Chapter 31

Koopman modes

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S O FAR WE HAVE mostly focused on computation of eigenvalues of evolution operators. Here we shall discuss the role of their eigenfunctions. This is easiest to explain for systems with stable equilibria and periodic orbits, for which the dynamics is described by Koopman operators. We shall show how here how the *nonlinear* dynamics of transient states on the way to a stable solution is captured by the eigenfunctions of the *linear* Koopman operator.

31.1 Koopmania

The Koopman operator action on an observable a(x) (a bounded and smooth state space function that associates a scalar to state x) is to replace it by its downstream value time t later, $a(x) \rightarrow a(x(t))$, evaluated at the trajectory point x(t):

$$\begin{bmatrix} \mathcal{K}^t a \end{bmatrix} (x) = a(f^t(x)) = \int_{\mathcal{M}} dy \, \mathcal{K}^t(x, y) \, a(y)$$
$$\mathcal{K}^t(x, y) = \delta \Big(y - f^t(x) \Big) \,. \tag{31.1}$$

Given an initial density of representative points $\rho(x)$, the state space average of a(x) evolves as

$$\begin{split} \langle a \rangle_{\rho}(t) &= \frac{1}{|\rho_{\mathcal{M}}|} \int_{\mathcal{M}} dx \, a(f^{t}(x)) \, \rho(x) \, = \, \frac{1}{|\rho_{\mathcal{M}}|} \int_{\mathcal{M}} dx \, \left[\mathcal{K}^{t} a \right](x) \, \rho(x) \\ &= \, \frac{1}{|\rho_{\mathcal{M}}|} \int_{\mathcal{M}} dx \, dy \, a(y) \, \delta\left(y - f^{t}(x)\right) \rho(x) \, . \end{split}$$

The 'propagator' $\delta(y - f^t(x))$ can be interpreted as belonging to the Perron-Frobenius operator (19.10), so the two operators are adjoint to each other,

$$\int_{\mathcal{M}} dx \left[\mathcal{K}^{t} a \right](x) \rho(x) = \int_{\mathcal{M}} dy \, a(y) \left[\mathcal{L}^{t} \rho \right](y) \,. \tag{31.2}$$

The Koopman and Perron-Frobenius operators describe the dynamics in complementary ways. Koopman advances the trajectory by time t, Perron-Frobenius depends on the trajectory point time t in the past. Perron-Frobenius propagates a conserved quantity (a density of initial conditions) forward in time. The growth (or decay) of the density depends on the compression (or expansion) of a volume occupied by a set of trajectories. The dynamics of an observable depends on the other hand on one single trajectory.

The family of Koopman operators $\{\mathcal{K}^t\}_{t \in \mathbb{R}_+}$ forms a semigroup parameterized by time, $\mathcal{K}^t \mathcal{K}^{t'} = \mathcal{K}^{t+t'}$, $\mathcal{K}^0 = \mathbf{1}$ with the generator of infinitesimal time translations defined by

$$\mathcal{A}^{\dagger} = \lim_{t\to 0^+} \frac{1}{t} \left(\mathcal{K}^t - \mathbf{1} \right).$$

If the flow is finite-dimensional and invertible, \mathcal{A}^{\dagger} is a generator of a group. The explicit form of \mathcal{A}^{\dagger} follows from expanding dynamical evolution up to first order, as in (2.6):

$$\mathcal{A}^{\dagger}a(x) = \lim_{t \to 0^+} \frac{1}{t} \left(a(f^t(x)) - a(x) \right) = v_i(x) \partial_i a(x) \,. \tag{31.3}$$

This is by definition the time derivative, so the time-evolution equation for a(x) is

$$\left(\frac{d}{dt} - \mathcal{A}^{\dagger}\right)a(x) = 0.$$
(31.4)

We formally write the solution to (31.4) as

$$a(x(t)) = e^{t\mathcal{A}^{\mathsf{T}}}a(x_0) = \mathcal{K}^t a(x_0),$$

so the finite time Koopman operator (31.1) can be recovered by exponentiating the time-evolution generator \mathcal{A}^{\dagger} . The generator \mathcal{A}^{\dagger} looks very much like the generator of translations. For example, for a constant velocity field dynamical evolution is nothing but a translation by time × velocity:

$$e^{tv\frac{\partial}{\partial x}}a(x) = a(x+tv).$$
(31.5)

As we will not need to implement a computational formula for general $e^{t\mathcal{A}}$ in what follows, we relegate making sense of such operators to appendix A31.2.

The Koopman / Perron-Frobenius operators are non-normal, non-self-adjoint operators, so their left and right eigenvectors differ. The right eigenvectors of a Perron-Frobenius operator are the left eigenvectors of the Koopman, and vice versa. That is,

$$\mathcal{A}\phi_{\alpha}(x) = s_{\alpha}\phi_{\alpha}(x), \quad \mathcal{A}^{\dagger}\psi_{\alpha}(x) = s_{\alpha}^{*}\psi_{\alpha}(x), \qquad \alpha = 0, 1, 2, \cdots$$

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appendix A31.2

exercise 31.1

exercise A31.1

exercise 19.10

appendix A31.2

The left and right eigenfunctions satisfy the bi-orhogonality condition with respect to L^2 norm,

$$\int_{\mathcal{M}} dx \,\phi_{\alpha}^* \psi_{\beta} = \delta_{\alpha\beta} \,. \tag{31.6}$$

While one might think of a Koopman operator as an 'inverse' of the Perron-Frobenius operator, the notion of *adjoint* is the right one, especially in settings where flow is not time-reversible, as is the case for dissipative PDEs (infinite dimensional flows contracting forward in time) and for stochastic flows.

Given the left and right eigenfunctions, we can express the evolution of an observable as

$$a(x(t)) = \left[\mathcal{K}^t a\right](x_0) = \sum_{\alpha} c_{\alpha} e^{s_{\alpha} t} \psi_{\alpha}(x_0)$$
(31.7)

where

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$$c_{\alpha} = \int_{\mathcal{M}} dx \, a(x) \, \phi_{\alpha}^*(x) \ .$$

This expansion suggests an alternative description of nonlinear dynamics, which is the (linear) evolution of observables in an infinite-dimensional space. In principle, this allows the study of full nonlinear dynamics using linear operator-theoretical tools.



31.2 Koopman eigenvalues for a limit cycle

The $[(d-1)\times(d-1)]$ -dimensional monodromy matrix $\mathbf{M}_{ij} = \partial_j P_i(\hat{x}_a)$ of dimension governs the dynamics of the small perturbation $\delta \hat{x}$ within a Poincaré section.

Even though the monodromy matrix $\mathbf{M}(\hat{x})$ depends upon \hat{x} (the 'starting' point of the periodic orbit), its eigenvalues do not, so we may write for its eigenvectors $\mathbf{e}^{(j)}$ (sometimes referred to as 'covariant Lyapunov vectors,' or, for periodic orbits, as 'Floquet vectors')

$$\mathbf{M}(x) \mathbf{e}^{(j)}(x) = \Lambda_j \mathbf{e}^{(j)}(x), \qquad \Lambda_j = e^{\lambda^{(j)}T}.$$
(31.8)

where Floquet exponents $\lambda^{(j)} = \mu^{(j)} \pm i\omega^{(j)}$ are independent of *x*. We order the Floquet multipliers as

$$|\Lambda_1| \ge |\Lambda_2| \ge \dots \ge |\Lambda_{d-1}|. \tag{31.9}$$

The limit cycle is stable if $|\Lambda_1| < 1$.

The two most important characteristics of the limit cycle are thus the fundamental frequency and the leading Lyapunov exponent, defined by

$$\omega = \frac{2\pi}{T}, \qquad \mu = \frac{1}{T} \ln |\Lambda_1|, \qquad (31.10)$$

respectively.

Here we follow the derivations chapter 21, except that the analysis is restricted to the simpler case of a stable limit cycle. The trace of the Koopman operator is,

$$\operatorname{tr} \mathcal{K}^t = \int_{\mathcal{M}} \mathcal{K}^t(x, x) dx.$$

where \mathcal{K}^t is the kernel. Inspired by this definition, we define the trace of Koopman operator as

$$\operatorname{tr} \mathcal{K}^{t} = \int_{\mathcal{M}} \delta(x - f^{t}(x)) dx.$$
(31.11)

From (31.11), one observes that the trace \mathcal{K}^t receives a contribution whenever the trajectory returns to the starting point after *r* repeats of the limit cycle period *T*.

To proceed, we decompose the propagator f_t into two parts, the (d-1)-dimensional return map P and a 1-dimensional return-time function τ . The return map captures only the transverse part of the periodic dynamics, since the flow component tangent to the trajectory, which is not in the span of the Poincaré section, has not been taken into account. Assuming the longitudinal state component has a certain mean velocity v as it traverses the limit cycle, one may transform this component to a time coordinate system using the relation vdt. Thus the full dynamics is described by the return map P and by the first return function $\tau(\hat{x})$ that provides the (non-constant) time interval between successive points \hat{x} on Poincaré section, e.g. $t_{k+1} = t_k + \tau(\hat{x}_k)$. Applying τ recursively, we may write ((k+1)th time as a function first point and initial time,

$$t_{k+1} = t_1 + \sum_{j=0}^{k-1} \tau(P^j \hat{x}_1).$$
(31.12)

Now, factor the kernel of \mathcal{K}^t (31.11) into two parts

$$\operatorname{tr} \mathcal{K}^{t} = \int_{\mathcal{P}(\hat{\$})=0} d\hat{x} \int_{0}^{\tau(\hat{x})} dt \,\delta\!\left(\hat{x} - P^{k}\hat{x}\right) \delta\!\left(t - \sum_{j=0}^{k-1} \tau(P^{j}\hat{x})\right),$$
(31.13)

where P^k and τ are defined above and in (31.12), respectively. We treat the two Dirac delta functions separately, starting with P^k . First recall that the Dirac delta function applied to a scalar-valued function g(x), is

$$\int \delta(g(x))dx = \int \delta(x)|g'(0)^{-1}|dx = \sum_{j} \frac{1}{|g'(x_j)|}$$

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where x_j are the roots of g(x). This property may be generalized to d-1 dimensions and applied to the Dirac-delta in (31.13),

$$\int_{\mathcal{P}(\mathbf{u})=0} d\hat{x}\,\delta(\hat{x} - P^k(\hat{x})) = \frac{1}{|\det\left(\mathbf{I} - \mathbf{M}^r\right)|},\tag{31.14}$$

where I denotes the identity matrix. The second part of the trace can be written as

$$\int_{0}^{\tau(\hat{x})} \delta(t - \sum_{j=0}^{k-1} \tau(P^{j}\hat{x})) dt = T \sum_{r=1}^{\infty} \delta(t - rT).$$
(31.15)

Inserting the identities (31.14) and (31.15) in (31.13), we get the trace formula for a single limit cycle of period *T*,

$$\operatorname{tr} \mathcal{K}^{t} = T \sum_{r=1}^{\infty} \frac{\delta(t - rT)}{|\det (\mathbf{I} - \mathbf{M}^{r})|}, \qquad (31.16)$$

which was first derived in ref. [1], here given in the special case of a single limit cycle. The trace formula is a sum whose terms are nonzero only for integers of the cycle period. The *r*th nonzero term describes how much after the *r*th return to the Poincaré section a small neighborhood volume (i.e. a tube) of the stable limit cycle has retracted. This relation thus connects the trace of \mathcal{K}^t to the dynamics in the local stable manifold of the limit cycle.

The Koopman eigenvalues are the poles of the Laplace transform of trace of \mathcal{K}^t

$$\int_0^\infty e^{-st} \operatorname{tr} \mathcal{K}^t dt = \operatorname{tr} \frac{1}{s - \mathcal{A}},$$

i.e., the poles of the resolvent of \mathcal{A} . By inserting (31.16) in the left-hand side of above equation one obtains,

$$\operatorname{tr} \frac{1}{s - \mathcal{A}} = \frac{\partial}{\partial s} \ln(\det(s - \mathcal{A})),$$

where det $(s - \mathcal{A})$ is the spectral determinant,

$$\det(s - \mathcal{A}) = \exp\left[-\sum_{r=1}^{\infty} \frac{1}{r} \frac{e^{-sTr}}{|\det(\mathbf{I} - \mathbf{M}^r)|}\right].$$

Now, since the determinant does not depend on the basis which \mathbf{M} is described in, we may write it in terms of the eigenvalues of \mathbf{M} ,

$$\frac{1}{|\det\left(\mathbf{I} - \mathbf{M}^{r}\right)|} = \prod_{k=1}^{d-1} \frac{1}{1 - \Lambda_{k}^{r}},$$
(31.17)

where we have assumed that $|\Lambda_k| < 1$ for all *k*.

Denominators can be expanded in Taylor series such as

$$(1-x)^{-1}(1-y)^{-1} = 1 + x + y + x^{2} + xy + y^{2} + \dots,$$

when |x| < 1, |y| < 1. Each term in the product (31.17) may thus be written as an infinite sum. Define a *multi-index* as an array of *d* non-negative integers $j_k = 0, 1, 2, ...$:

$$\boldsymbol{j} = [j_1, j_2, \ldots, j_d] \in \mathbb{N}^d,$$

Consider next the product of d - 1 Floquet multipliers

$$\mathbf{\Lambda} = \mathbf{\Lambda}_1 \mathbf{\Lambda}_2 \cdots \mathbf{\Lambda}_{d-1} = e^{T(\mu^{(1)} + \mu^{(2)} + \cdots + \mu^{(d-1)})},$$

(the imaginary parts of complex pairs cancel in the exponent), and define

$$\boldsymbol{\mu} = [\mu^{(1)}, \mu^{(2)}, \cdots, \mu^{(d-1)}] \in \mathbb{R}^d.$$

 Λ can now be raised to *j*th power as

$$\mathbf{\Lambda}^{j} = e^{T \boldsymbol{\mu} \cdot j} = \Lambda_{1}^{j_{1}} \Lambda_{2}^{j_{2}} \cdots \Lambda_{d-1}^{j_{d-1}} \,. \tag{31.18}$$

Using multi-index notation (31.18) we may write (31.17) as

$$\frac{1}{|\det\left(\mathbf{I}-\mathbf{M}^{r}\right)|}=\sum_{j}\Lambda^{rj},$$

and consequently the spectral determinant as

$$\det (s - \mathcal{A}) = \exp \left[-\sum_{r=1}^{\infty} \frac{1}{r} (e^{-sT} \sum_{j} \Lambda^{j})^{r} \right].$$

Applying the identity $\sum x^r/r = -\ln(1-x)$, we obtain the final form of the spectral determinant for a stable limit cycle

$$\det(s - \mathcal{A}) = \prod_{j=1}^{\infty} \left(1 - e^{-sT} \Lambda^{j}\right).$$
(31.19)

The zeros of det $(s - \mathcal{A}) = 0$ are given by the zeros of individual terms in the product:

$$e^{-T(s-\mu \cdot j)} = 1$$

Taking the logarithm of both sides, we obtain

$$s_{j,m} = \boldsymbol{\mu} \cdot \boldsymbol{j} + 2\pi i m/T = \boldsymbol{\mu} \cdot \boldsymbol{j} + i m \omega$$
(31.20)

with $m = 0, \pm 1, \pm 2, \ldots$ For our particular choice of analytic observables the spectrum of \mathcal{K}^t is reduced to its minimal components, namely any integer multiple of the stability eigenvalues. Thus, for any stable limit cycle, the Koopman eigenvalues form a lattice on the lower half of the complex plane. The marginal eigenvalues on the horizontal imaginary axis corresponding to j = 0 correspond to the non-decaying time-averaged mean (m = 0) and periodic dynamics ($m \neq 0$) on the limit cycle. The remaining eigenvalues $j \neq 0$ are decaying and describe the transient behavior of flow in the local stable manifold of the limit cycle.



Remark 31.1. Koopman operators. The "Heisenberg picture" in dynamical systems theory has been introduced by Koopman and Von Neumann [3, 5], see also ref. [4]. Inspired by the contemporary advances in quantum mechanics, Koopman [3] observed in 1931 that \mathcal{K}^t is unitary on $L^2(\mu)$ Hilbert spaces. The Koopman operator is the classical analogue of the quantum evolution operator $\exp(i\hat{H}t/\hbar)$ – the kernel of $\mathcal{L}^t(y, x)$ introduced in (19.13) (see also sect. 20.2) is the analogue of the Green function discussed here in chapter 36. The relation between the spectrum of the Koopman operator and classical ergodicity was formalized by von Neumann [5]. We shall not use Hilbert spaces here and the operators that we shall study *will not* be unitary. For a discussion of the relation between the Perron-Frobenius operators and the Koopman operators for finite dimensional deterministic invertible flows, infinite dimensional contracting flows, and stochastic flows, see Lasota-Mackey [4] and Gaspard [2].

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31.3 Examples

Example 31.1. Spectrum of a 1D linear system. Consider a 1D system with a single equilibrium

$$\dot{x} = \lambda x, \tag{31.21}$$

If the observable a(x) is a smooth, real-analytical function, the Koopman operator spectrum can be identified from its Taylor expansion,

$$\begin{cases} s_k = k\lambda \\ \phi_k = \delta^{(k)}(x) & \text{when } \lambda < 0 \quad (\text{attractor}) \\ \psi_k = x^k \end{cases}$$
(31.22)

and

$$\begin{cases} s_k = -(k+1)\lambda \\ \phi_k = x^k & \text{when } \lambda > 0 \quad \text{(repeller)} \\ \psi_k = \delta^{(k)}(x) \end{cases}$$
(31.23)

for $k = 0, 1, \cdots$. Here the superscript ^(k) refers to the *k*th derivative. We observe the duality between the right/left eigenfunctions and the repelling/attracting points. When $\lambda < 0$, any neighborhood of representative points shrinks to a point and asymptotically the density becomes a singular function. On the other hand, any smooth observable has the asymptotic limit *a*(0). Koopman operator \mathcal{K}^t is thus the appropriate evolution operator to represent the dynamics in stable manifolds, since the observable dynamics goes along with the flow.

Example 31.2. Spectrum of a 1D nonlinear system. As an example of how the effects of nonlinearity are captured by expansion into eigenfunctions of the Koopman operator, consider the stable nonlinear system:

$$\dot{x} = \lambda x - x^3, \qquad \lambda < 0 \tag{31.24}$$

where the only equilibrium point is the attracting fixed point $x_q = 0$. The difference between (31.24) and the linear system in (31.21), is the presence of a cubic nonlinear term. However, the nonlinear coordinate transformation

$$y = g(x) = \frac{x}{\sqrt{x^2 - \lambda}}$$
(31.25)

transforms (31.24) into a linear system $\dot{y} = \lambda y$, whose spectrum is already determined by (31.22). The Koopman spectrum in terms of the coordinate *x* is thus

$$\begin{cases} s_k = k\lambda \\ \phi_k(x) = \delta^{(k)} \left(x - g^{-1}(y) \right) |_{y=0} \\ \psi_k(x) = \left(x/\sqrt{x^2 - \lambda} \right)^k \end{cases}$$
(31.26)

where $k = 0, 1, \cdots$ and the derivative of δ is with respect to y. Comparing to (31.22), the Koopman eigenvalues are not modified by the cubic nonlinear term in (31.24), but the term $\sqrt{x^2 - \lambda}$ appears in the Koopman eigenfunctions.

Consider the expansion (31.7) of a position x(t) at time *t* considered as an observable, a(x(t)) = x(t),

$$x(t) = \left(\frac{-\lambda}{x_0^2 - \lambda}\right)^{1/2} x_0 e^{\lambda t} + \frac{1}{\sqrt{-\lambda}} \left(\frac{x_0}{x_0^2 - \lambda}\right)^{3/2} e^{3\lambda t} + \dots$$
(31.27)

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Figure 31.1: (black line) The trajectory x(t) of (31.24) plotted on logarithmic scale as a function of time, for $\lambda = -0.6$. (red lines) Reconstructions of the trajectory based on the expansion (31.27) – including up to the ϕ_1 , ϕ_3 , ϕ_5 or ϕ_7 left eigenfunction of \mathcal{K}^t . (dashed line) The trajectory of the linearized system, with x^3 neglected in (31.24).

Figure 31.2: State trajectory starting close to $x_q = 0$ and with $\mu = 1/10$ for the system (31.28) in *x*, *y*-plane (left) and the (*x*, *z*)-plane (right).



In figure 31.1, the trajectory x(t) (black line) obtained by integrating (31.24) starts out by a rapid decay to the stable manifold of the stable fixed point, followed by an exponential decay along the manifold to $x_q = 0$. In a purely linear analysis, the state evolves as $x_{lim}(t) = x_0 e^{\lambda t}$ (dashed black line in the figure). A linear analysis provides the exponential decay rate, but fails to describe the curved trajectory in its initial stages. In the figure the first non-zero expansion terms and the superposition of gradually increasing number of modes are shown with red lines. Whereas the Koopman eigenvalues provide the asymptotic decay rate, the Koopman eigenfunctions provide the direction as well as an amplitude. Including higher order terms in the expansion, eventually the full state trajectory can be recovered by a number of Koopman eigenfunctions, and thus the transient nonlinear dynamics preceding the infinitesimal linear region can be captured.

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Example 31.3. Spectrum of a stable limit cycle. system

Consider the three dimensional

1	(X	=	$\mu x - y - xz$	
{	ý	=	$\mu y - x - yz$	(31.28)
	ż	=	$-z+x^2+y^2,.$	

for $\mu \gtrsim 0$. The system has an unstable fixed point

$$x_q = (x, y, z) = 0,$$

and an attracting limit cycle

 $x_a = (\sqrt{\mu} \cos t, \sqrt{\mu} \sin t, \mu).$

In figure 31.2, a typical trajectory starting near x_q is shown. The trajectory grows exponentially with the exponent $\lambda_q > 0$ and after a transient time, approaches the stable limit cycle exponentially fast with the exponent $\lambda_a < 0$.

The set of discrete Koopman/Perron-Frobenius eigenvalues is simply the union of the eigenvalues associated with the fixed point and the limit cycle. One may thus treat the two critical elements separately using the formulas derived from the trace of the operators. Here we only consider the spectrum pertaining to stable limit cycle. By considering the Poincaré section given by the plane y = 0 and its associated monodromy matrix, one arrives at

$$\Lambda = -2\mu, \qquad \omega = 2\pi.$$

According to formula (31.20) the Koopman/Perron-Frobenius eigenvalues $\{j, m\} = \{j_1, 0, ..., 0, m\}$ corresponding to this leading Floquet exponent are,

$$s_{j,m} = j\Lambda + im\omega = -2\mu j + mi2\pi$$

for j = 0, 1, 2, ... and $m = 0, \pm 1, \pm 2, ...$ The expansion of the state observable into the leading complex Koopman eigenfunctions (j = 0, 1 and m = 0, 1) associated with (31.28) is

$$x(t) = v_{0,0} + v_{0,1} e^{it} + v_{1,0} e^{-2\mu t} + c.c + \dots$$

with,

$$v_{0,0} = (0,0,\mu), \tag{31.29}$$

$$v_{0,1} = \frac{\sqrt{\mu}}{2}(1,0,0) + \frac{i\sqrt{\mu}}{2}(0,1,0), \qquad (31.30)$$

$$v_{1,0} = \frac{c \sqrt{\mu}}{2} (0, 0, \frac{r^2 - \mu}{r^2}), \qquad (31.31)$$

where *c* is some constant and $r^2 = x^2 + y^2$.

The first two modes resolve the attractor dynamics; $v_{0,0}$ represents the average asymptotic value, and $v_{0,1}$ the periodic asymptotic solution with unit frequency on the attractor. These two Koopman modes correspond to the three first (real) empirical Karhunen-Loève or proper orthogonal decomposition modes. A robust low-order representation of the flow should in addition to the limit cycle also, at least in some sense, capture the dynamics of the corresponding attracting inertial manifold, that connects the unstable fixed point with the limit cycle. This is the role of the transient mode $v_{1,0}$; the function $(r^2 - \mu)/r^2$ is singular near the fixed point and zero at the limit cycle and points in the direction z, i.e. from x_q to x_a .

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Exercises

- 31.1. **Perron-Frobenius operator is the adjoint of the Koopman operator.** Check (31.2) - it might be wrong as it stands. Pay attention to presence/absence of a Jacobian.
- 31.2. Nonlinear system mapped into a linear one. (31.24) and the linear system in (31.21), is the presence of a cubic nonlinear term. Show the nonlinear coordinate trans-

formation (31.25)

$$y = g(x) = \frac{x}{\sqrt{x^2 - \lambda}}$$

transforms (31.24) into a linear system $\dot{y} = \lambda y$.

31.3. Stability of a limit cycle. Show that the system (31.28) has an attracting limit cycle $x_a = (\sqrt{\mu} \cos t, \sqrt{\mu} \sin t, \mu)$.