KAM theory for particles in periodic potentials

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Abstract. It is shown that the system of the form $\ddot{x} + V'(x) = p(t)$ with periodic V and p and with $\langle p \rangle = 0$ is near-integrable for large energies. In particular, most (in the sense of Lebesgue measure) fast solutions are quasiperiodic, provided $V \in C^{(5)}$ and $p \in L^1$; furthermore, for any solution x(t) there exists a velocity bound c for all time: |x(t)| < c for all $t \in \mathbb{R}$. For any real number r there exists a solution with that average velocity, and when r is rational, this solution can be chosen to be periodic.

1. Introduction

The result of this note states that any system consisting of a particle in a periodic potential subject to periodic external forcing possesses KAM tori, physically corresponding to quasiperiodic translational motion. The only assumptions are the $C^{(5)}$ smoothness of the potential and the zero average of the forcing. In particular, forcing need not be small. This note was stimulated by J. Franks' extension of the Poincaré-Birkhoff theorem to the case when the boundaries of the annulus are noninvariant. This extension was proven and applied (the latter in collaboration with Moeckel and Robinson) in [5] to the conservative pendulum with periodic forcing

$$\ddot{x} + \sin x = p(t), \quad \int_0^1 p(t) dt = 0,$$
 (1)

where p(t+1) = p(t), to show that periodic solutions of any rational rotation number exist.

The standard version [2] of the Poincaré-Birkhoff theorem may not seem applicable in this case since no annulus with invariant boundaries is available a priori. We will show that such boundaries actually do exist, using Moser's invariant curve theorem [8], [13], [16].

We will look at the systems of the form

$$\ddot{x} + V'(x) = p(t), \quad V(x+1) = V(x), \quad p(t+1) = p(t)$$
 (2)

describing the motion of a particle in a periodic potential with external periodic forcing p(t). This could be a simple model of an electron in an atomic lattice subject

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to a periodically varying potential, or of charge-density waves [6]. We will show that the associated Poincaré map $F:(x, \dot{x})_{t=0} \mapsto (x, \dot{x})_{t=1}$ of the phase cylinder $(x \mod 1, \dot{x})$ onto itself possesses noncontractible invariant circles. The results are stated fully in § 2. We mention a related result by Zehnder and Dieckerhoff [3, 4] on the existence of KAM circles for the particle in a superquadratic potential

$$\ddot{x} + V_x(x, t) = 0,$$

$$V(x, t) = x^{2n} + a_1 x^{2n-1} + \dots + a_{2n}, \quad n > 1$$
(3)

with lower coefficients $a_i(t)$ periodic in t. The superquadratic nature of the potential provided the twist needed to apply KAM. In the case at hand, the twist is provided by a different effect, essentially, by the shear in the (x, \dot{x}) -plane whose physical manifestation lies in the obvious fact that the faster particles travel further. The invariant circles on the phase torus turn out to be approximately straight for large energies; this eliminates the need of a preliminary change into action-angle variables, making the proofs simpler than in the superquadratic case (3).

We mention also the earlier results by Jacobowitz and Struble [9] and by Hartman [7], where the superquadratic nature of the potential was used to apply the Poincaré-Birkhoff theorem to prove the existence of periodic solutions in a class of systems of the form (3).

2. Results

THEOREM 1. Assume that $V(x) \in C^{(5)}$ and that p(t) is continuous (actually, summable is enough) with $\int_0^1 p(t) dt = 0$.

For any $0 < \omega < 1$ satisfying for some $c_0 > 0$ and $\mu > 0$ the set of inequalities

$$\left|\omega-\frac{m}{n}\right|>\frac{c_0}{n^{2+\mu}}\quad\forall m,\,n\in\mathbb{Z},\,n\neq0,$$

there exists an integer $k_0 = k(c_0, \mu) > 0$ such that Poincaré map $F: (x, \dot{x})_{t=0} \mapsto (x, \dot{x})_{t=1}$ of eq. (2) possesses a countable set of invariant curves $y = f_{\omega+k}(x) \equiv f_{\omega+k}(x+1)$, for all integers $|k| \ge k_0$ with translation numbers $\omega + k$. The corresponding invariant circles in the phase cylinder $(x \mod 1, \dot{x})$ have rotation numbers ω . For large |k| we have

$$f_{\omega+k+1}(x) - f_{\omega+k}(x) = 1 + O(k^{-1})$$
 and $f'_{\omega+k} = O(k^{-1})$.

Relative measure of invariant circles in an annulus $N \le \dot{x} \le N+1$ tends to one as $N \to \infty$.

Applying a recent result of Herman [8] on the existence of invariant curves for $C^{(3)}$ -small perturbations of the twist maps, one can lower the smoothness assumption to $V \in C^{(4)}$, at the expense of replacing the Diophantine condition on ω by the requirement that ω be of constant type. One also loses the statement on the relative measure of invariant circles.

Each such invariant circle sweeps out an invariant torus in the extended phase space $\{(x \mod 1, \dot{x}, t \mod 1)\} = S^1 \times \mathbb{R} \times S^1$. Each orbit on such a torus is quasiperiodic with basic frequencies 1 and $\omega + k$.

Physically, these orbits correspond to quasiperiodic rotations with average angular velocity $\omega + k$, or to quasiperiodic translations (in the potential well interpretation) with the average speed $\omega + k$. The basic frequencies of the quasiperiodic solutions are 1 and $\omega + k$.

The existence of invariant circles implies at once the following:

COROLLARY 1. Any solution of (2) is bounded in the phase cylinder $\{(x \mod 1, \dot{x})\} = S^1 \times \mathbb{R}$; in other words, any solution of (2) has bounded angular velocity.

Since Poincaré map F defined above is a composition of monotone twist maps, we can apply the Aubry-Mather theorem [1, 12, 13], obtaining

COROLLARY 2. For any real number ω there exists a Birkhoff orbit with that rotation number. Physically, there exists a motion with any average angular velocity. Furthermore, as a consequence of the Poincaré-Birkhoff's theorem, for any rational $\omega = p/q$ there exists a periodic solution satisfying x(t+q) = x(t) + q.

A note added in proof. After this paper had been submitted I learned that Jürgen Moser had proved a similar statement for a more general equation $\ddot{x} + W_x(x, t) = 0$ with W_x periodic in both arguments, satisfying the exactness condition $\int_0^1 \int_0^1 W_x(x, t) \, dx \, dt = 0$ and smooth enough [17]. Moser's proof is based on a variational approach; the proof given in the present note is different—it is based on the application of Moser's invariant curve theorem [13]. The proof given here carries over almost verbatim to the more general case when the dependence on x and t is not separate. The argument requires, however, the differentiability in t as well, as it does in [17]; it suffices to assume $V \in C^{(5)}(\mathbb{R}^2)$. In the special case (2) no smoothness in t is assumed.

3. Proof

We will show that F is an exact map of the cylinder which is $C^{(4)}$ -close to the linear shear for large $|y| = |\dot{x}|$.

3.1. Exactness of the Poincaré map

The exactness of the cylinder map F is due, as it turns out, to the zero-average property of p(t) - this was observed previously by Moeckel, Robinson [5] and others. For completeness, we provide a proof.

Let C_0 be an arbitrary noncontractible circle going once around the cylinder, and let C_0 be its image under the flow of eq. (2):

$$\dot{z} = f(z, t), \quad z = \begin{pmatrix} x \\ y \end{pmatrix}, \quad f = \begin{pmatrix} y \\ -V'(x) + p(t) \end{pmatrix}.$$
 (4)

Thus $C_1 = FC_0$; we have to show that

$$\int_{C_0} y \, dx = \int_{C_1} y \, dx. \tag{5}$$

Let A_t be the annulus bounded by the horizontal circle $H = \{y = 0\}$ of the x-axis (oriented in the positive direction) and by C_t (oriented in the opposite direction to the x-axis), figure 1.

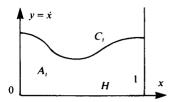


FIGURE 1. Proof of exactness.

Differentiating the area $\iint_{A_t} dx \, dy$ and observing that only one component C_t of the boundary is moving with the flow (4), we obtain:

$$\frac{d}{dt} \int \int_{A_t} dx \, dy = - \int_{C_t} f \cdot n \, ds,$$

where n is the outward unit normal vector.

Using the divergence theorem, we rewrite the flux on the right-hand side as

$$-\int_{C_{t}} f \cdot n \, ds = \int_{H} f \cdot n \, ds - \int \int_{A_{t}} \operatorname{div} f \, dx \, dy \stackrel{\text{(A)}}{=} \int_{H} f \cdot n \, ds$$
$$= \int_{0}^{1} V'(x) \, dx + \int_{0}^{1} p(t) \, dx = \int_{0}^{1} p(t) \, dt \stackrel{\text{(B)}}{=} 0,$$

where the Hamiltonian (i.e., divergence-free) character of f was used in (A) and zero-average property of p was used in (B). We conclude that

$$\iint_{A_0} dx \, dy = \iint_{A_1} dx \, dy,$$

which by Stokes' theorem is equivalent to the desired exactness property (5).

3.2. Near-integrability

To prove Theorem 1 it remains to show that the map F is $C^{(4)}$ -close to the twist for large y; we will show in fact, that

$$F\begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ v \end{pmatrix} + \begin{pmatrix} \bar{P} \\ 0 \end{pmatrix} + r(x, y), \tag{6}$$

where $\bar{P} = \int_0^1 \int_0^1 p(\tau) d\tau dt$ and $r = \text{col}(r_1, r_2)$ is $C^{(4)}$ -small: there exists a constant C depending on $V(\cdot)$ and $p(\cdot)$ only, such that

$$||r_1||_{C^4}, ||r_2||_{C^4} < C|y|^{-1}.$$
 (6a)

The idea of the proof is to show that for high angular velocities the effect of periodic potential averages out to zero.

To prove (6) and (6a) we let $z(t) \equiv z(t; s_1, s_2)$ be the solution of (4) with $z(0; s_1, s_2) = \operatorname{col}(s_1, s_2)$. To estimate r(x, y) we introduce the derivative vectors

$$z_i = \frac{\partial z}{\partial s_i}, \quad z_{ij} = \frac{\partial^2 z}{\partial s_i \partial s_j}, \quad z_{ijk} = \frac{\partial^3 z}{\partial s_i \partial s_i \partial s_k}, \quad z_{ijkl} = \frac{\partial^4 z}{\partial s_i \partial s_i \partial s_k \partial s_l},$$

where i, j, k, l=1 or 2 and show that for t=1

$$z_1(1) = {1 \choose 0} + O(|y|^{-1}), \quad z_2(1) = {1 \choose 1} + O(|y|^{-1}),$$

while

$$|z_{ij}(1)|, |z_{ijk}(1)|, |z_{ijkl}(1)| = O(|y|^{-1})$$
 for y large.

These vectors satisfy the linear, Hessian cubic and quartic versions of eq. (4):

$$\dot{z}_i = f_z(z, t)z, \quad z_1(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad z_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$
 (7a)

$$\dot{z}_{ii} = f_z z_{ii} + f_{zz}(z) [z_i, z_i], \quad z_{ii}(0) = 0, \tag{7b}$$

$$\dot{z}_{ijk} = f_z z_{ijk} + f_{zz}[z_k, z_{ij}] + f_{zz}[z_i, z_{jk}] + f_{zz}[z_{ik}, z_j] + f_{zz}[z_k, z_i, z_j], \quad z_{ijk}(0) = 0, \quad (7c)$$

and similarly for z_{ijkl} . The derivatives f_{zz} , f_{zzz} and f_{zzzz} are tensors (multilinear functions of their arguments) with coefficients being second, third and fourth mixed partials in x and y of the components of f(z). For f(z, t) as in (4), these depend only on $V^{(i)}(x)$ with $i \le 5$ and thus satisfy, for some C > 0 and for all $x \in \mathbb{R}$, the bounds

$$|f_{zz}[u,v]| \le C|u||v| \tag{8a}$$

$$|f_{zzz}[u, v, w]| \le C|u||v||w| \tag{8b}$$

$$|f_{zzzz}[u, v, w, \zeta]| \le C|u||v||w||\zeta|. \tag{8c}$$

To obtain the desired $C^{(4)}$ -estimate (6a) on the remainder we will use the following estimate on $z(t; x_0, y_0) \equiv z(t; z_0)$ valid for large $|y_0|$, given in Lemma 1 and in its two corollaries.

3.3. Auxiliary lemmas

LEMMA 1. Let $B = \max_{x} |V'(x)| + \max_{t} |p(t)|$. For any x_0 , y_0 , t with $y_0 \ge 8B$ and $0 \le t \le 1$, the solution $z(t; z_0)$ of (4) lies in the triangle shown in figure 2, i.e. satisfies

$$y_0 + \frac{2B}{y_0}(x(t; z_0) - x_0) \ge y(t; z_0) \ge y_0 - \frac{2B}{y_0}(x(t; z_0) - x_0), \tag{9a}$$

$$x_0 \le x(t; z_0) \le x_0 + 2y_0.$$
 (9b)

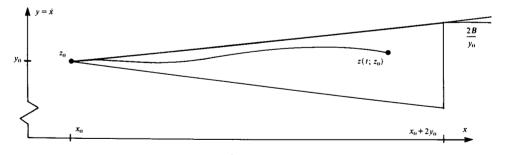


FIGURE 2. Estimate on $z(t; z_0)$ as given by Lemma 2.

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Proof of Lemma 1. We show that the solution $z(t; z_0)$ stays in the triangle defined by (9) during $0 \le t \le 1$ by proving first that $z(t, z_0)$ cannot leave through the sloped sides

$$y = y_0 \pm \frac{2B}{v_0} (x - x_0) \stackrel{\text{def}}{=} L_{\pm}(x), \quad x_0 \le x \le x_0 + 2y_0,$$

since the flow crosses these inwards. First we show that the lower boundary is crossed upwards: if $y(t) - L_{-}(x(t)) = 0$ and $x_0 \le x(t) \le x_0 + 2y$, then

$$\frac{d}{dt} \left[y - \left(y_0 - \frac{2B}{y_0} (x - x_0) \right) \right] = -V' + p + \frac{2B}{y_0} y$$

$$= -V' + p + \frac{2B}{y_0} \left(y_0 - \frac{2B}{y_0} (x - x_0) \right)$$

$$> -B + 2B - \frac{4B^2}{y_0^2} (x - x_0)$$

$$> B - \frac{4B^2}{y_0^2} \cdot 2y_0 = B - \frac{8B^2}{y_0} > 0, \text{ since } y_0 > 8B.$$

Second, the top boundary of the triangle defined by (9) is crossed downwards: for points (x, y) on the top boundary segment we have

$$\frac{d}{dt}[y - L_{+}(x)] = \frac{d}{dt} \left[y - \left(y_{0} + \frac{2B}{y_{0}} (x - x_{0}) \right) \right] = -V' + p - \frac{2B}{y_{0}} y$$

$$= -V' + p - \frac{2B}{y_{0}} \cdot \left(y_{0} + \frac{2B}{y_{0}} (x - x_{0}) \right)$$

$$< B - 2B - \frac{4B^{2}}{y_{0}^{2}} (x - x_{0}) < -B < 0.$$

Since z(t) stays below the line, it does not travel too fast to the right – this gives the estimate on x(t):

$$\dot{x} = y < y_0 + \frac{2B}{v_0}(x - x_0),$$

and thus

$$x(t) \le x_0 + \frac{y_0^2}{2B} (e^{2Bt/y_0} - 1)$$
 for $t \ge 0$,

which for $0 \le t \le 1$ and $y_0 \ge 8B$ gives

$$x(t) \le x_0 + 2y_0 t. \qquad \Box$$

COROLLARY 3. There exists a constant C > 0 independent of (x_0, y_0) such that for all $|y_0| \ge 8B$ and for all x_0

$$\left| \int_0^1 V^{(k)}(x(t, x_0, y_0)) dt \right| \le C|y_0|^{-1}, \quad k = 1, 2, 3, 4, 5.$$
 (10)

Proof of Corollary 3. The idea of the proof is simple: if x(t) had changed linearly with time, the integral in question would have been zero. Since x(t) changes

near-linearly by Lemma 1, the integral should be small. To make this rigorous, we choose x as the independent variable, obtaining:

$$\left| \int_0^1 V^{(k)}(x(t)) dt \right| = \left| \int_{x_0}^{x_1} V^{(k)}(x) \frac{1}{y(x)} dx \right|$$

$$= \left| \frac{V^{(k)}(x)}{y(x)} \Big|_{x_0}^{x_1} - \int_{x_0}^{x_1} \frac{V^{(k-1)}(x)y'(x)}{u^2(x)} dx \right| \le \frac{C}{|y_0|},$$

where Lemma 1 was used to estimate $y^2 \ge Cy_0^2$ from below and the estimates

$$|y'(x)| = \left| \frac{dy}{dx} \right| = \left| \frac{-V' + p}{y} \right| \le \frac{C}{|y_0|} \text{ and } |x_1 - x_0| < 2y_0$$

were incorporated, both following from Lemma 1.

COROLLARY 4. Let $g:[0,1] \to \mathbb{R}$ be C^1 -bounded: $|g(t)|, |g'(t)| < C_1$, let $V \in C^{(5)}$ and assume that $z(t; z_0)$ satisfies conclusion (9) of Lemma 1. Then $\exists C > 0$ such that for all $y_0 \ge 8B$ we have

$$\left| \int_0^1 g(t) V^{(k)}(x(t)) dt \right| < C|y_0|^{-1}, \quad 1 \le k \le 5.$$
 (11)

Proof of Corollary 4. The idea of the proof is similar to the one above. The added ingredient (implicit in our analytic argument) is the fact that g changes slowly with respect to x(t) so that the integrand averages out to near-zero over one full 2π -rotation of x.

With $h(x) \equiv V^{(k-1)}(x)$, we have, choosing x as the independent variable:

$$\left| \int_{0}^{1} gV^{(k)} dt \right| = \left| \int_{0}^{1} gh'(x(t)) dt \right| = \left| \int_{0}^{1} g(t) \frac{h'(x(t))}{y(x(t))} \dot{x} dt \right|$$

$$= \left| \int_{x_{0}}^{x_{1}} h'(x) \frac{g(t(x))}{y(x)} dx \right|$$

$$= \left| h(x) \frac{g(t(x))}{y(x)} \Big|_{x_{0}}^{x_{1}} - \int_{x_{0}}^{x_{1}} h(x) \frac{g' dt/dx y(x) - g(t(x))y'(x)}{y^{2}(x)} dx \right|$$

$$\leq \left| h(x) \frac{g(t(x))}{y(x)} \Big|_{x_{0}}^{x_{1}} \right| + |x_{1} - x_{0}| \frac{\max |g' - gy'|}{\min y^{2}}.$$

Since h, g are bounded and $|y| \ge |y_0| - 4B$ (Lemma 1), the first term in the last sum satisfies the desired estimate. Similarly, the second term is less than $C|y_0|^{-1}$ since $|x_1 - x_0| \le 2|y_0|$, and

$$|y'(x)| = \left| \frac{dy}{dx} \frac{dt}{dx} \right| = \left| \frac{\dot{y}}{\dot{x}} \right| = \left| \frac{-V' + p}{y} \right| \le \frac{B}{|y|}.$$

3.4. End of the proof of Theorem 1

We now begin the end of the proof of the theorem.

As the first step, we estimate the position $z(1; z_0)$ after one period. Integrating the second component of eq. (3), we obtain for $0 \le t \le 1$:

$$y(t) = y_0 + \int_0^t (-V' + p) dt = y_0 + \int_0^t p(\tau) d\tau + O\left(\frac{1}{|y_0|}\right),$$
 (12)

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using Corollary 3; in particular, for t = 1 we obtain

$$y(1) = y_0 + O(|y_0|^{-1}).$$

Furthermore, integrating (12), we obtain

$$x(1) = x_0 + \int_0^1 y(t) dt = x_0 + \int_0^1 \left[y_0 + \int_0^t p(\tau) d\tau + O(|y_0|^{-1}) \right] dt$$
$$= x_0 + y_0 + \bar{P} + O(|y_0|^{-1}).$$

This proves the C^0 -smallness of the remainder r in (6). To get the C^1 -estimate, we evaluate $z_i(1)$: introducing matrices $A(t) = f_z(z(t))$ and $B(t) = \int_0^t A(\tau) d\tau$, we obtain from the linearized equation (7a):

$$z_i(1) = z_i(0) + \int_0^1 A(t)z_i(t) dt = z_i(0) + \int_0^1 B'(t)z_i(t) dt$$
$$= z_i(0) + B(1)z_i(1) - \int_0^1 B(t)A(t)z_i(t) dt;$$

the last step involved integration by parts. Using Corollary 3 on the elements of the matrix B we obtain

$$B(1) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + O(|y_0|^{-1}),$$

while Corollary 4 gives

$$\int_0^1 B(t)A(t)z_i(t) dt = O(|y_0|^{-1}),$$

resulting in

$$z_i(1) = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} z_i(0) + O(|y_0|^{-1}),$$

proving the C^1 -estimate on r.

The last argument shows also that the fundamental solution matrix Φ for the linearized equation (7a) satisfies

$$\Phi(t,\tau) = \begin{pmatrix} 1 & t-\tau \\ 0 & 1 \end{pmatrix} + O(|y_0|^{-1}), \quad 0 \le \tau \le t \le 1.$$

This will be used in the remaining estimates.

Equation (7b) is inhomogeneous in z_{ij} , but the inhomogeneity has been estimated in the previous steps. To show that $z_{ij}(1) = O(|y_0|^{-1})$, we use the variation of constant formula to obtain

$$z_{ij}(1) = z_{ij}(0) + \Phi(1; 0)z_{ij}(0) + \int_0^1 \Phi(1; t)f_{zz}[z_1, z_j] dt$$
$$= \int_0^1 \Phi(1; t)f_{zz}[z_i(t), z_j(t)] dt.$$

Using the above estimate on $\Phi(t; \tau)$ together with the observation that the components of f_{zz} are either 0 or -V'''(x(t)), we can apply Corollary 4 to conclude that $z_{ij}(t) = O(|y_0|^{-1})$ for $0 \le t \le 1$.

The estimate $z_{ijk}(1) = O(|y_0|^{-1})$ is obtained in precisely the same way, by using all previous estimates on z, z_i , z_{ij} together with Corollary 4. The last estimate $z_{ijkl}(1) = O(|y_0|^{-1})$ is obtained analogously. This argument makes it clear that the remainder r is C^k -small for large y_0 if $V \in C^{k+1}$.

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