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STATISTICAL MECHANICS OF NONLINEAR WAVE EQUATIONS

Dedicated to Fritz John on the occasion of his 80th birthday, with the wish that he may find something entertaining here, and in recognition of his deep influence on the subject of wave equations, stretching over more productive years than most of us can hope to see.

V. E. Zakharov asked the audience of the 6th I. G. Petrovskii Memorial Meeting of the Moscow Mathematical Society, January 1983, to explain the numerical observation that solutions of[1] $\Box Q + Q^3 = 0$ on the circle return (more or less) to their initial shape after an interlude of complicated motion. In classical mechanics, such returns are guaranteed by the existence of a (micro-) canonical measure which is invariant under the flow and of total mass $< \infty$[2], and so it was proposed to write the equation in the Hamiltonian format[3]

$$Q^\bullet = P = \partial H/\partial P, P^\bullet = Q'' - Q^3 = -\partial H/\partial Q$$

with

$$H = \int_0^1 \left[\frac{1}{2}P^2 + \frac{1}{2}(Q')^2 + \frac{1}{4}Q^4\right] dx$$

and to verify that the flow preserves the canonical ensemble based upon the "measure":

$$dM = e^{-H} d^\infty P d^\infty Q,$$

with a suitable interpretation of this object. Friedlander [1985] put forward such an explanation but it was over-complicated and, in part, mistaken. It is the purpose of the present paper to make this attractive

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[1] $\Box$ is the wave operator $\partial^2/\partial t^2 - \partial^2/\partial x^2$.

[2] This is the recurrence theorem of Poincaré [1912].

[3] $\bullet = \partial/\partial'$, $= \partial/\partial x \bullet$ $\partial/\partial P$ and $\partial/\partial Q$ are gradients in function space.

idea work for the more general wave equation $\Box Q + f(Q) = 0$ with odd "restoring" force[4] $f(Q)$ and energy

$$H = \int_0^1 \left[\frac{1}{2}P^2 + \frac{1}{2}(Q')^2 + F(Q)\right] dx.$$

in which $F(Q) = \int_0^Q f$, as for $f(Q) = Q^3$. The rest of the introduction sketches the contents of the paper under the following headings:
1. Canonical ensemble
2. The flow (with cutoff)
3. Alternating flows (with cutoff)
4. Invariance of canonical ensemble (with cutoff)
5. Cutoff removed
6. The whole line
7. Sinh-Gordon
8. Sine-Gordon
9. Metric transitivity

The section numbers and titles in the main text follow the same plan.

1.1. Canonical ensemble. The meaning of the formal expression $dM = e^{-H} d^\infty P d^\infty Q$ is simple: with the appropriate (infinite) normalizing constants,

$$e^{-H} d^\infty P d^\infty Q = \frac{e^{-(1/2)\int_0^1 P^2}}{(2\pi/0+)^{\infty/2}} d^\infty P \otimes \frac{e^{-(1/2)\int_0^1 (Q')^2}}{(2\pi 0+)^{\infty/2}} d^\infty Q \times e^{-\int_0^1 F(Q)},$$

in which the first piece is the law of white noise; the second is the law of (circular) Brownian motion; and the third is simply a density factor. Here is more detail. The first piece is an honest measure of total mass 1: it is the Gaussian measure on the Sobolev space H^{-1} with zero mean and correlation = the identity operator. The second piece is construed as for standard Brownian motion, except that $Q(0)$ and $Q(1)$ are identified (by conditioning) and this common value $Q(0) = Q(1) = h$ is distributed over the line according to Lebesgue measure dh :

$$\int_B \frac{e^{-(1/2)\int_0^1 (Q')^2}}{(2\pi 0+)^{\infty/2}} d^\infty Q = \int_{-\infty}^{\infty} P_{00}(Q + h \in B) dh.$$

[4]The adjective means that, like $Q^3, f(Q)$ has the same signature as Q.

where P_{00} is the law of Brownian motion, conditioned (tied) so that $Q(0) = 0 = Q(1)$. For example, if $x_0 = 0 < x_1 < \ldots < x_n < 1$ and $a_0 < b_0$ etc. are fixed, then the measure of

$$B = (Q : a_0 \leq Q(x_0) < b_0, a_1 \leq Q(x_1) < b_1, \ldots, a_n \leq Q(x_n) < b_n)$$

is

$$\int_{a_0}^{b_0} dQ_0 \int_{a_1}^{b_1} dQ_1 \ldots \int_{a_n}^{b_n} dQ_n$$

$$\frac{e^{-(Q_1-Q_0)^2/2(x_1-x_0)}}{\sqrt{2\pi(x_1-x_0)}} \frac{e^{-(Q_2-Q_1)^2/2(x_2-x_1)}}{\sqrt{2\pi(x_2-x_1)}} \cdots \frac{e^{-(Q_0-Q_n)^2/2(1-x_n)}}{\sqrt{2\pi(1-x_n)}}.$$

This is a perfectly fine measure on the space of continuous paths $x \in [0,1) \to Q(x)$ of period 1, only its total mass is $+\infty$. Note that $\int_0^1 (Q')^2 = \infty$ where the measure lives, so that neither $exp[-(1/2)\int(Q')^2]$, nor $(2\pi 0+)^{\infty/2}$, nor $d^\infty Q$ makes any sense by itself; only these three together are kosher. The third piece $exp[-\int F(Q)]$ makes perfect sense because the Brownian motion lives in $C[(0,1)$. The total mass $Z = \int dM$ may even be finite, depending on the strength of the restoring force $f(Q)$: indeed,[5]

$$Z = \int E_{00}\, exp[-\int_0^1 F(Q+h)]dh \leq \infty$$

according as $\int_0^\infty e^{-F(h)}dh$ is finite or not.

Proof. $Z/2 =^6 \int_0^\infty E_{00}\, exp[-\int_0^1 F(Q+h)]dh$ is split in two pieces according as $m = |Q|_\infty \leq h/2$ or not. The first piece contributes something between

$$\int_0^\infty e^{-F(3h/2)} P_{00}(m \leq h/2)dh \geq P_{00}(m \leq 1/2) \int_1^\infty e^{-F(3h/2)}dh$$

and

$$\int_0^\infty e^{-F(h/2)} P_{00}(m \leq h/2)dh \leq \int_0^\infty e^{-F(h/2)}dh;$$

[5] E_{00} is the tied Brownian expectation.

[6] $Q \to -Q$ preserves P_{00} and $F(Q)$ is even, so $0 \leq h < \infty$ suffices.

the second is neglected in view of $P_{00}(m > h/2) \le aexp(-bh^2)$ for suitable $ab > 0$.

The bulk of the paper is devoted to proving that $dM = e^{-H} d^\infty P d^\infty Q$ is invariant under the flow of $\Box Q + f(Q) = 0$. The odd function $f(Q)$ is taken to be of class C^1 (with corners if you like) and $\ge kQ$ for a suitable constant $k > 0$ and big $Q \ge 0$ so that $F(Q) \ge kQ^2/2$ far out or nearly so and $Z < \infty$; for simplicity, $k = 1$ below.

1.2–1.4. Flows/invariance of canonical ensenble (with cutoff). The existence of the flow in the canonical ensemble must be established before anything else. This is easy if $f(Q)$ has bounded slope. The flow may be interpreted in an integrated form and its existence confirmed by a self-evident fixed-point argument, applicable not only to nice data, but to the unpleasant data of the canonical ensemble as well. It is convenient to bring into evidence the fact that $f(Q) \ge Q$ by writing $f(Q) + Q$ in its place. Then $\Box Q + Q + f(Q) = 0$ is expressed by means of the vector field

$$X : \begin{bmatrix} Q \\ P \end{bmatrix} \to \begin{bmatrix} P \\ Q'' - Q - f(Q) \end{bmatrix}$$

is the formal sum of two fields.

$$X_0 : \begin{bmatrix} Q \\ P \end{bmatrix} \to \begin{bmatrix} P \\ Q'' \quad -Q \end{bmatrix} \text{ and } X_* : \begin{bmatrix} Q \\ P \end{bmatrix} \to \begin{bmatrix} 0 \\ -f(Q) \end{bmatrix}$$

with the advantage over X that the associated flows may be computed explicitly: with $\Delta = \sqrt{1 - D^2}$,

$$e^{tX_0} \begin{bmatrix} Q \\ P \end{bmatrix} = \begin{bmatrix} \cos \Delta t & \Delta^{-1} \sin \Delta t \\ -\Delta \sin \Delta t & \cos \Delta t \end{bmatrix} \begin{bmatrix} Q \\ P \end{bmatrix}$$

$$\text{and } e^{tX_*} \begin{bmatrix} Q \\ P \end{bmatrix} = \begin{bmatrix} Q \\ P - tf(Q) \end{bmatrix}.$$

The canonical measure $dM = e^{-H} d^\infty P d^\infty Q$ is now expressed as

$$\frac{e^{-(1/2)\int P^2}}{(2\pi/0+)^{\infty/2}} d^\infty P \otimes \frac{e^{-(1/2)\int[(Q')^2+Q^2]}}{(2\pi 0+)^{\infty/2}} d^\infty Q \times e^{-\int F(Q)} = e^{-\int F(Q)} dM_0,$$

with the new $F(Q) =$ the old $F(Q) - Q^2/2$, and it is easy to see that the first (Klein–Gordon) flow preserves dM_0 : indeed, if P and Q are so distributed, i.e., P white and Q circular Ornstein-Uhlenbeck, then P and ΔQ are white and independent, and this is maintained by the flow

$$e^{tX_0} \begin{bmatrix} \Delta Q \\ P \end{bmatrix} \to \begin{bmatrix} \cos & \sin \\ -\sin & \cos \end{bmatrix} (\Delta t) \begin{bmatrix} \Delta Q \\ P \end{bmatrix}$$

since the matrix belongs to $S0(2)$, i.e., the flow preserves M up to a change in the density

$$exp[-\int F(Q)] \to exp[-\int F(e^{tX_0}Q)].$$

The second flow fixes Q and so also M, up to a change of the white factor in accordance with the rule of Cameron–Martin [1945]: formally, and also in truth[7]

$$\frac{e^{-(1/2)\int P^2}}{(2\pi/0+)^{\infty/2}} d^\infty P \to \frac{e^{-(1/2)\int P^2}}{(2\pi/0+)^{\infty/2}} d^\infty P \times e^{t\int f(Q)P-(t^2/2)\int f^2(Q)}.$$

In short, each flow distorts the canonical measure in its own simple way, and these distortions cancel more or less, as can be seen from the formal development

$$exp[-\int F(e^{tX_0}Q)] = exp[-\int F(\cos \Delta t Q + \Delta^{-1} \sin \Delta t P)]$$

$$= exp[-\int F(Q) - t\int f(Q)P + 0(t^2)]$$

leaving a total distortion, due to the application of $e^{tX_*}e^{tX_0}$, in the amount $1+o(t)$ for small values of t. But now $(e^{hX_0}e^{hX_*})^N$ approximates e^{TX} for $hN = T + o(1)$ and distorts M in the amount $[1+o(h)]^N \cong 1$. In this way, the true invariance of the canonical measure is proved (with cutoff).

1.5. Cutiff removed. For the general force $f(Q)$, the existence of the flow and the invariance of the canonical ensemble under it are proved by a Borel-Cantelli trick. Introduce the cutoff force with bounded slope so that $F_n(Q) = \int_0^Q f_n$ increases to the true $F(Q) = \int_0^Q f$ and $F_n(Q) = F(Q)$ for $|Q| \leq n$, let M_0 be the (white) $\times(OU)$ measure, as before, and note that it has total mass $Z_0 < \infty$. Then $dM_n = exp[-\int F_n(Q)]dM_0$ is invariant under the flow e^{tX_n} for $\Box Q + f_n(Q) = 0$ and exceeds the canonical measure $dM_\infty = exp[-\int F(Q)]dM_0$. Fix $T < \infty$. Then[8]

$$M_\infty \left[\max_{t\leq T}|e^{tX_n}Q|_\infty \geq n\right] \leq M_n[ditto] \leq \frac{T}{n}\int\int_0^1 |Q|dM_0 + o(\frac{1}{n})$$

[7] $\int f(Q)P$ is the Brownian integral; it makes sense because Q is independent of P.
[8] $e^{tX_n}Q(x)$ is continuous, jointly in t and x.

as simple estimates confirm, so, by the cheap half of the Borel-Cantelli lemma, the nth flow does not feel the cutoff before time T if n is sufficiently big, the actual level n required being dependent upon the data QP, with exceptions of measure 0. This leads at once to the existence of the flow in the canonical ensemble and to the invariance of the latter under the former in full generality. It is germane to remark that current (nonstatistical) proofs of the existence of the flow fail because they rely upon $H < \infty$ which is nowhere verified in the canonical ansemble: compare STRAUSS [1970] for the state of the art.

1.6. The whole line[9]. The (normalized) canonical ensemble can be formed for the circle of any perimeter L, and it is interesting to see what happens as $L \uparrow \infty$. The discussion is facilitated by a well-known trick. Let ψ_0 the groundstate of $Q_0 = -(1/2)d^2/dQ^2 + F(Q)$ and put $m = \psi_0'/\psi_0$. Then the Q-part of dM is nothing but the law

$$\frac{e^{-(1/2)\int_0^1 (Q')^2}}{(2\pi 0+)^{\infty/2}} d^\infty Q \times e^{\int_0^1 m dQ - (1/2)\int_0^1 m^2 dx}.$$

of the (circular) diffusion with infinitesimal operator $\mathcal{G} = (1/2)d^2/dQ^2 + m(Q)d/dQ$ up to a constant factor washed out by the normalization, and, for $L = \infty, P$ is still white but now Q is an independent copy of stationary diffusion with infinitesimal operator $\mathcal{G}$. This ensemble is invariant under the flow, the existence of the latter being immediate from the fact that $\Box Q + f(Q) = 0$ propagates at speed 1. This diffusion format also provides a nice formal insight into why the canonical ensemble is invariant. $P = a$ is white and $Q' = b + m(Q)$ with an independent white noise b. Now[10]

$$a^\bullet = Q'' - f(Q) = b' + m'(Q)Q' + \frac{1}{2}m''(Q) - \frac{1}{2}m''(Q) - mm'(Q) = b' + m'(Q)b$$

and

$$b^\bullet = [Q' - m(Q)]^\bullet = P' - m'(Q)P = a' - m'(Q)a,$$

i.e.,

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} D + \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} m'(Q) : \begin{bmatrix} a \\ b \end{bmatrix} \to \begin{bmatrix} a^\bullet \\ b^\bullet \end{bmatrix},$$

and this map is skew, which is to say it is an infinitessimal rotation, preserving the statistical character of a and b.

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[9] The original notation is used: $f(Q)$ is the full restoring force.

[10] $dm(Q) = m'(Q)dQ + (1/2)m''(Q)(dQ)^2$ and $(dQ)^2 = dx$, by Ito's lemma. $f(Q) = (1/2)(m' + m^2)'$.

1.7–1.8. Special example.

$$1) \text{ sinh-GORDON:} \quad \Box Q + \sinh Q = 0,$$
$$2) \text{ sine-GORDON:} \quad \Box Q + \sin Q = 0.$$

1) is a wave equation of the kind considered before, but with the extra feature of complete integrability so that it has many (additive) constants of motion[11] which can be used to form additional (diffusion-type) canonical ensembles invariant under the flow. This is an artefact of integrability alone, having *nothing to do with change of phase; esp.* the several canonical measures so produced live in different parts of function space. The situation is compared to the results of Chulaevskii [1983] and Gurevich [1986/90]. Gurevich [1986] conjectured that extra Gibbs states arise in classical mechanics only from extra "additive" constants of motion. The adjective means that the integral I splits into a sum I (class 1) + I (class 2), or nearly so, if the particles fall into two classes at a large distance, one from the other. Gurevich [1990] then proved the following remarkable fact: if[12] $H = P^2/2 + \sum_{i<j} U(|Q_i - Q_j|)$ with smooth potential $U(r)$ varying between $+\infty$ at $r = 0+$ to 0 at $r = +\infty$, then nonclassical additive constants of motion are present only if $d = 1$, and then only for the Calogero-Moser potentials $U(r) = r^{-2}$ and $U(r) = sh^{-2}r$. Ya. G. Sinai conjectured and V. A. Chulaevskii [1983] proved that, in fact, CM with an infinite number of degrees of freedom enjoys additional Gibbs states. The parallel conjecture would be that $\Box Q + f(Q) = 0$ with odd restoring force has nonclassical (additive) constants of motion only if $f(Q) = Q$ or $f(Q) = shQ$. Note the rule of inverse squares: $Q \to r^{-2}$ and $shQ \to sh^{-2}r$, whatever that means! 2) is also integrable and so exhibits the same phenomenon.

1.9. Metric transitivity. This issue arises in connection with GUREVICH [1986/90]. It is conjectured that, for the wave equation $\Box Q + f(Q) = 0$ with odd restoring force, the flow is always metrically transitive if $L = \infty$, and likewise if $L < \infty$ unless $f(Q) = Q$ or $f(Q) = shQ$. The former statement is made plausible by the hope that, for $t \uparrow \infty$ and any fixed interval $-\infty < a \le x \le b < \infty, e^{tX}QP(x) : a \le x \le b$ should depend less and less upon the data $QP(x) : a' \le x \le b'$ in any other

[11] The basic Hamiltonian $H = \frac{1}{2}\int[P^2 + (Q')^2] + \int(chQ - 1)$ illustrates the idea of additivity: $H(QP) = H(Q_1P_1) + H(Q_2P_2)$ if Q_1P_1 and Q_2P_2 live in disjoint parts of the line.

[12] $PQ \in (R^d)^n$ are classical coordinates for n d-dimensional particles.

fixed interval. Then any invariant function such as[13]

$$H(QP) = \lim_{T\uparrow\infty} \frac{1}{T} \int_0^T e^{tX} I(QP)dt$$

would be measurable over the (spatial) tail field of QP and, as P is white and Q is mixing, so this field is trivial, i.e., H is constant, as metric transitivity would have it.

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[13] $e^X I(GP) = I(e^X GP)$.