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Cubic Schrödinger: The Petit Canonical Ensemble

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§1. Introduction

This report describes some aspects of the Gibbsian petit canonical ensemble for the cubic Schrödinger equation in the space of functions of period 1, say. $\S2-5$ (defocussing case) represent joint work with K. Vaninsky¹). $\S6$ is a brief report on the much more difficult focussing case. The original hope, that the petit ensemble might provide a picture of the typical solution, is far from being achieved.

1.1. $Preliminaries^{2}$

The mechanical state is a pair QP of nice functions of period 1, moving according to the defocussing flow:

$$rac{\partial Q}{\partial t} = -rac{\partial^2 P}{\partial x^2} + (Q^2 + P^2) P = rac{\partial H_3}{\partial P}$$

 $rac{\partial P}{\partial t} = +rac{\partial^2 Q}{\partial x^2} - (Q^2 + P^2) Q = -rac{\partial H_3}{\partial Q}$

This is a Hamiltonian system, relative to the classical bracket in function space, with Hamiltonian

$$H_{3} = \frac{1}{2} \int_{0}^{1} \left[\left(Q' \right)^{2} + \left(P' \right)^{2} \right] + \frac{1}{4} \int_{0}^{1} \left(Q^{2} + P^{2} \right).$$

It is integrable in the full technical sense of the word, having an infinite series of (commuting) constants of motion $H_1 = \frac{1}{2} \int_0^1 (Q^2 + P^2)$, $H_2 = \int_0^1 Q'P$, H_3 , and so on. The flow is integrated with the help of the Dirac equation

$$M' = \begin{bmatrix} \begin{pmatrix} Q & P \\ P & -Q \end{pmatrix} + \frac{\lambda}{2} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \end{bmatrix} M$$

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¹⁾ McKean-Vaninsky [1997]

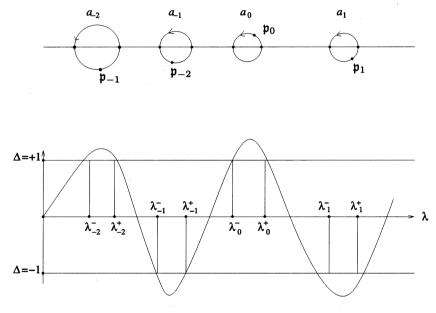
²⁾ Manakov et al. [1984] and/or McKean-Vaninsky [1997]

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for the 2 × 2 monodromy matrix $M = [m_{ij} : 1 < i, j \leq 2]$ with M(x = 0) = I. Introduce the "discriminant" $\Delta(\lambda) = \frac{1}{2} sp M(x = 1)$ and the associated "Dirac curve" \mathfrak{M} with points $\mathfrak{p} = [\lambda, \sqrt{\Delta^2(\lambda) - 1}]$. The latter is a double cover of the complex plane where λ lives, ramified over the roots

 $\dots \lambda_{-1}^{-} \leq \lambda_{-1}^{+} < \lambda_{-1}^{-} \leq \lambda_{-1}^{+} < \lambda_{0}^{-} \leq \lambda_{0}^{+} < \lambda_{1}^{-} \leq \lambda_{1}^{+} < \dots, \lambda_{n}^{\pm} \simeq 2\pi n \quad etc.$ of $\Delta(\lambda) = \pm 1$ indicated in the figure. These comprise the periodic/anti-

periodic spectrum of the Dirac equation and may be interpreted as a



complete list of constants of motion, commuting among themselves and with the prior constants, H_1, H_2, H_3 , etc. The cycles $a_n : n \in \mathbb{Z}$ seen in the upper part of the figure are the "real ovals" of \mathfrak{M} covering the "gaps" $[\lambda_n^-, \lambda_n^+]$, these being all open for QP in general position, as is mostly assumed below. QP is encoded into a divisor $\mathfrak{P} = [\mathfrak{p}_n : n \in \mathbb{Z}]$ of \mathfrak{M} having 1 point on each real oval: the numbers $\lambda(\mathfrak{p}_n) \equiv \mu_n \in [\lambda_n^-, \lambda_n^+]$ are the roots of $m_{12}(\mu) = 0^{3}$ and the radical $\sqrt{\Delta^2 - 1}(\mathfrak{p}_n)$ is declared to be $\frac{1}{2}(m_{11} - m_{12})(\mu_n)^{4}$. The map $QP \to \mathfrak{P}$ is 1:1 or to the product

³⁾ $m_{12}(\lambda)$ looks much like $-\sin(\lambda/2)$.

⁴⁾ det M(1) = 1 so $m_{11} m_{12} = 1$ if $m_{12} = 0$ and $m_{11} + m_{12} = 2\Delta$ always, whence this possibility.

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of all the ovals. The next actor in the play is the "Abel map" of the divisor into the (real) Jacobi variety Jac of \mathfrak{M} , determined as follows. DFK = the "differentials of the first kind" of \mathfrak{M} are of the form $\omega = \phi_n(\lambda) d\lambda / \sqrt{\Delta^2(\lambda) - 1}$ with certain entire functions ϕ , and a basis may be chosen so that $a_i(\omega_j) = 2\pi$ or 0 according as i = j or not.⁵⁾ \mathfrak{P} is now mapped to Jac via the "angles" $\theta_n = \sum_{k \in \mathbb{Z}} \int_{\mathfrak{o}_k}^{\mathfrak{p}_k} \omega_n$ construed mod 2π ,⁶⁾ *i.e.*

$$\mathfrak{P} o \Theta = [heta_n : n \in \mathbb{Z}] \in (\mathbb{R}/2\pi \, \mathbb{Z})^\infty = \, \operatorname{Jac},$$

and this map likewise is 1:1 and onto. Now you have the composite map $QP \rightarrow \text{divisor} \rightarrow \text{Jac}$, the point of the whole exercise being that the (complicated) flow of QP is converted thereby into (simple) straight-line motion at constant speed in Jac which may be mapped back to the original (mechanical) variables with the help of a Riemann-like "theta" function. In this way, the flow is "integrated".

§2. Petit Ensemble at Levels 1 & 3

Level 1 is a warm-up for "level 3" to be described below. Introduce the "level 1 actions" $I_n = \frac{1}{4\pi} a_n (ch^{-1} \Delta, d\lambda)^{7}$ and note the trace formula $H_1 = \frac{1}{2} \int (Q^2 + P^2) = \sum_{\mathbb{Z}} I_n$. The petit ensemble⁸⁾

$$e^{-H_1} d^{\infty} Q \, d^{\infty} P = \frac{e^{-\frac{1}{2} \int_0^1 Q^2}}{(2\pi/0_+)^{\infty/2}} d^{\infty} Q \times \frac{e^{-\frac{1}{2} \int_0^1 P^2}}{(2\pi/0_+)^{\infty/2}} \, d^{\infty} P$$
$$= \prod_{\mathbb{Z}} e^{-I_n} \, dI_n \times \prod_{\mathbb{Z}} d\theta_n / 2\pi :$$

is descriptive of 2 independent copies of white noise; line 2 comes from the trace formula plus the formal identification of the volume elements $d^{\infty}Q d^{\infty}P \& d^{\infty}I d^{\infty}\theta/2\pi$ prompted by the fact that actions & angles are canonically conjugate and together form a full coordinate system in QP-space. Naturally, line 2 requires proof as does the invariance of the ensemble under the flow, for which see McKean-Vaninsky [1997].

⁷⁾ The name will be justified in ^{§4}.

⁸⁾ Here and below, I will be free and easy with possibly infinite norming constants.

⁵⁾ I should say differentials of the third kind as they have simple poles at the 2 points of \mathfrak{M} covering ∞ , but as they play the role of classical DFK, I keep the name. $\phi_n(\lambda)$ looks much like $m_{12}(\lambda)$ divided by $\lambda - \mu$, *i.e.* with 1 root left out.

⁶⁾ $\mathfrak{o}_k = [\lambda_k^-, 0]$, some such choice being necessary for the convergence of the sum.

Level 3. The petit ensemble at "level 3":

$$e^{-H_3} d^{\infty}Q d^{\infty}P = \frac{e^{-\frac{1}{2}\int_0^1 (Q')^2}}{(2\pi 0_+)^{\infty/2}} d^{\infty}Q \frac{e^{-\frac{1}{2}\int_0^1 (P')^2}}{(2\pi 0_+)^{\infty/2}} d^{\infty}P \times e^{-\frac{1}{4}\int_0^1 (Q^2 + P^2)^2}$$

is descriptive of 2 independent "circular" Brownian motions⁹⁾ coupled by the third factor; it is invariant under the flow as for level 1. To describe it in•action/angle language requires a revision: DFK at level 3 is as before (level 1) but with a new basis $\omega'_n : n \in \mathbb{Z}$ normalized as in $a_i(\lambda^2 \omega'_j) = 2\pi$ or 0 according as i = j or not. The level 3 actions are $I'_n = \frac{1}{q_\pi} a_n(\lambda^2 ch^{-1} \Delta d\lambda)$ and you have the trace formula $H_3 = \sum_{\mathbb{Z}} I'_n$, whence

$$e^{-H_3} d^{\infty} Q \, d^{\infty} P = \prod_{\mathbb{Z}} e^{-I'_n} \times \left[d^{\infty} Q d^{\infty} P = d^{\infty} I \, d^{\infty} \frac{d\theta}{2\pi} \text{ at level } 1 \right]$$

= $\prod_{\mathbb{Z}} e^{-I'_n} \, dI'_n \prod_{\mathbb{Z}} d \, \frac{\theta_n}{2\pi} \times \det \frac{\partial I}{\partial I'} ,$

in which the third (Jacobian) factor is still to be understood. The level 3 actions are canonically paired to the level 3 angles¹⁰) $\theta'_n = \sum_{r \in \mathbb{Z}} \int_{\mathfrak{o}_k}^{\mathfrak{p}_k} \omega'_n$, so

$$\det \frac{\partial I}{\partial I'} = \det \frac{\partial \theta'}{\partial \theta} = \frac{\det \left[\omega'_i / d\lambda(\mathfrak{p}_j) \right]}{\det \left[\omega_i / d\lambda(\mathfrak{p}_j) \right]} \times \int \frac{\det \prod_{i>j} (\mu_i - \mu_j)}{\prod_{\mathbb{Z}} \sqrt{\Delta^2 - 1(\mathfrak{p}_n)}} d^{\infty} \mu divided by \int \prod_{\mathbb{Z}} \mu^2 \times \text{ the same "volume element".}$$

This rather fanciful expression comes from level 2 in case all but N gaps are closed and making $N \uparrow \infty$ with an (unpardonable) disregard of normalizing factors. Now the "volume element" seen in line 3 is

⁹⁾ CBM is standard Brownian motion, conditioned to end where it began, with this common displacement distributed over \mathbb{R} by flat Lebesgue measure. The coupling holds down the total mass so that normalization is possible.

¹⁰⁾ These must be construed, not $mod 2\pi$, but relative to another, pretty complicated lattice of periods.

nothing but an un-normalized expression of the flat (level 1) volume element $d^{\infty}\theta/2\pi$ on Jac, written out in the language of the divisor; also $m_{12}(\lambda) = \frac{1}{2} (\mu_0 - \lambda) \prod_{\mathbb{Z}} (2\pi n)^{-1} (\mu_n - \lambda)$ precisely; and so it is an educated guess that, after proper normalization, the Jacobian det $\partial I/\partial I'$ ought to be the reciprocal of $N = \int_{Jac} m_{12}^2(0) d^{\infty} \theta/2\pi$.

This is correct as far as it $goes^{11}$, but what does N really look like? It is a function of actions alone, so the level 1 angles are still independent of them, with the same flat distribution as before. There are 10 integrals of products of 2 entries of M(1), and I know 9 relations among them involving the constants of motion Δ and Δ^{\bullet} , but the value of N is not revealed by these. Too bad! Crude estimates of N can be had but do not help to describe how the actions couple. I leave the subject in this unsatisfactory state.

§3. Some Tricks

I record here 3 amusing examples of averaging over Jac with respect to $d^{\infty}\theta/2\pi$, but first a general principle. Think of the (still to be normalized) expression

$$d^{\infty} \, rac{ heta}{2\pi} = \prod_{i>j} \left(\mu_i - \mu_j
ight) d^{\infty} \mu \, ext{divided by } \prod_{\mathbb{Z}} \sqrt{\Delta^2 - 1} \; (\mathfrak{p}_n)$$

encountered in §3. The top, considered as a function of μ_n , say, is proportional to $m_{12}^{\bullet}(\mu_n)$, so you have the "splitting rule at $n \in \mathbb{Z}$ ":

$$d^\infty rac{ heta}{2\pi} = rac{m_{12}^ullet(\mu_n)}{\sqrt{\Delta^2-1}\,(m{\mathfrak{p}}_n)} \quad ext{on the oval } a_n$$

 \times a volume element on the product of all the other ovals.

This principle is now applied in 3 ways:

Example 1. $m_{12}(\lambda)$ looks like $-\sin(\lambda/2)$ and $\Delta(\lambda)$ like $\cos(\lambda/2)$, so you may expect $2\Delta^{\bullet} - m_{12}$ to be of "degree 1 lower" than m_{12} and that Lagrange interpolation would apply. This is correct:

$$2\Delta^{\bullet}(\lambda) - m_{12}(\lambda) = {}^{12)}\sum_{\mathbb{Z}} \frac{2\Delta^{\bullet}(\mu_n)}{m_{12}^{\bullet}(\mu_n)} \frac{m_{12}(\lambda)}{\lambda - \mu_n}$$

¹¹⁾ McKean-Vaninsky [1997].

¹²⁾ $m_{12}(\mu_n) = 0$ of course.

Now average over Jac, exchange sum and average, and split the volume at $n\in\mathbb{Z}$ to produce

$$2\Delta^{\bullet}(\lambda) - \int_{\text{Jac}} m_{12}(\lambda) \, \frac{d^{\infty}\theta}{2\pi} = \sum_{\mathbb{Z}} 2 \int_{\substack{\lambda = a_k \\ k \neq n}} \frac{m_{12}(\lambda)}{\lambda - \mu_n} \int_{a_n} \frac{\Delta^{\bullet} d\mu_n}{\sqrt{\Delta^2 - 1}} = {}^{13)}0,$$

i.e. $2\Delta^{\bullet} = \text{average } m_{12}$.

Example 2. The numerator ϕ_n of $\omega_n \in \text{DFK}$ at level 1 looks like m_{12} with 1 root factored out, so it, too, should be capable of interpolation:

$$\phi_n(\lambda) = \sum_{i \in \mathbb{Z}} rac{\phi(\mu_i)}{m_{12}^ullet(\mu_i)} rac{m_{12}^ullet(\lambda)}{\lambda - \mu_i} \; .$$

But this object has nothing to do with angles, so an average over Jac does it no harm, and proceeding as in ex. 1, you find

$$\begin{split} \phi_n(\lambda) &= \sum_{\substack{i \in \mathbb{Z} \\ j \neq i}} \int_{\substack{\lambda = \mu_i \\ j \neq i}} \frac{m_{12}(\lambda)}{\lambda - \mu_i} \int_{a_i} \frac{\phi_n(\mu_i) \, d\mu_i}{\sqrt{\Delta^2 - 1}} (\mathfrak{p}_i) \\ &= \int_{\substack{\lambda = \mu_i \\ j \neq n}} \frac{m_{12}(\lambda)}{\lambda - \mu_n} \times 2\pi \\ &= \int_{\substack{\lambda = \mu_i \\ \lambda = \mu_i}} \frac{m_{12}(\lambda)}{m_{12}^{\bullet}(\mu_n)(\lambda - \mu_n)} \, d^{\infty} \, \frac{\theta}{2\pi} \end{split}$$

divided by

$$\frac{1}{2\pi} \int\limits_{a_n} \frac{d\mu}{\sqrt{\Delta^2 - 1}} \; :$$

i.e.

$$\omega_n = - ext{average} - rac{m_{12}(\lambda)}{m_{12}^{ullet}(\mu_n)(\lambda - \mu_n)} ext{ normalized to have mass } 2\pi ext{ on } a_n ext{ .}$$

This seems to be a new way of writing DFK.

¹³⁾ $\Delta^{\bullet}/\sqrt{\Delta^2 - 1} = d ch^{-1} \Delta.$

Example 3 identifies $I_n = \frac{1}{4\pi} a_n (ch^{-1} \Delta d\lambda)$ with a true mechanical action, as promised at start of §3.¹⁴ The physical actions are $A_n = (2\pi)^{-1}a_n(PdQ) : n \in \mathbb{Z}$. To implement their evaluation, take the flow $e^{t\mathbb{X}}$ with Hamiltonian I_n which carries \mathfrak{p}_n once about its private cycle a_n in time 2π , leaving the rest of the divisor fixed, and equate A_n with

$$\frac{1}{2\pi}\int_0^{2\pi}e^{t\mathbb{X}}\left[\int_0^1 P(x)\,\mathbb{X}\,Q(x)\,dx\right]dt.$$

Now A_n has nothing to do with angles, so you can average over Jac, exchange this average with the time-average, and use the invariance of the flat volume under the present flow and the flow of translation produced by $H_2 = \int_0^1 Q' P$ to reduce the previous display to $\int_{\text{Jac}} P(0) X Q(0) d^{\infty} \theta / 2\pi$. Here,

$$\mathbb{X} Q(0) = rac{1}{4\pi} \int_{a_n} (1/2) \left(m_{12} + m_{21}
ight) \; rac{d\lambda}{\sqrt{\Delta^2 - 1}} \; ,$$

 $m_{12} - m_{21}$ is invariant under the "phase flow" $Q^{\bullet} = P$ and $P^{\bullet} = -Q$ produced by $H_1 = \frac{1}{2} \int_0^1 (Q^2 + P^2)$, and the average of P(0) under this flow is 0, permitting a further reduction to

$$A_n = \frac{1}{4\pi} \int_{a_n} \frac{d\lambda}{\sqrt{\Delta^2 - 1}} \int_{\text{Jac}} P(0) \left[m_{12}(\lambda) - 2\Delta^{\bullet}(\lambda) \right] d^{\infty} \frac{\theta}{2\pi} \ .$$

The trace formula $P(0) = {}^{15)}\frac{1}{2}\sum (\mu_i - \lambda_i)$ and the interpolation of $2\Delta^{\bullet} - m_{12}$ from example 1 are now inserted under the average, sums and avarage are exchanged, and the volume element $d^{\infty}\theta/2\pi$ is split at

¹⁵⁾ $\lambda_n^{\bullet} : n \in \mathbb{Z}$ are the roots of $\Delta^{\bullet}(\lambda) = 0$.

 $^{^{14)}}$ The level 3 actions have also a mechanical interpretation, but I do not go into it here.

 $j \in \mathbb{Z}$, with the result that

$$\begin{split} A_n &= \frac{1}{4\pi} \int_{a_n} \frac{d\lambda}{\sqrt{\Delta^2 - 1}} \sum_{i \in \mathbb{Z}} \sum_{j \in \mathbb{Z}} \int_{\substack{x a_k \\ k \neq j}} \frac{m_{12}}{\lambda - \mu_j} \int_{a_j} (\lambda_i^{\bullet} - \mu_i) \, d \, c h^{-1} \, \Delta(\mathfrak{p}_j) \\ &= \frac{1}{4\pi} \int_{a_n} \frac{d\lambda}{\sqrt{\Delta^2 - 1}} \sum_{i \in \mathbb{Z}} \int_{\substack{x a_k \\ k \neq i}} \frac{m_{12}}{\lambda - \mu_i} \int_{a_n} c h^{-1} \, \Delta \, d\mu_i \\ &= \frac{1}{2\pi} \int_{a_n} \frac{d\lambda}{\sqrt{\Delta^2 - 1}} \sum_{i \in \mathbb{Z}} \begin{cases} \int_{x a_k = \text{ Jac. }} \frac{m_{12}}{m_{12}^{\bullet}(\mu_i)(\lambda - \mu_i)} \, d^{\infty} \frac{\theta}{2\pi} \\ & \text{divided by } \frac{1}{2\pi} \int_{a_i} \frac{d\mu_i}{\sqrt{\Delta^2 - 1}} \\ & \text{multiplied by } \frac{1}{4\pi} \int_{a_i} c h^{-1} \, \Delta \, d\mu_i \\ &= \frac{1}{2\pi} \int_{a_n} \frac{d\lambda}{\sqrt{\Delta^2 - 1}} \sum_{i \in \mathbb{Z}} \phi_i \, I_i \\ &= I_n, \end{split}$$

as advertised.

§4. Thermodynamic Limit

Now let Q & P have period L and take the large volume limit $L \uparrow \infty$. What happens to the petit ensemble $e^{-H_3} d^{\infty}Q d^{\infty}P$? The answer is nice and simple. Let ψ be the ground state of $-\frac{1}{2}\Delta + \frac{1}{4}r^4$ in \mathbb{R}^2 . Then the mechanical variables $[Q(x), P(x)] : x \in \mathbb{R}$ tend (in law) to the stationary diffusion with infinitessimal operator $\frac{1}{2}\Delta + (\operatorname{grad} \ell n \psi) \cdot \operatorname{grad}$. This is even easy to prove.

§5. Focussing Case

This is much harder. The Hamiltonian is changed to $\frac{1}{2}\int [(Q')^2 + (P')^2]$ minus $\frac{1}{4}\int (Q^2 + P^2)$ and the associated petit ensemble has total mass $+\infty$. This prompted Lebowitz-Rose-Speer [1989] to introduce the microcanonical ensemble obtained by conditioning upon the value N of the constant of motion $H_1 = \frac{1}{2} \int (Q^2 + P^2) \cdot P^{(1)}$ Their interest was in the thermodynamic limit: with fixed "density" D, "particle number" N = DL, and $L \uparrow \infty$, they found by numerical simulation, that the temperature dependent ensemble $e^{-H_3/T} d^{\infty}Q d^{\infty}P$ favors "solitons"/"radiation" at low/high temperatures, *i.e.* some kind of phase change takes place. Chorin [private communication] used a more sophisticated simulation of the Brownian motion and found the opposite: no phase change. This made me curious and, subsequently¹⁷, I claimed to prove that the thermodynamical limit does not exist, explaining (as I thought) the discrepancy just described. But alas, all the big boys were wrong: in fact, my student B. Rider¹⁸) proved that, at any values of temperature and density, the whole ensemble collapses onto $Q \equiv 0$ & $P \equiv 0$. A pity.

Bibliography

- LEBOWITZ, J., H. A. ROSE, and E. R. SPEER: Statistical mechanics of the nonlinear Schrödinger equation(2). Mean field approximation. J. Stat. Phys. 54 (1989), 17-56.
- MANKOV, S.V., S. NOVIKOV, L. P. PITAEVSKII, and V. E. ZAKAROV: Theory of Solitons. The Inverse Scattering Method. Contemporary Soviet Math., Consultants Bureau, New York-London, 1984.
- MCKEAN, H. P. : Statistical mechanics of nonlinear wave equations (4): cubic Schrödinger. Comm. Math. Phys. 168 (1995), 479–491; erratum: 173 (1995) 675.
- , H. P. : A Martin boundary connected with the ∞ -volume limit of the focussing cubic Schrödinger equation. Itô's Stochastic Calculus and Probability Theory, ed. Ikeda et al., pp. 251–260, Springer-Verlag, Tokyo, 1995.
- MCKEAN, H. P. and K. VANINSKY: Action-angle variables for the cubic Schrödinger equation. CPAM 50 (1997), 489–562.

_____: Cubic Schrödinger: the petit canonical ensemble in action-angle variables. CPAM 50 (1997), 593–622.

RIDER, B. : On the ∞ -volume limit of the focussing cubic Schrödinger equation. CPAM 55 (2002), 1231–1248.

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¹⁷⁾ McKean [1995]

¹⁶⁾ The total mass is now finite, so the ensemble can be normalized. For a probabilistic proof of the existence of the flow and for the invariance of the micro-canonical ensemble under it, see McKean [1995].

¹⁸⁾ Rider [2002]