} u_0 - \nu\tanh(\omega t - c_0) & \nu\,\mathrm{sech}(\omega t - c_0)\,\mathrm{e}^{-\mathrm{i}\phi_0} \\ \nu\,\mathrm{sech}(\omega t - c_0)\,\mathrm{e}^{\mathrm{i}\phi_0} & u_0 + \nu\tanh(\omega t - c_0) \end{pmatrix}. \tag{10}$$

A straightforward calculation shows that the eigenvalues of H_t are time independent, and that

$$\lim_{t\to\infty} H_t = \frac{1}{2}\begin{pmatrix} u_0 - \nu & 0 \\ 0 & u_0 + \nu \end{pmatrix}. \tag{11}$$

Thus, the Hamiltonian is asymptotically diagonalized in the G-basis. Observe that $\mathrm{tr}H_t$ and $\det H_t$ are conserved quantities. Therefore, the flow induced by (6) for fixed initial values u_0 and $|\mathbf{n}_0|$ is confined to a 2-sphere $\mathcal{L}$, which can be identified with the state space of a two-level system (i.e. the complex projective line). Since u_t and $|\mathbf{n}_t|$ are constant, in what follows we shall fix these two variables and focus our attention upon the associated sphere $\mathcal{L}$ parameterized by the dynamical coordinates (θ_t, ϕ_t).

The fact that (6) defines a gradient flow

$$\mathrm{d}x^a = -\tfrac{1}{2}\lambda\nu g^{ab}\nabla_b G(x)\,\mathrm{d}t \tag{12}$$

on $\mathcal{L}$, where we use local coordinates $(x^1, x^2) = (\theta, \phi)$ on the sphere, can be seen as follows. First, in terms of these coordinates the inverse metric on the sphere is

$$g^{ab} = \frac{4}{\sin^2\theta}\begin{pmatrix} \sin^2\theta & 0 \\ 0 & 1 \end{pmatrix}. \tag{13}$$

We define a function $G(x)$ on the sphere $\mathcal{L}$ as follows:

$$G(\theta, \phi) = \tfrac{1}{2}(\upsilon + \mu\cos\theta). \tag{14}$$

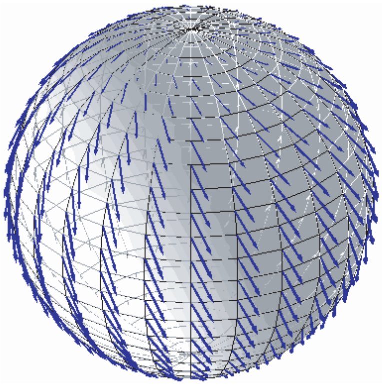

Figure 1. Flow on the sphere $\mathcal{L}$. The vector field generated by the unitarily-modified gradient flow (15) is plotted. The first term in (15) generates a rotation around the G-axis, while the second term generates geodesic flows towards the south pole. The axis $\mathbf{n}_0$ of the initial Hamiltonian H_0 spirals around the G-axis $\mathbf{g}$ and is asymptotically aligned with the latter.

This is obtained by taking the 'expectation' of reference Hamiltonian G in a pure state corresponding to the point (θ, ϕ) on $\mathcal{L}$. Then, a short calculation using (12), (13) and (14) shows that the dynamical equations (8) correspond to the gradient flow (12).

We remark, incidentally, that the dynamical equation (1) can be modified to include a unitary term

$$\frac{\mathrm{d}H_t}{\mathrm{d}t} = -\mathrm{i}[H_t, G] - \lambda\,[H_t, [H_t, G]]\,, \tag{15}$$

without greatly affecting its physical characteristics. In the 2×2 example considered here, the only change occurs in the phase, so that instead of $\phi_t = \phi_0$ we have $\phi_t = \phi_0 + \mu t$. Thus, according to (1) the eigenvectors of H_t evolve 'straight' towards those of G (i.e., along geodesics), whereas under (15) they 'spiral' towards those of G. This is illustrated in figure 1 where we plot the vector field on the sphere defined by the dynamical equation (15).

We also note that the diagonalization property of the double-bracket evolution (1) has been applied to the analysis of Toda lattices [5], dispersions in the Euler–Poincaré equations [6], couplings in photorefractive media [7], and flow equations in renormalization group [8]. Although here we consider the case in which G is fixed, it is possible to vary G in time (that is, vary the direction of $\mathbf{g}$). Then the dynamical equation (1) can be used to characterize *quantum control* (cf [9] for a related idea). In this context it would be interesting to investigate the role of *geometric phases for observables*, when the control Hamiltonian G is varied along a loop in $\mathcal{L}$.

Having defined a natural gradient flow on the invariant 2-spheres foliating the space of Hamiltonians, we now consider a dynamical model on a given sphere $\mathcal{L}$ such that an arbitrary initial Hamiltonian H_0 evolves—according to (1)—towards the reference frame determined by G, but at the same time is randomly perturbed in all directions in $\mathcal{L}$ by a pair of independent Brownian motions. The dynamical model, in particular, will possess the following properties: (i) the eigenvalues of H_t remain constant in time, and (ii) the probability distribution over $\mathcal{L}$ evolves towards an equilibrium distribution characterized by the standard canonical density function. Although rather elaborate, this model can be treated analytically by identifying any given surface of the foliation with the space of pure states of a two-level system, which permits application of the model for the thermalization of quantum states introduced in [10].

We consider first a stochastic differential equation of the form

$$\mathrm{d}x^a = \mu^a\,\mathrm{d}t + \kappa\sigma_i^a\,\mathrm{d}W_t^i \tag{16}$$

on $\mathcal{L}$ (viewed as a real 2-sphere). Here κ is a constant, the drift μ^a is a vector field on $\mathcal{L}$, and the vectors $\{\sigma_i^a\}_{i=1,2}$ constitute an orthonormal basis in the tangent space of $\mathcal{L}$ such that $g^{ab} = \sigma_i^a\sigma_j^b\delta^{ij}$ and $\sigma_i^a\sigma_j^b g_{ab} = \delta_{ij}$. We note that $\mathrm{d}x^a$ is the covariant Ito differential [11], and that the standard two-dimensional Wiener process $\{W_t^i\}$ satisfies $\mathrm{d}W_t^i\,\mathrm{d}W_t^j = \delta^{ij}\,\mathrm{d}t$. By straightforward calculation one verifies [10] that the density function $\rho_t(x)$ on $\mathcal{L}$ associated with the stochastic evolution (16) satisfies the Fokker–Planck equation

$$\frac{\partial}{\partial t}\rho_t(x) = -\nabla_a(\mu^a\rho_t) + \frac{1}{2}\kappa^2\nabla^2\rho_t. \tag{17}$$

For our model we require that the drift vector μ^a represents the double-bracket gradient flow (1). This is achieved by choosing $\mu^a = -\frac{1}{2}\kappa^2\lambda\nabla^a G$, where $\kappa^2 = \nu$. Then it follows from a theorem of Zeeman [12] that there exists a unique stationary solution to (17), given by the canonical density

$$\rho(x) = \frac{\exp(-\lambda G(x))}{\int_{\mathcal{P}}\exp(-\lambda G(x))\,\mathrm{d}V}. \tag{18}$$

To illustrate these results in more explicit terms we consider a system consisting of a single spin-$\frac{1}{2}$ particle immersed in an external magnetic field. The Hamiltonian is then $H = -\mathbf{B}\cdot\mathbf{S}$, where $\mathbf{B}$ denotes the field and $\mathbf{S}$ the spin vector. The direction of the field $\mathbf{B}$, however, is subject to fluctuations around its stable direction, specified by G (directed along the z-axis). Calculating the orthonormal basis σ_i^a on the sphere, we obtain the stochastic equations for the variables (θ,ϕ):

$$\begin{cases} \mathrm{d}\theta_t = \omega\sin\theta_t\,\mathrm{d}t + \sqrt{2\nu}\left(\mathrm{d}W_t^1 + \mathrm{d}W_t^2\right) \\ \mathrm{d}\phi_t = -\dfrac{1}{\sin\theta_t}\sqrt{2\nu}\left(\mathrm{d}W_t^1 - \mathrm{d}W_t^2\right). \end{cases} \tag{19}$$

The associated Fokker–Planck equation reads

$$\dot{\rho} = -\omega(\cos\theta + \sin\theta\,\partial_\theta)\rho + 2\nu\left(\partial_\theta^2 + \frac{1}{\sin^2\theta}\partial_\phi^2\right)\rho, \tag{20}$$

where $\partial_\theta = \partial/\partial\theta$ and $\partial_\phi = \partial/\partial\phi$. The asymptotic solution is the following canonical density function:

$$\rho(\theta,\phi) = \frac{\lambda\mu}{2\pi\sinh\left(\frac{1}{2}\lambda\mu\right)}\exp\left(-\frac{1}{2}\lambda\mu\cos\theta\right). \tag{21}$$

Direct substitution shows that (21) is the stationary solution to (20). It follows from (21) and the use of the spherical (Fubini-Study) volume element $\mathrm{d}V = \frac{1}{4}\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi$ that the equilibrium mean Hamiltonian is

$$\langle H\rangle = \frac{1}{2}\begin{pmatrix} u_0 + \nu\langle\cos\theta\rangle_\lambda & 0 \\ 0 & u_0 - \nu\langle\cos\theta\rangle_\lambda, \end{pmatrix}, \tag{22}$$

where $\langle\cos\theta\rangle_\lambda = 2/\lambda\mu - 1/\tanh\left(\frac{1}{2}\lambda\mu\right)$. We may regard the parameter λ as representing the 'inverse temperature' for the Hamiltonian: if the noise level is high ($\lambda \ll 1$), then the direction of the external field $\mathbf{B}$ on the average lies close to the xy-plane so that $\langle\cos\theta\rangle_\lambda \simeq 0$, whereas if the noise level is low $\lambda \gg 1$, then the field $\mathbf{B}$ on the average is parallel to the z-axis and we have $\langle\cos\theta\rangle_\lambda \simeq -1$.

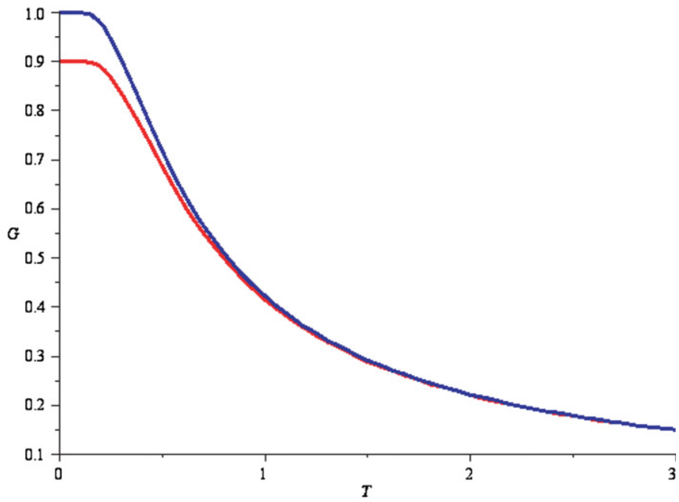

Figure 2. Quenched and annealed averages of G. The functions $\langle G\rangle_Q$ and $\langle G\rangle_A$ are plotted against the temperature $T = \beta^{-1}$, where we set $\lambda^{-1} = 0.1$, $\upsilon = 0$, $\nu = 1$ and $\mu = 2$ so that $G = \sigma_z$. The 'quenched magnetization' $\langle\sigma_z\rangle_Q$ does not attain the maximum value 1.0 at zero temperature unless $\lambda^{-1} = 0$.

Let us now consider how the statistical theory of Hamiltonians presented here can be applied to quantum statistical mechanics. In this context it is natural to borrow ideas from the spin glass literature [1]. We may take the averaged Hamiltonian $\langle H\rangle_\lambda$ as the starting point of the analysis—this gives the analogue of an *annealed* average. In this regime the expectation of an observable O is given by

$$\langle O\rangle_A = \frac{\mathrm{tr}(O\,\mathrm{e}^{-\beta\langle H\rangle_\lambda})}{\mathrm{tr}(\mathrm{e}^{-\beta\langle H\rangle_\lambda})}. \tag{23}$$

Such an expectation, however, will involve the use of the averaged Hamiltonian $\langle H\rangle_\lambda$ whose eigenvalues differ from those of H. Alternatively, we may use the 'unaveraged' Hamiltonian to compute the thermal expectation of an observable O, regarded as a function on a specified invariant surface in the above described foliation of the space of Hamiltonians, and then take its average—this gives the analogue of a *quenched* average:

$$\langle O\rangle_Q = \left\langle \frac{\mathrm{tr}(O\,\mathrm{e}^{-\beta H})}{\mathrm{tr}(\mathrm{e}^{-\beta H})}\right\rangle_\lambda. \tag{24}$$

A short calculation shows that the canonical quenched average of the Hamiltonian G is

$$\langle G\rangle_Q = \frac{1}{2}\mu\tanh\left(\frac{1}{2}\beta\nu\right)\left(\frac{1}{\tanh\left(\frac{1}{2}\lambda\mu\right)} - \frac{2}{\lambda\mu}\right), \tag{25}$$

whereas the canonical annealed average of G is

$$\langle G\rangle_A = \frac{1}{2}\mu\tanh\left[\frac{1}{2}\beta\nu\left(\frac{1}{\tanh\left(\frac{1}{2}\lambda\mu\right)} - \frac{2}{\lambda\mu}\right)\right]. \tag{26}$$

These averages are plotted in figure 2. These results suggest a new line of studies on the extended quantum statistical mechanics of disordered systems.

The explicit analysis presented above is for the most part confined to 2×2 systems. In higher dimensions, the double-bracket evolution equation (1) still defines an isospectral gradient flow in the space of Hamiltonians. Thus, the procedure for a statistical analysis of Hamiltonians as outlined above is naturally extendable to higher dimensions. However, in higher dimensions the equivalence of the Schrödinger and Heisenberg picture for the nonunitary motion (1) breaks down (that is to say, the generic surface foliating the space of Hamiltonians is not isomorphic to the associated space of pure states). Instead, in higher dimensions, the relevant foliation consists of certain subspaces of higher-dimensional spheres. Nevertheless, there exist unitary-invariant measures on these spaces, which can be used to formulate the theory in an analogous manner. In particular, the equilibrium state resulting from the thermalization dynamics remains canonical in the sense that it is proportional to the canonical density $\exp(-\lambda \mathrm{tr}(GH))$ just as in the 2×2 example (cf [13]). The remaining open problem is the precise geometrical description of the relevant gradient flows in higher dimensions, and the specification of the associated measures to calculate partition functions.

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