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LETTER TO THE EDITOR

A note on the Klein inequality

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Abstract. The Klein inequality is translated into a dynamical mechanism embedded in the quantum-Liouville equation $\forall t \in R$. The results can be stated for arbitrary convex (concave) measure functions with a certain entropy function as a special case.

Take an arbitrary convex ($\cap$) (concave $\cup$) function f defined on the interval [0, 1] and a density matrix ρ. Defining a new density matrix $\sigma = \mathrm{diag}(\rho)$, then by the Klein inequality (Wehrl 1978) it follows that

$$\mathrm{Tr}\, f(\rho) \underset{(\geqslant)}{\leqslant} \mathrm{Tr}\, f(\sigma). \tag{1}$$

Clearly

$$\mathrm{Tr}\, f(\sigma) = \sum_p f(\rho_{pp}) = S(t) \tag{2}$$

say. If at $t = t_1$, $\rho = \sigma(t_1)$ then $S(t)$ has a turning point there which is, in fact, independent of the dynamics according to (1). This result is well known (e.g. Tolman 1962a). However, what is apparently not appreciated is the nature of the mechanism in the dynamics that accounts for it. From (2) it follows that

$$\dot{S} = \sum_p f'(\rho_{pp})\dot{\rho}_{pp}$$

and

$$\ddot{S} = \sum_p [f''\dot{\rho}_{pp}^2 + f'\ddot{\rho}_{pp}]. \tag{3}$$

Putting

$$J_1 = \sum_p f''\dot{\rho}_{pp}^2$$

yields immediately

$$J_1 \underset{(\geqslant)}{\leqslant} 0 \qquad \forall t \in R \tag{4}$$

depending on the convexity of f. The standard quantum-Liouville equation (e.g. Tolman 1962b) gives the time evolution of $\dot{\rho}_{ij}$ in the form:

$$\dot{\rho}_{ij} = -\frac{\mathrm{i}}{\hbar}\sum_k (H_{ik}\rho_{kj} - \rho_{ik}H_{kj}) = -\frac{\mathrm{i}}{\hbar}[H, \rho]_{ij}. \tag{5}$$

Therefore, $\ddot{\rho}_{pp}$ for use in (3) is given by

$$\ddot{\rho}_{pp} = -\frac{\mathrm{i}}{\hbar}[\dot{H}, \rho]_{pp} - \frac{\mathrm{i}}{\hbar}[H, \dot{\rho}]_{pp}$$

$$= -\frac{\mathrm{i}}{\hbar}[\dot{H}, \rho]_{pp} - \frac{1}{\hbar^2}[H, [H, \rho]]_{pp} \tag{6}$$

where the matrix elements of the Hamiltonian may be time dependent. Putting $\rho = \sigma + \tau$ yields (6) in the final form:

$$\ddot{\rho}_{pp} = -\frac{\mathrm{i}}{\hbar}[\dot{H}, \tau]_{pp} - \frac{1}{\hbar^2}[H, [H, \sigma]]_{pp} - \frac{1}{\hbar^2}[H, [H, \tau]]_{pp}. \tag{7}$$

The middle contribution of (7) yields the following:

$$[H, [H, \sigma]]_{pp} = 2\sum_k H_{pk}H_{kp}\rho_{pp} - 2\sum_k H_{pk}H_{kp}\rho_{kk}.$$

Putting $H_{pk}H_{kp} = H_{pk}H^*_{pk} = \alpha^2_{pk}$ gives the result that

$$\sum_p f'(\rho_{pp})\ddot{\rho}_{pp} = \sum_p f'(\rho_{pp})\left(-\frac{\mathrm{i}}{\hbar}[\dot{H}, \tau]_{pp} - \frac{1}{\hbar^2}[H, [H, \tau]]_{pp}\right)$$

$$-\frac{2}{\hbar^2}\sum_{p,k}\{\rho_{pp}f'(\rho_{pp})\alpha^2_{pk} - \rho_{kk}f'(\rho_{pp})\alpha^2_{pk}\}$$

$$= J_2 + \Lambda. \tag{8}$$

From (8) Λ can be expressed in the alternative form as

$$\Lambda = -\frac{1}{\hbar^2}\sum_{p,k}\alpha^2_{pk}(\rho_{pp} - \rho_{kk})\left(\frac{\partial f(\rho_{pp})}{\partial \rho_{pp}} - \frac{\partial f(\rho_{kk})}{\partial \rho_{kk}}\right) \tag{9}$$

with the sign of Λ depending only on the convexity of f. Specifically

$$\Lambda \underset{(\leqslant)}{\geqslant} 0 \qquad \forall t \in R. \tag{10}$$

For the exact dynamics, the quantity S varies such that for any convex function the quantity Λ is a source term and for any concave function Λ is a sink term. Equation (9) is essentially identical in structure to the evolution of $\dot{S}$ obtained from a master equation for irreversible flow (van Kampen 1981). If at $t = t_1$, $\rho = \sigma(t_1)$ then $\dot{S}(t_1) = 0$ and $\ddot{S}(t_1) = \Lambda$. Hence the inequality (10) holds for the exact dynamics with the requirement that the Hamiltonian matrix is Hermitian. The evolution of the measure function $S(t)$ satisfies

$$\ddot{S}(t) = J_1(t) + J_2(t) + \Lambda(t) \tag{11}$$

and the Λ term is essentially responsible for the evolution of the Klein inequality with J_1 and Λ satisfying the inequalities (4) and (10) respectively. J_2 has no obvious sign interpretation. For the standard entropy measure ($f(x) = -x \ln x$) the quantity Λ is given by

$$\Lambda = \frac{1}{\hbar^2}\sum_{p,k}\alpha^2_{pk}(\rho_{pp} - \rho_{kk})\ln\frac{\rho_{pp}}{\rho_{kk}} \geqslant 0 \tag{12}$$

and only becomes zero under the condition that the ρ_{pp} are identical.

Wehrl (1978) has claimed that the concept of entropy does not appear in any equation of motion. Andrew (1984) has also made this point. This letter has shown that any convex (concave) function leads to a measure which separates out the dynamical interactions according to (11). The concept of entropy as defined by (2) with $f(x) = -x \ln x$ becomes a special case of (1) with an embedded source term of the form (12). In contrast to the quantum case, Tapp (1990) has shown that there are strong purely dynamical reasons why the function $\pm x \ln x$ is unique for the classical case.

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