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# **Phase-space tomography and construction of invariant tori in gravitationally bound systems**

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Collisionless Boltzmann:

$$\frac{\partial f}{\partial t} + \langle v, \nabla_x f \rangle - \langle \nabla \Phi, \nabla_v f \rangle = \frac{\partial f}{\partial t} + [f, H] = 0 \quad (1)$$

Steady-state assumption:  $\partial f / \partial t = 0 = \partial \Phi / \partial t$ , i.e.,  $f = f(x, v)$  and  $\Phi = \Phi(x)$ .

data: measurements of  $(x, v)$  for stars or equivalent units of matter for one epoch

Can (and should) have several  $f_i$ ; all relaxed to steady-state Vlasov equilibrium.

Dark matter and bias factors allowed ( $\rho$  from  $f$  need not fulfill Poisson self-consistently; data fragmented).

**Phase-space tomography or generalized Newton's inverse problem of dynamics.** *Given a large number of observed  $(x, v)$  (for any motion markers such as stars or other matter and possibly in different populations  $P_i$ ) in a domain  $\Omega \subset \mathbb{R}^3 \times \mathbb{R}^3$  in a gravitationally bound steady-state system, deduce the potential  $\Phi(x)$  of the system, and the distribution function(s)  $f(x, v)$  of the observed matter in  $\Omega$ .*

(Kaasalainen 2008, Inverse Problems and Imaging **2**, 527)

## Uniqueness

Approximate the system by an integrable one: in  $\Phi(x)$ ,  $x \in \mathbb{R}^3$ , all orbits are approximately confined to 3-tori in  $\mathbb{R}_x^3 \times \mathbb{R}_v^3$  that are each defined by three action (Poincaré) integrals  $J_i$ ,  $i = 1..3$ , a class of isolating integrals  $I$ :

$$J_i = \frac{1}{2\pi} \oint_{P_i} \langle p, dq \rangle, \quad (2)$$

where  $p \in \mathbb{R}^3$  and  $q \in \mathbb{R}^3$  are any canonically conjugate momenta and coordinates, and  $P_i$  is a path that cannot be continuously deformed into a point (for other paths, the integral vanishes). By Jeans' theorem,

$$f(x, v) = f[I_1(x, v), \dots, I_3(x, v)] := f[I(x, v)]. \quad (3)$$

**Lemma.** *Let the potential  $\Phi(x)$  generate an integrable system, and let  $\mathcal{T}$  denote the corresponding set of 3-tori in  $\mathbb{R}^3 \times \mathbb{R}^3$ . Then  $\Phi(x)$  is the only integrable potential (up to an additive constant) that creates any chosen subset  $\hat{\mathcal{T}}$  of arbitrarily small patches  $\Gamma$  on any tori of  $\mathcal{T}$  such that  $\hat{\mathcal{T}}$  covers all of  $\mathbb{R}_x^3$  (accessible to the system) in a connected manner.*

[The lemma can also be expanded to concern all potentials (not just integrable systems) by defining  $\Gamma$  to be sections of orbits having common points  $x$ . In fact, just one chaotic orbit is sufficient as it eventually defines  $\Phi(x)$  at all  $x \in \mathbb{R}^3$ . More generally,  $\Gamma$  can denote parts of any structures on which  $E$  is constant, or parts of isosurfaces of functions of the form  $f(E)$ .]

The lemma states that even highly fragmentary information on the shape of the tori in phase space is well sufficient to determine the integrable potential  $\Phi(x)$  uniquely. The 3-surfaces formed by the intersection of three 5-surfaces  $f_i(I)$  are 3-tori (defined by  $I$  as well). Then, by the lemma, any collection of parts of surfaces  $f_i$  sufficient to determine a connected chain of torus patches uniquely determines  $\Phi(x)$ . We can now state the following result:

**Uniqueness theorem.** *Let three independent steady-state distribution functions  $f_i(x, v)$ ,  $i = 1..3$  ( $f : \mathbb{R}^3 \times \mathbb{R}^3 \rightarrow \mathbb{R}$ ) of matter in an integrable system be defined in some common domains of  $\mathbb{R}^3 \times \mathbb{R}^3$  such that a set of parts of the surfaces  $f_i(x, v) = \text{const.}$  forms a succession of torus patches connected in  $x$ . Then the  $f_i(x, v)$  uniquely determine the potential  $\Phi(x)$ .*

*Also, we can expect that one distribution function  $f(x, v)$ , defined everywhere in  $\mathbb{R}^3 \times \mathbb{R}^3$ , uniquely determines  $\Phi(x)$ .*

The theorem is constructive for three  $f$ 's (from which we directly get  $\Phi(x)$  with the procedure of the lemma), while the case of one  $f$  is non-constructive. Finding the integrable  $\Phi(x)$  corresponding to one  $f$  is not obvious since there are no general procedures for finding and exploring integrable potentials. In practice, we can circumvent this difficulty by allowing the use of non-integrable potentials and approximate tori

The theorem generalizes to observations of  $g_i(x, v) = \gamma(x, v) f_i(x, v) > 0$ , where  $\gamma$  is a bias function. Also, *we can expect that, if  $\gamma(x)$  depends on  $x$  only:  $\gamma : \mathbb{R}_x^3 \rightarrow \mathbb{R}$ , even the single product  $\gamma(x)f(x, v)$  determines the potential  $\Phi(x)$  of the system.*

## Tomography in 6D

Have distribution  $f(x)$ ,  $x \in \mathbb{R}^N$  and a linear transformation  $w = Rx$ ,  $\det R = 1$ . The marginal distribution function  $h(z)$  along  $z$ , any one of the new coordinate axes denoted by the set  $W(R)$ , is

$$h(z) = \int_{W(R) \setminus z} f(R^{-1}w) d^{N-1}w, \quad (4)$$

and its cumulative distribution function  $C(z)$  is

$$C(z) = \int_{z_{\min}}^z h(z') dz', \quad (5)$$

usually with  $z_{\min} \rightarrow -\infty$ . Since  $h(z) = dC(z)/dz$  uniquely defines  $h(z)$  from a given  $C(z)$ , we know from tomographic theory (another reason why this inverse problem can be called dynamical or phase-space tomography) that:

*The probability distribution  $f(x)$ ,  $x \in \mathbb{R}^N$ , is uniquely determined by the cumulative distributions  $C(z)$  of its marginal distributions  $h(z)$  along all line directions in  $\mathbb{R}^N$  that define the coordinate  $z$ .*

Two one-dimensional distributions can be compared via their cumulative distribution functions. In the case of observations and a model, we denote the observational distribution of  $K$  observations at  $z_i$  (arranged in ascending order by  $z$ ) by

$$S_K(z) = i, \quad z_i \leq z < z_{i+1}, \quad (6)$$

for number density, or, if mass is included in our problem,

$$S_K(z) = \sum_{j=1}^i m_j, \quad z_i \leq z < z_{i+1}, \quad (7)$$

with  $S_K(z) = 0$  for  $z < z_1$ .

$$\chi^2 = \sum_{ij} [S_K^{(i)}(z_j) - C^{(i)}(z_j)]^2. \quad (8)$$

Generally, with  $q = (x, v)$  and  $w = R_i q$ , we evaluate each  $h_i(z)$  corresponding to the choice for  $z$  ordered by  $i$ :

$$h_i(z) = \int \gamma(R_i^{-1}w) f(R_i^{-1}w) d^5w, \quad (9)$$

and find, via  $S_K^{(i)}(z)$  and  $C^{(i)}(z)$ , the best model parameters of  $\Phi(x)$ ,  $f(x, v)$ , and  $\gamma(x)$  minimizing (8).

We can also include errors: when the number of data points is high, the real probability  $f(w)$  is blurred by error convolution function  $\epsilon(w - w')$ :

$$\tilde{f}(w) = \int_{\mathbb{R}^6} f(w') \epsilon(w - w') d^6w' \quad (10)$$

which results in a transformed CDF.

As a computational device, we can maximize the product of likelihoods, or  $\log P = \sum_i \log p_f(w_i)$ . Since  $P \rightarrow 0$  always ( $p_f(w_i) < 1$ ), the result is not a proper measure and only gives the relative goodness-of-fit between different models. To know how good the actual fit is, we need to evaluate the CDFs. Instead of CDF integrals, we can draw simulated data sets via MCMC (and include error distributions in these as well) and compare these with the observed set.

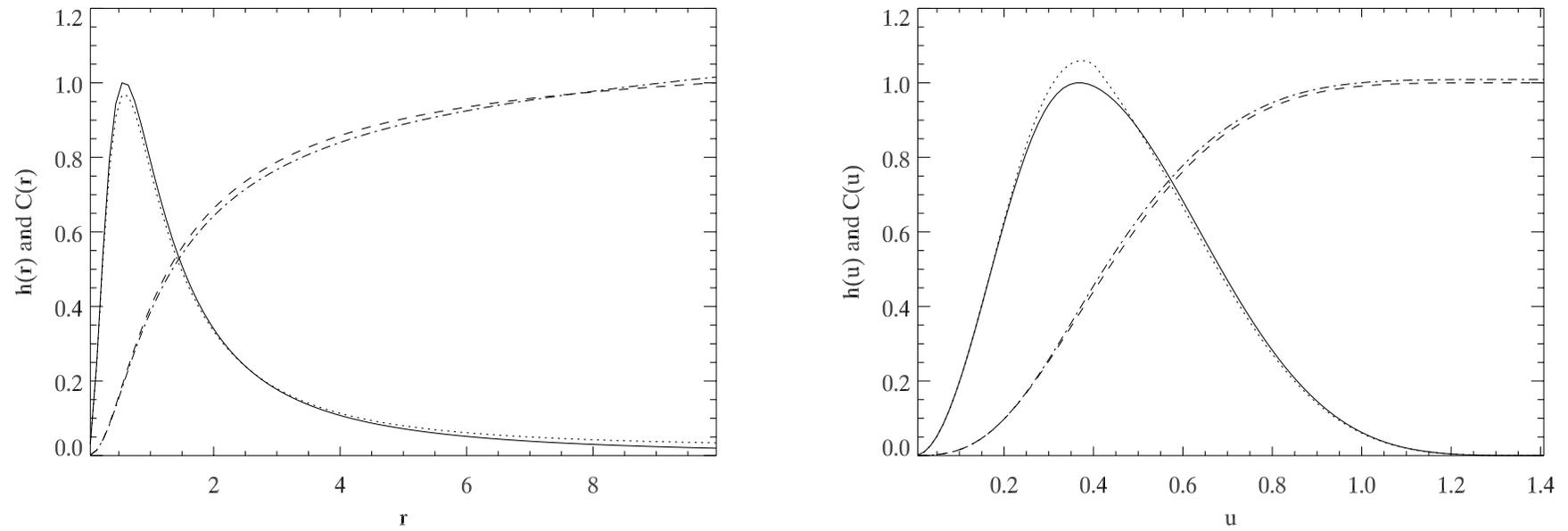


Figure 1: (a) Marginal and cumulative distributions in  $r$  and (b)  $u$  from the isochrone distribution ( $h$  in solid line,  $S_K$  from samples in dashed line), and the distributions with the best-fit model ( $h$  in dotted line,  $C$  in dot-dash).

## Torus construction

Torus construction can be seen as a way of solving the inverse problem of determining an integrable Hamiltonian  $H_0$  of which the near-integrable  $H$  is a perturbation:

$$H(J, \theta) = H_0(J) + \epsilon H_1(J, \theta), \quad (11)$$

where  $J \in \mathbb{R}^n$  and  $\theta \in \mathbb{T}^n$  are canonically conjugate actions and angles. Poincaré called the direct problem of perturbation “the fundamental problem of dynamics”, so we can call our problem the inverse Poincaré problem of dynamics. Torus construction defines the mapping

$$(\theta, J) \leftrightarrow (q, p) \quad (12)$$

between actions-angles (or their approximations) and the Cartesian canonical phase-space coordinates  $q \in \mathbb{R}^n, p \in \mathbb{R}^n$ .

We can classify the various types of methods of torus construction (or goals essentially equivalent to this) as

$$M(i, j) = M([1 : \text{canonical map}, 2 : \text{embedding}], [1 : \text{phase - space sampling}, 2 : \text{orbit integration}]). \quad (13)$$

(Kaasalainen and De Simone, in preparation)

M(1,1):

Have  $(I, \phi)$  of some known integrable  $H_I$  and thus know the mapping

$$(\theta, J) \leftrightarrow (\phi, I) \leftrightarrow (q, p) \quad (14)$$

Now we can write  $S(\phi, J) : \mathbb{T}^2 \times \mathbb{R}^2 \rightarrow \mathbb{R}$  with the (finite) Fourier series

$$S(\phi, J) = \phi \cdot J - i \sum_{n \in \mathbb{Z}^2 \setminus \{0\}} S_n(J) e^{in \cdot \phi}, \quad (15)$$

and taking into account the time symmetry and real-valuedness, we have

$$S(\phi, J) = \phi \cdot J + 2 \sum_{n \in \mathbb{Z}_+^2} S_n(J) \sin n \cdot \phi \quad (16)$$

so that the transformations between the canonical coordinates are

$$I = \frac{\partial S}{\partial \phi} = J + 2 \sum_n n S_n(J) \cos n \cdot \phi \quad (17)$$

and

$$\theta = \frac{\partial S}{\partial J} = \phi + 2 \sum_n \frac{\partial S_n(J)}{\partial J} \sin n \cdot \phi. \quad (18)$$

For an integrable  $H_0(w)$ ,  $w := (q, p) \in \mathbb{R}^2 \times \mathbb{R}^2$ , we must have

$$\frac{\partial H_0}{\partial \theta} = 0, \quad \frac{\partial H_0}{\partial J} = \omega, \quad (19)$$

Setting  $\partial H / \partial \theta = 0$  with  $\partial H / \partial \phi = 0$  everywhere gives the torus fitting routine for  $S_n(J)$  (Binney et al., Kaasalainen et al.; also done as  $M(1, 2)$  by a long orbit integration (Warnock et al.): only OK for real KAM tori).

If  $\frac{\partial S_n(J)}{\partial J}$  are needed for angle transformation (e.g. for smooth interpolation between tori):

$$\frac{\partial H}{\partial J} = \frac{\partial H}{\partial w} \frac{\partial w}{\partial I} \frac{\partial I}{\partial J} = \omega \quad (20)$$

where

$$\frac{\partial I}{\partial J} = \mathbb{I}_{2 \times 2} + 2 \sum_n \left[ n_i \frac{\partial S_n(J)}{\partial J_j} \right]_{ij \in 2 \times 2} \cos n \cdot \phi, \quad (21)$$

so the requirement of fulfilling (20) at  $J$  for a set of sample  $\phi^{(l)}$ ,  $S_n(J)$  given, can be written in the form of two sets of linear equations for the two unknown vectors  $(\omega_j, \frac{\partial S_n(J)}{\partial J_j})$ ,  $j = 1, 2$ :

$$\omega_j - \frac{\partial H}{\partial w} \sum_{i=1}^2 \frac{\partial w}{\partial I_i} \Big|_{J, \phi^{(l)}} \sum_n n_i \frac{\partial S_n(J)}{\partial J_j} \cos(n \cdot \phi^{(l)}) = \frac{\partial H}{\partial w} \frac{\partial w}{\partial I_j} \Big|_{J, \phi^{(l)}} \quad (22)$$

(also done as  $M(1, 2)$  with integrated orbit strips: OK for any tori, not only KAM). Can also use  $\omega$  to label the desired torus.

M(2,1):

We can also consider the desired torus simply as a manifold in  $\mathbb{R}^2 \times \mathbb{R}^2$  and aim at defining a suitable embedding  $\Phi : \mathbb{T}^n \rightarrow \mathbb{R}^{2n}$

$$\Phi(\theta; \alpha) = [q(\theta), p(\theta)] \quad (23)$$

where the parameter vector  $\alpha \in \mathbb{R}^n$  denotes the constraints we want our torus to fulfill: these can be either the desired actions  $J$  or frequencies  $\omega$ .

Now we minimize the norm  $\|e\|$  of the error vector

$$e(\theta') = \mathbb{J}_{4 \times 4} \nabla_{(q,p)} H[\Phi(\theta)] - \partial_\omega \Phi(\theta), \quad (24)$$

where  $\mathbb{J}$  is the symplectic matrix

$$\begin{pmatrix} 0 & \mathbb{I} \\ -\mathbb{I} & 0 \end{pmatrix}. \quad (25)$$

We can express  $[q(\theta), p(\theta)]$  as the Fourier series

$$q(\theta) = \sum_n q_n e^{i(n \cdot \theta)}, \quad p(\theta) = \sum_n p_n e^{i(n \cdot \theta)}. \quad (26)$$

The first two components  $e_A(\theta)$  of the error vector  $e(\theta)$  are now given by

$$e_A(\theta) = p(\theta) - \sum_n i(n \cdot \omega) q_n e^{i(n \cdot \theta)}. \quad (27)$$

This implies that  $e_A(\theta)$  identically vanishes if we set

$$p_n = i(n \cdot \omega) q_n. \quad (28)$$

The remaining components  $e_B(\theta)$  to be minimized in the norm can be written as

$$e_B(\theta) = \partial_q H(q, p) + i(n \cdot \omega) p_n e^{i(n \cdot \theta)}, \quad (29)$$

or, using the condition (28),

$$e_B(\theta) = \partial_q H(q, p) - (n \cdot \omega)^2 q_n e^{i(n \cdot \theta)}. \quad (30)$$

This is well known: e.g. Ratcliff-Chang-Schwarzschild. But RCS i) used a bad method for determining  $q_n$  and ii) did not treat this as a potentially ill-posed inverse problem: constraints needed/useful (especially when not a KAM torus). Also, might not want to set  $e_A = 0$ : then  $\|e_B\|$  and  $\|e\|$  may be larger than they would with free  $p_n$  as well.

One regularization function:

$$R_H(\theta) = |H(\theta) - \langle H \rangle_\theta|, \quad (31)$$

Another:  $J$  on the torus should be constant, so

$$\begin{aligned} J_1 &= \frac{1}{2\pi} \sum_j \sum_{kl} \sum_{mn} p_{kl}^j q_{mn}^j e^{i(l+n)\theta_2} i m \int_0^{2\pi} e^{i(k+m)\theta_1} d\theta_1 \\ &= \sum_{jkl n} (-ik) p_{kl}^j q_{-kn}^j e^{i(l+n)\theta_2}. \end{aligned} \quad (32)$$

Likewise,

$$J_2 = \sum_{jkl n} (-in) p_{kn}^j q_{l-n}^j e^{i(k+l)\theta_1}. \quad (33)$$

Since  $J_i$  should not depend on  $\theta_j$ , we define the actions  $J^T$  of our torus to be the mean values of the above series, i.e.,

$$J_1^T = \sum_{jkl} (-ik) p_{kl}^j q_{kl}^{j*}, \quad J_2^T = \sum_{jkl} (-il) p_{kl}^j q_{kl}^{j*}, \quad (34)$$

with  $q_{-n} = q_n^*$  due to the real-valuedness of  $q$ . Our constraint is that  $\theta$ -dependence should vanish:

$$\forall L \neq 0 : \sum_{jkl} (-ik) p_{kl}^j q_{-k, L-l}^j = 0, \quad \forall K \neq 0 : \sum_{jkl} (-il) p_{kl}^j q_{K-k, -l}^j = 0. \quad (35)$$

as noted in Binney-Spergel.

For example, minimize

$$\chi_S^2 = \sum_i \|e_A(\theta_i)\|^2 + \|e_B(\theta_i)\|^2 + \lambda_H R_H(\theta_i)^2 + \lambda_J R_J(\theta_i)^2, \quad (36)$$

where  $\lambda_i$  are suitable regularization weights, and

$$R_J(\theta) = |J_i(\theta) - J_i^T|. \quad (37)$$

When a KAM torus exists for  $\omega$  in  $H$ , the requirement  $\|e\| = 0$  directly implies  $J = J^T$  and  $H = \langle H \rangle$  on the torus.

M(2,2):

An alternative scheme is to use strips of numerically integrated orbits starting at a set of  $\theta_0$ , and demanding that the surface of the final torus deviate as little as possible from the strips in phase space:

$$\chi_I^2 = \sum_i \|p_I^i - p(\theta_i)\|^2 + \|q_I^i - q(\theta_i)\|^2 + \lambda_H R_H(\theta_i)^2 + \lambda_J R_J(\theta_i)^2, \quad (38)$$

where  $q_I^i, p_I^i$  are the numerically integrated phase-space points at times  $t_i$  starting from  $q(\theta_{0i}), p(\theta_{0i})$ , and

$$\theta_i = \theta_{0i} + \omega t_i. \quad (39)$$

Other things:

- We can use adaptive interpolation on a random grid (rather than a fixed grid) to probe the  $J$ -space efficiently.
- Quadratically convergent algorithm for polishing off an almost-there torus
- Don't like Fourier series? Then do the above by straight manifold triangulation: distribute  $\theta$  among vertices in  $\mathbb{R}^{2n}$ , interpolate  $\Phi$  and  $\theta$  between vertices (on facets) such that  $\|e\|$  is minimized
- $M(1, *)$  works for most orbits (at least in 2 effective dimensions);  $M(2, *)$  for cases requiring brute force