文章编号:1000 - 582x(2000)03 - 0080 - 04

Non-collision Closed Orbits with Fixed Energy for Symmetrical Singular Hamiltonian Systems*

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ABSTRACT: Under a weak force type condition, we study the existence of non-collision periodic solutions with fixed energy for a singular Hamiltonian systems. Our methods depend on the Mountain Pass Lemma and the estimates of Morse index and the number of collisions.

KEYWORDS: singular Hamiltonian systems; Morse index; non-collision solutions
CLC number: O 175.7 **Document Code**: A

We consider the existence of non - collision periodic solutions of

$$(Ph)\quad \begin{cases} \ddot{q} + \nabla V(q) = 0, \text{in } R^n & (Ph.1) \\ \frac{1}{2}|\dot{q}(t)|^2 + V(q(t)) = h, \text{in } R^n & (Ph.2) \end{cases}$$

where $q = (q_1, \cdots, q_n) \in R^n$ and $V \in C^1(R^n \setminus \{0\}, R)$. (Ph) is related with the two - body problems with potential V and energy h, it is important in mechanics and physics.

Recently there have been several papers which deal via variational methods with the prescribed energy problems ([1 ~5]).in [5], Tanaka proved the existence of generalized solutions that may enter the singularity under suitable assumptions for singular potentials through the relation between the Morse index and the number of collisions of generalized solutions. Tanaka also got the existence of classical solutions of (Ph) under some stronger assumptions. In this paper, through the Mountain Pass Lemma and the estimates of Morse index of critical point and the relation between the Morse index and the number of collisions, we prove the existence of a classical (non - collision) solution of (Ph) for a symmetrical singular Hamiltonian system with weak force:

Theorem 1 Assume that V satisfies the following conditions:

(V1) $V(q) \in C^2(R^n \setminus \{0\}, R)$

(V2) $V(-q) = V(q), \forall q \in R^n \setminus \{0\}$

(V3) $V(q) < 0$ for all $q \in R^n \setminus \{0\}$ and $V(q) \to 0$ as $|q| \to \infty$

(V4) There is an $\alpha_1 \in (0,2)$ such that $\nabla V(q)q \geq -\alpha_1 V(q), \forall q \in R^n \setminus \{0\}$

(V5) There is an $\alpha_2 \in (0,2)$ and $R_0 > 0$ such that $\nabla V(q)q \leq -\alpha_2 V(q), \ \forall 0 \leq |q| \leq R_0$

(V6) $V(q) = -1/|q|^\alpha + W(q)$, where $\alpha \in (0, 2)$ and $|q|^\alpha W(q)$, $|q|^{\alpha+1}\nabla W(q)$, $|q|^{\alpha+2}\nabla^2 W(q) \to 0$ as $|q| \to 0$.

Then for any $h < 0$, there exists at least one classical (non - collision) solution of (Ph).

Remark It follows from (V3) ~ (V5) that for some constants $a_1, a_2, a_3 > 0$

$$\frac{a_1}{|q|^{\alpha_1}} \leq -V(q) \leq \frac{a_2}{|q|^{\alpha_2}} \quad \text{for} \quad 0 < |q| \leq R_0 \tag{1}$$

* Received date: : 1999-08-22
Foundation item: : Supported by National Natural Science Foundation (19871096)
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$$-V(q) \leqslant \frac{a_3}{|q|^{\alpha_1}} \text{ for } |q| \geqslant R_0 \qquad (2)$$

Comparing Theorem 1 with the theorem of Tanaka [5], we add the symmetry assumption (V2) for V, but we get the existence of one classical non-collision periodic solution for (Ph), this is different from Tanaka [5].

1 Proof of Main Result

Let us introduce the following notations:

$$H = H^{1,2}(S^1, R^n)$$

$$E = \{u \in H \mid u\left(t + \frac{1}{2}\right) = -u(t)\}$$

$$\Lambda_0 = \{u \in E \mid u(t) \neq 0, \ \forall t \in [0,1]\}$$

$$< u, v > = \int \dot{u}\dot{v}, \ \|u\|_E^2 = \int |\dot{u}|^2 \quad (u, v \in E)$$

Here and always in the sequel $\int$ stands for $\int_0^1 dt$. It is well known that $\|u\|_E$ is a norm on E equivalent to the usual one and one has

$$\|u\|_E \geqslant 4|u|_\infty \qquad (3)$$

Define the following function on Λ_0:

$$I(u) = \frac{1}{2}\|u\|_E^2 \cdot \int[h - V(u)] \qquad (4)$$

Formally, it is known ([1]) that the critical point of I on Λ_0 gives rise, after a rescaling of time, to periodic solutions of (Ph). Since Λ_0 is an open subset of E and we deal with the potential with weak force, it is difficult to verify the Palais - Smale compactness condition for I(u). To get the Palais - Smale compactness condition, we introduce the modified function:

$$I_\beta(u) = \frac{1}{2}\int_0^1 |\dot{u}|^2 d\tau \cdot \left[h + \int_0^1 \left[-V(u) + \frac{\beta}{|u|^2}\right] d\tau\right] \qquad (5)$$

$$I_{\beta,\varepsilon}(u) = \frac{1}{2}\int_0^1 |\dot{u}|^2 d\tau \left[h + \int_0^1 \left[-V(u) + \frac{\beta}{|u|^2}\right] d\tau\right] + \int_0^1 \frac{\varepsilon}{|u|^2} d\tau \qquad (6)$$

Lemma 1 Assume (V1) - (V4) and $h < 0$. Then for $\beta \in (0,1]$ and $\varepsilon \in (0,1]$, $I_{\beta,\varepsilon}(u)$ satisfies (PS^+). That is, for any $s > 0$, if a sequence $\{u_j \mid j = 1,2,\cdots,\} \subset \Lambda_0$ satisfies $I_{\beta,\varepsilon}(u_j) \to s$ and $I'_{\beta,\varepsilon}(u_j) \to 0$ *in* E^*, then u_j possesses a subsequence converging to some $u \in \Lambda_0$.

The critical point of $I_{\beta,\varepsilon}$ on Λ_0 will be found by means of the Mountain Pass Theorem ([6]).

Lemma 2 Let (V1) - (V5) hold. Then there exist $\rho, m > 0$ such that

(i) $I_{\beta,\varepsilon}(u) \geqslant m$ for all $\varepsilon > 0$, $\beta > 0$ and all $u \in \Lambda_0$, $\|u\|_E = \rho$;

(ii) there exist $\varepsilon_0 > 0, \beta_0 > 0$, $u_0, u_1 \in \Lambda_0$ with $\|u_0\|_E < \rho < \|u_1\|_E$, such that $I_{\beta,\varepsilon}(u_0), I_{\beta,\varepsilon}(u_1) < m$, $\forall 0 < \varepsilon \leqslant \varepsilon_0, \forall 0 < \beta \leqslant \beta_0$

Proof. (i). Using (1) and (3) we have

$$I_{\beta,\varepsilon}(u) \geqslant \frac{1}{2}\|u\|_E^2\int[h - V(u)] \geqslant \frac{1}{2}\|u\|_E^2\int\left[h + \frac{a_1}{|u|^{\alpha_1}}\right] \geqslant \frac{h}{2}\|u\|_E^2 + C_1\|u\|_E^{2-\alpha_1}, \text{for } \|u\|_E \text{ small} \qquad (7)$$

This proves (i).

(ii) we take $u^* = (\cos 2\pi t, \sin 2\pi t, 0, \cdots, 0) \in \Lambda_0$. Then

$$|u^*|^2 = 1, \|u^*\|_E^2 = \int_0^1 |\dot{u}^*(t)|^2 dt = 4\pi^2$$

and

$$I_{\beta,\varepsilon}(Ru^*) = 2\pi^2 R^2\left[\int_0^1 \cdot \left[(h - V(Ru^*) + \frac{\beta}{R^2}\right] d\tau\right] + \frac{\varepsilon}{R^2} \qquad (8)$$

By (V3) and $h < 0$, we have $I_{\beta,\varepsilon}(Ru^*) \to -\infty$ as $R \to \infty$. This proves the existence of $u_1 \in \Lambda_0$ such that $\|u_1\| > \rho$ and $I_{\beta,\varepsilon}(u_1) < m$ for enough small ε and β.

Lastly, let $r > 0$ be small enough. Then by (1) and (3) we have

$$I_{\beta,\varepsilon}(ru) \leqslant 2\pi^2 r^2(h + a_2 r^{-\alpha_2} + \beta r^{-2}) + \varepsilon r^{-2} = 2\pi^2 hr^2 + 2\pi^2 a_2 r^{2-\alpha_2} + 2\pi^2\beta + \varepsilon r^{-2} \quad (9)$$

Since $0 < \alpha_2 < 2$, then the existence of $\varepsilon_0 > 0, \beta_0 > 0$ and u_0 satisfying (ii) follows.

Lemma 3. Assume (V1) - (V5) and $h < 0$. Then for any $\beta \in (0, \beta_0]$ and $\varepsilon \in (0, \varepsilon_0]$, $I_{\beta,\varepsilon}(u)$ possesses a critical point $u_{\beta,\varepsilon}(\tau) \in \Lambda_0$ such that

(i) $I'_{\beta,\varepsilon}(u_{\beta,\varepsilon}) = 0$, $I_{\beta,\varepsilon}(u_{\beta,\varepsilon}) \in [m, M]$, $I'_{\beta,\varepsilon}(u_{\beta,\varepsilon}) = 0$ where $0 < m < M$ are independent of β and ε.

(ii) there are $C > 0$ such that $0 < \|u_{\beta,\varepsilon}\|_E \leqslant C$, $\forall \beta \in (0, \beta_0], \forall \varepsilon \in (0, \varepsilon_0]$.

(iii) index $I''_{\beta,\varepsilon}(u_{\beta,\varepsilon}) \leqslant 1$

Proof. (i) Lemma 1 and Lemma 2 allow us to apply the Mountain Pass Theorem ([6]) yielding a critical point $u_{\beta,\varepsilon} \in \Lambda_0$ of $I_{\beta,\varepsilon}$. From the min - max characterization of $I_{\beta,\varepsilon}$

$(u_{\beta,\epsilon})$ it follows:

$$0 < m \leqslant I_{\beta,\epsilon}(u_{\beta,\epsilon}) \leqslant \max_{R>0} I_{\beta,\epsilon}(Ru^*) \leqslant \max_{R>0} I_{\beta_0,\epsilon_0}(Ru^*) = M > 0 \qquad (10)$$

(ii) Since $I'_{\beta,\epsilon}(u_{\beta,\epsilon}) = 0$, we have $I'_{\beta,\epsilon}(u_{\beta,\epsilon})u_{\beta,\epsilon} = 0$, i.e.,

$$\| \dot{u}_{\beta,\epsilon} \|_\epsilon^2 [h + \int_0^1 [-V(u_{\beta,\epsilon}) - \frac{1}{2}\nabla V(u_{\beta,\epsilon})u_{\beta,\epsilon}]d\tau = \int_0^1 \frac{2\epsilon}{|u_{\beta,\epsilon}|^2} \qquad (11)$$

By (i), $u_{\beta,\epsilon}(\tau) \neq \text{const}$, $\| \dot{u}_{\beta,\epsilon} \|_2 > 0$, we get from (2.9) and (V4),

$$\frac{2-\alpha_1}{2}\int_0^1 -V(u_{\beta,\epsilon})d\tau \geqslant \int_0^1 [-V(u_{\beta,\epsilon}) - \frac{1}{2}\nabla V(u_{\beta,\epsilon})u_{\beta,\epsilon}]d\tau \geqslant -h \qquad (12)$$

Thus

$$h + \int_0^1 [-V(u_{\beta,\epsilon}) + \frac{\beta}{|u_{\beta,\epsilon}|^2}]d\tau \geqslant \frac{-\alpha_1 h}{2-\alpha_1} > 0 \qquad (13)$$

$$M \geqslant I_{\beta,\epsilon}(u_{\beta,\epsilon}) \geqslant \frac{-\alpha_1 h}{2(2-\alpha_1)} \| u_{\beta,\epsilon} \|_\epsilon^2 \qquad (14)$$

Therefore $\| u_{\beta,\epsilon} \| \leqslant C$ for some positive constant number C independent of β and ϵ.

(iii) follows from the estimate of Morse index about the Mountain Pass critical point (see[7]).

Definition 1.([5]) By a generalized (collision) solution, we mean a function $q(t)$ such that

(i) $q(t) \in C(R, R^N)$ is a periodic function.

(ii) $D = \{t \in R \mid q(t) = 0\}$ is a set of measure 0.

(iii) $q(t) \in C^2(R \setminus D, R^N)$ and $q(t)$ satisfies (Ph) on $R \setminus D$.

Similar to the proof of Tanaka [5], we can prove that $\bar{u}(\tau) = \lim_{\beta\to 0}\lim_{\epsilon\to 0} u_{\beta,\epsilon}(\tau)$ is a generalized solution for (Ph). In the following, we further prove that $\bar{u}(\tau)$ is actually a non-collision solution for (Ph).

Lemma 4([5]) Assume (V6) and $u_\beta(\tau) = \lim_{\epsilon\to 0} u_{\beta,\epsilon}(\tau)$. Then

$$\liminf_{\beta\to 0} \text{index } I''_\beta(u_\beta) \geqslant (n-2)i(\alpha)\upsilon \qquad (15)$$

where υ is the number of times at which $\bar{u}(\tau)$ enters the singularity 0, that is,

$$\upsilon = \#\{\tau \in (0,1] \mid \bar{u}(\tau) = 0\} \in N \cup \{\infty\} \qquad (16)$$

and $i(\alpha) \in N$ is an integer defined by

$$i(\alpha) = \max\{k \in N \mid k < \frac{2}{2-\alpha}\} \qquad (17)$$

Now Theoreme 1.1 can be proved by Lemma 2.4 and Lemma 2.3.

In fact, by Lemma 2.3 and the lower semicontinuity of Morse index we have

$$\liminf_{\beta\to 0} \text{index } I''_\beta(u_\beta) \leqslant 1 \qquad (18)$$

By $0 < \alpha < 2$ we have $i(\alpha) \geqslant 1$. Hence $\upsilon \leqslant 1$ by (2.13). Symmetry property $\bar{u}(t + \frac{1}{2}) = -\bar{u}(t)$ implies $\upsilon = 0$.

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给定能量对称奇异哈米尔顿系统的非碰撞闭轨

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摘　要：在弱力型条件下，依据于山路引理、Morse 指数及碰撞次数的估计，研究了给定能量的对称奇异哈米尔顿系统的非碰撞周期解的存在性。

关键词：奇异哈米尔顿系统；Morse 指标；非碰撞解

（责任编辑　张小强）

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AB Intio Study on the Interaction between CH_4 and the Coal Surface

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ABSTRACT: The atom cluster model of coal surface is proposed. Quantum chemical ab initio calculation with base set STO 4-31G indicates that the interaction between CH_4 and coal surface is anisotropy and the maximum interaction potential (or adsorption potential) is 2.65 kJ/mol, rotation potential barrier is 1.34 kJ/mol. These results have shown that the adsorption of methane on coal surface should be a physical process (that is, freezing on surface).

KEYWORDS: coal; CH_4; interaction potential; quantum chemistry; ab initio calculation

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