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An energy dispersion estimate

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Given the density operator ρ_1 as an initial value of a Hamiltonian motion that evolves in a time interval Δt to ρ_2. Then $\Delta t\,\Delta E$, ΔE being the energy dispersion (or energy uncertainty) of the motion, can be estimated from below by comparing the length of the Hamiltonian curve with a geodesic joining the initial and the final density operator The lengths are calculated in the Bures metric.

Let the curve of the density operators $t\mapsto\rho=\rho(t)$ be a solution of

$$i\hbar\dot\rho=[H,\rho],\quad H=H(t)\,, \tag{1}$$

and assume $\rho_j=\rho(t_j)$ for $j=1, 2$ with $t_1<t_2$. Using an idea of ref. [1] it is my aim to derive the a priori inequality

$$\int_{t_1}^{t_2}\sqrt{\operatorname{tr}\rho H^2-(\operatorname{tr}\rho H)^2}\,\mathrm{d}t\geqslant\hbar\gamma_{12}\,, \tag{2}$$

where

$$0\leqslant\gamma_{12}\leqslant\tfrac{1}{2}\pi\,,$$
$$\cos\gamma_{12}=\tau_{12}:=\operatorname{tr}\sqrt{\rho_1^{1/2}\rho_2\rho_1^{1/2}}\,. \tag{3}$$

The physical meaning of the quantity τ_{12} is as follows [2]: Let ψ_1 and ψ_2 be two pure vector states of a (possibly fictitious) larger quantum system and let their reduced density operators coincide with ρ_1 and ρ_2. Then $|\langle\psi_1,\psi_2\rangle|$ should be not larger than τ_{12}, and τ_{12} is the smallest number with that property. In short, τ_{12} is the supremum of $|\langle\psi_1,\psi_2\rangle|$ if the pair of unit vectors ψ_1 and ψ_2 runs through all possible simultaneous purifications of the pair ρ_1 and ρ_2.

In case the Hamiltonian is time independent, the expectation values $\bar E$ and $\bar{E^2}$ of H and H^2 are constants of motion and inequality (2) simplifies to

$$\Delta t\,\Delta E\geqslant\hbar\arccos\tau_{12}\,,$$
$$\Delta t=t_2-t_1,\quad\Delta E=\sqrt{\bar{E^2}-(\bar E)^2}\,. \tag{4}$$

A further important special case appears if $\rho(t)=|\varphi(t)\rangle\langle\varphi(t)|$ describes a curve of pure states which is a solution of a Schrödinger equation $i\hbar\dot\varphi=H\varphi$. Now eq. (4) looks like [3]

$$\Delta t\,\Delta E\geqslant\hbar\arccos|\langle\varphi(t_1),\varphi(t_2)\rangle|\,. \tag{5}$$

Finally, if $\varphi(t_1)$ and $\varphi(t_2)$ are orthogonal then the right-hand side of (5) takes its maximal value $\frac{1}{4}h$. This is a result of Anandan and Aharonov [1].

The *proof* of (2) and (3) is in two steps, and will be done for non-singular density operators. The general case follows by continuity.

The first step starts by lifting the curve of density operators into the Hilbert space of Hilbert–Schmidt operators, W, with scalar product

$$\langle W,W'\rangle=\operatorname{tr}W'W^*\,, \tag{6}$$

i.e. we purify this curve by an ansatz

$$t\mapsto W=W(t),\quad\text{with }\rho(t)=WW^*\,. \tag{7}$$

There is a gauge freedom $W(t)\to W(t)U(t)$ with arbitrary unitaries $U(t)$ for these purifications. The freedom can be diminished by choosing a curve (7) which is as short as possible in the metric given by the scalar product (6). This variational demand produces the parallelity condition [4–6]

$$W^*\dot W=\dot W^*W\,. \tag{8}$$

Eq. (8) can be satisfied, as shown in ref. [5], by a Schrödinger motion

$$i\hbar\dot{W}=HW-W\tilde{H},\quad \tilde{H}=\tilde{H}^*,\tag{9}$$

where

$$\tilde{H}=2W^*YW,\quad \text{with } H=\rho Y+Y\rho,\tag{10}$$

and the last equation uniquely determines an operator $Y=Y(t)$. Inserting (9) into (8) yields

$$2W^*HW=W^*W\tilde{H}+\tilde{H}W^*W.\tag{11}$$

As is easily seen (9) is compatible with (1) and implies in addition

$$i\hbar\frac{\partial}{\partial t}\tilde{\rho}=[\tilde{H},\tilde{\rho}],\quad \text{with } \tilde{\rho}=W^*W.\tag{12}$$

Now inserting (9) into $\langle\dot{W},\dot{W}\rangle$ and using (11) gives

$$\hbar^2\langle\dot{W},\dot{W}\rangle=\operatorname{tr}\rho H^2-\operatorname{tr}\tilde{\rho}\tilde{H}^2.\tag{13}$$

Taking the trace of (11) yields

$$\operatorname{tr}\tilde{\rho}\tilde{H}=\operatorname{tr}\rho H.\tag{14}$$

Taking this into account one gets by the help of the Schwarz inequality from (13) the relation

$$\operatorname{tr}\rho H^2-(\operatorname{tr}\rho H)^2\geqslant\hbar^2\langle\dot{W},\dot{W}\rangle,\tag{15}$$

with which step one of the proof is done.

The final step is in proving

$$\int_{t_1}^{t_2}\sqrt{\langle\dot{W},\dot{W}\rangle}\,dt\geqslant\gamma_{12},\tag{16}$$

which gives, together with (15), the desired inequality (2). This will be done by the aid of the Bures metrics [7]. To calculate the Bures distance between ρ_1 and ρ_2 one considers a general simultaneous purification

$$W_1=W(t_1)U_1,\quad W_2=W(t_2)U_2,\quad \rho_j=W_jW_j^*,\tag{17}$$

in order to get

$$\|\rho_2-\rho_1\|_{\text{Bures}}=\inf\sqrt{\langle W_1-W_2,W_1-W_2\rangle}=\sqrt{2-2\tau_{12}},\tag{18}$$

where the infimum runs through the unitaries U_1 and U_2. The τ_{12} is given by (3). The proof of (18) can be found in refs. [2,8]. Now let W_1 and W_2 be a pair of points on the unit sphere $\operatorname{tr}WW^*=1$. Its Hilbert space distance d equals $d=2\sin\frac{1}{2}\gamma$, where γ denotes the length of a geodesic arc on the unit sphere connecting W_1 and W_2. This follows because the geodesic arc is a part of a large circle on the unit sphere crossing W_1 and W_2. But the length of any curve on the unit sphere of the W-space connecting W_1 and W_2 cannot be shorter than γ. Therefore, having in mind (18) and (3), the left-hand side of (16) cannot be smaller than γ_{12}. However, γ_{12} fulfills

$$2\sin\tfrac{1}{2}\gamma_{12}=\sqrt{2-2\tau_{12}}=\|\rho_2-\rho_1\|_{\text{Bures}}\tag{19}$$

and this relation implies (3). This finishes the proof.

Remarks. (i) Appropriate changes of the operator H and the parameter t produce mathematically equivalent but physically different inequalities. As an example one may choose instead of H the projection of the angular momentum onto an axis and the rotation angle instead of the time parameter.

(ii) Under the condition (8) the right-hand side of (15) is equal to the line element of the Bures metric (up to the square of the Planck constant and restricted to the density operators). Defining G by

$$\dot{\rho}=\rho G+G\rho\tag{20}$$

according to refs. [5,9] one gets $\dot{W}=GW$ for curves satisfying the parallelity condition (8), and this gives

$$\left(\frac{ds}{dt}\right)^2_{\text{Bures}}=\operatorname{tr}\rho G^2=\tfrac{1}{2}\operatorname{tr}G\dot{\rho}.\tag{21}$$

Thus the inequality (15) can be rewritten as

$$\operatorname{tr}\rho H^2-(\operatorname{tr}\rho H)^2\geqslant\tfrac{1}{2}\hbar^2\operatorname{tr}G\dot{\rho}.\tag{22}$$

(iii) Restricting on pure states there is no need of the step one of the given proof. Furthermore, for pure states the metric of Bures is nothing but the Fubini–Study metric. Based on that the inequality (5), also in the form including time dependent Hamiltonians, has been derived already in ref. [3].

(iv) The square of τ_{12} as given by (3) has been called a (*generalized*) *transition probability* in ref. [2]. Using results of ref. [10] it could be shown in ref. [11] that the same expression results from a quite different definition given in ref. [12].

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