在哈密顿动力学中，广义坐标 $q_\alpha\ (\alpha=1,2,\cdots,s)$ 和广义动量 $p_\alpha\ (\alpha=1,2,\cdots,s)$. 变换：

$$\begin{cases} P_\alpha = P_\alpha(p,q,t) \\ Q_\alpha = Q_\alpha(p,q,t) \end{cases} (\alpha=1,2,\cdots,s)$$

要求变换后的动力学方程仍然是哈密顿正则方程 → 正则变换. 如何满足？

$$\delta\int_{t_1}^{t_2}\left[\sum_{\alpha=1}^{s} p_\alpha \dot q_\alpha - H(p,q,t)\right]dt \overset{\text{等价}}{\Longleftrightarrow} \delta\int_{t_1}^{t_2}\left[\sum_{\alpha=1}^{s} P_\alpha \dot Q_\alpha - K(P,Q,t)\right]dt = 0$$

可以相差某个函数 U 对时间的全导数

$$\left(\sum_{\alpha=1}^{s} p_\alpha \dot q_\alpha - H\right) - \left(\sum_{\alpha=1}^{s} P_\alpha \dot Q_\alpha - K\right) = \frac{dU}{dt} \quad \text{即} \quad \sum_{\alpha=1}^{s} p_\alpha dq_\alpha - \sum_{\alpha=1}^{s} P_\alpha dQ_\alpha + (K-H)\,dt = dU$$

若用 $U_1 = U_1(q,Q,t)$，则参照 有：

$$\begin{cases} p_\alpha = \dfrac{\partial U_1}{\partial q_\alpha},\quad P_\alpha = -\dfrac{\partial U_1}{\partial Q_\alpha} \quad (\alpha=1,2,\cdots,s) \\ K-H = \dfrac{\partial U_1}{\partial t} \end{cases}$$

若用 $U_3(q,P,t) = U_1(q,Q,t) + \sum_{\alpha=1}^{s} P_\alpha Q_\alpha$（勒让德变换），则

$$\begin{aligned} dU_3 &= dU_1 + \sum_{\alpha=1}^{s} P_\alpha dQ_\alpha + \sum_{\alpha=1}^{s} Q_\alpha dP_\alpha \\ &= \sum_{\alpha=1}^{s} p_\alpha dq_\alpha + \sum_{\alpha=1}^{s} Q_\alpha dP_\alpha + (K-H)\,dt \end{aligned}$$ 有

$$\begin{cases} p_\alpha = \dfrac{\partial U_3}{\partial q_\alpha},\quad Q_\alpha = \dfrac{\partial U_3}{\partial P_\alpha} \quad (\alpha=1,2,\cdots,s), \\ K-H = \dfrac{\partial U_3}{\partial t} \end{cases}$$

正则变换的目标：若 $K(P,Q,t)=0$，则

$$\begin{cases} \dot P_\alpha = -\dfrac{\partial K}{\partial Q_\alpha} = 0 \\ \dot Q_\alpha = \dfrac{\partial K}{\partial P_\alpha} = 0 \end{cases}$$

由上面 $K-H = \frac{\partial U_3}{\partial t}$，若 $K=0$，则

$$H(q,p,t) + \frac{\partial U_3}{\partial t} = 0 \Rightarrow H\left(q_1,q_2,\cdots,q_s,\frac{\partial U_3}{\partial q_1},\frac{\partial U_3}{\partial q_2},\cdots,\frac{\partial U_3}{\partial q_s},t\right) + \frac{\partial U_3}{\partial t} = 0.$$

→ 哈密顿-雅可比方程、解：哈密顿主函数 $S(q,P,t)$.

$$\begin{aligned} \frac{dS}{dt} &= \sum_{\alpha=1}^{s} \frac{\partial S}{\partial q_\alpha}\dot q_\alpha + \sum_{\alpha=1}^{s} \frac{\partial S}{\partial P_\alpha}\dot P_\alpha + \frac{\partial S}{\partial t} \\ &= \sum_{\alpha=1}^{s} p_\alpha \dot q_\alpha + 0 + (0-H) \\ &= L \end{aligned}$$

由此 $S = \int L\,dt$.

若 H 不显含时间，则可以把哈密顿-雅可比方程中的 q 与 t 分离.

令 $S(q,P,t) = W(q,P) + f(t)$，则 $H\left(q,\frac{\partial W}{\partial q}\right) = -f'(t)$. 分解为

$$\begin{cases} f'(t) = -E \\ H\left(q_1,q_2,\cdots,q_s,\dfrac{\partial W}{\partial q_1},\dfrac{\partial W}{\partial q_2},\cdots,\dfrac{\partial W}{\partial q_s}\right) = E \end{cases} \qquad \begin{aligned} &\Rightarrow f(t) = -Et \\ &\Rightarrow K = H + \frac{\partial W}{\partial t} = H = E \end{aligned}$$

$W(q,P)$ 叫哈密顿特征函数.

例：用哈密顿－雅可比方程求解谐振子问题.

$$H=\frac{1}{2m}p^2+\frac{1}{2}kx^2$$

解：H不显含t ⇒ 求W.

$\Rightarrow K=E.$

$$H=\frac{1}{2m}p^2+\frac{1}{2}kx^2 \Rightarrow \frac{1}{2m}\left(\frac{\partial W}{\partial x}\right)^2+\frac{1}{2}kx^2=E.$$

$$\Rightarrow W(x,E)=\sqrt{mk}\int\sqrt{\frac{2E}{k}-x^2}\,dx$$

变换后的"P".

$$\dot{X}=\frac{\partial K}{\partial P}=\frac{\partial K}{\partial E}=1 \Rightarrow X=t-t_0$$

$$X=\frac{\partial W}{\partial P}=\frac{\partial W}{\partial E}=\sqrt{\frac{m}{k}}\int\frac{dx}{\sqrt{\frac{2E}{k}-x^2}}=\sqrt{\frac{m}{k}}\arcsin\left(x\sqrt{\frac{k}{2E}}\right)$$

$$x=\sqrt{\frac{2E}{k}}\sin\left(\sqrt{\frac{k}{m}}X\right)$$

$$=\sqrt{\frac{2E}{k}}\sin\left(\sqrt{\frac{k}{m}}t-\sqrt{\frac{k}{m}}t_0\right)$$