拉格朗日动力学 $L=L(q,\dot q,t)$

哈密顿动力学 $H=H(q,p,t)$ $\quad p_\alpha=\frac{\partial L}{\partial \dot q_\alpha}$

$[p_\alpha q_\alpha]=\left[\frac{\partial L}{\partial \dot q_\alpha}q_\alpha\right]=\left[\frac{L}{q_\alpha/t}q_\alpha\right]=[Lt]$ 具有作用量量纲!

量子论的量子化条件是把作用量加以量子化

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可作为从经典力学到量子力学的跳板

系统：只有完整约束 主动力都有(广义)势能

拉格朗日方程：$\frac{d}{dt}\frac{\partial L}{\partial \dot q_\alpha}-\frac{\partial L}{\partial q_\alpha}=0 \quad (\alpha=1,2,\cdots,s)$

⇓

定义 $p_\alpha=\frac{\partial L}{\partial \dot q_\alpha} \Rightarrow \dot p_\alpha=\frac{\partial L}{\partial q_\alpha}$

$L=L[q,\dot q(q,p),t] \quad \dot q_\beta=\dot q_\beta(q,p,t) \quad (\beta=1,2,\cdots,s)$

$\bar L(q,p,t)=L[q,\dot q(q,p,t),t]$

$$\begin{cases}\frac{\partial \bar L}{\partial q_\alpha}=\frac{\partial L}{\partial q_\alpha}+\sum_{\beta=1}^{s}\frac{\partial L}{\partial \dot q_\beta}\frac{\partial \dot q_\beta}{\partial q_\alpha}=\dot p_\alpha+\sum_{\beta=1}^{s}p_\beta\frac{\partial \dot q_\beta}{\partial q_\alpha}=\dot p_\alpha+\sum_{\beta=1}^{s}\frac{\partial}{\partial q_\alpha}(p_\beta\dot q_\beta)\\ \frac{\partial \bar L}{\partial p_\alpha}=\sum_{\beta=1}^{s}\frac{\partial L}{\partial \dot q_\beta}\frac{\partial \dot q_\beta}{\partial p_\alpha}=\sum_{\beta=1}^{s}p_\beta\frac{\partial \dot q_\beta}{\partial p_\alpha}=\sum_{\beta=1}^{s}\frac{\partial}{\partial p_\alpha}(p_\beta\dot q_\beta)-\dot q_\alpha\end{cases}$$

$(\alpha=1,2,\cdots,s)$ 记住各p各q相互独立, $\dot q_\beta=\dot q_\beta(q,p,t)$

$$\begin{cases}\frac{\partial}{\partial q_\alpha}\left(\sum_{\beta=1}^{s}p_\beta\dot q_\beta-\bar L\right)=-\dot p_\alpha\\ \frac{\partial}{\partial p_\alpha}\left(\sum_{\beta=1}^{s}p_\beta\dot q_\beta-\bar L\right)=\dot q_\alpha\end{cases}\quad(\alpha=1,2,\cdots,s)$$

定义 $\sum_{\beta=1}^{s}p_\beta\dot q_\beta-L=H$

$$\begin{cases}\frac{\partial H}{\partial q_\alpha}=-\dot p_\alpha\\ \frac{\partial H}{\partial p_\alpha}=\dot q_\alpha\end{cases}\quad(\alpha=1,2,\cdots,s)$$ 哈密顿正则方程

勒让德变换与哈密顿正则方程

$dL(q,\dot q,t)=\sum_{\alpha=1}^{s}\frac{\partial L}{\partial q_\alpha}dq_\alpha+\sum_{\alpha=1}^{s}\frac{\partial L}{\partial \dot q_\alpha}d\dot q_\alpha+\frac{\partial L}{\partial t}dt$

$\quad=\sum_{\alpha=1}^{s}\dot p_\alpha dq_\alpha+\sum_{\alpha=1}^{s}p_\alpha d\dot q_\alpha+\frac{\partial L}{\partial t}dt$

$d\bar L(q,p,t)=dL=\sum_{\alpha=1}^{s}\dot p_\alpha dq_\alpha+\sum_{\alpha=1}^{s}p_\alpha \underbrace{d\dot q_\alpha}_{dp_\alpha}+\frac{\partial L}{\partial t}dt$

$d\left(\sum_{\alpha=1}^{s}p_\alpha\dot q_\alpha\right)=\sum_{\alpha=1}^{s}\dot q_\alpha dp_\alpha+\sum_{\alpha=1}^{s}p_\alpha d\dot q_\alpha$

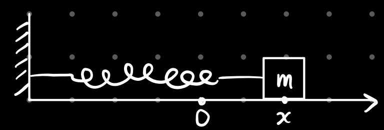
$dH=d\left(\sum_{\alpha=1}^{s}p_\alpha\dot q_\alpha-L\right)=\sum_{\alpha=1}^{s}(-\dot p_\alpha)dq_\alpha+\sum_{\alpha=1}^{s}\dot q_\alpha dp_\alpha-\frac{\partial L}{\partial t}dt$

又 $dH(p,q,t)=\sum_{\alpha=1}^{s}\frac{\partial H}{\partial q_\alpha}dq_\alpha+\sum_{\alpha=1}^{s}\frac{\partial H}{\partial p_\alpha}dp_\alpha+\frac{\partial H}{\partial t}dt$

$$\begin{cases}\frac{\partial H}{\partial q_\alpha}=-\dot p_\alpha\\ \frac{\partial H}{\partial p_\alpha}=p_\alpha\end{cases}\qquad \frac{\partial H}{\partial t}=-\frac{\partial L}{\partial t}$$

利用微分式 $d\left(\sum_{\alpha=1}^{s}p_\alpha\dot q_\alpha\right)$ 把变量从 $q,\dot q,t$ 改为 q,p,t，同时把起支配作用的函数L变换为函数 $\sum_{\alpha=1}^{s}p_\alpha\dot q_\alpha-L=H$ 这种方法叫勒让德变换

例：质量为m的物体在光滑水平面上沿x轴运动，弹簧的劲度系数为k.



解：自由度：1，广义坐标：x.

$L=T-V=\frac{1}{2}m\dot x^2-\frac{1}{2}kx^2$

$p=\frac{\partial L}{\partial \dot x}=m\dot x \Rightarrow \dot x=\frac{1}{m}p$

$H=p\dot x-L=\frac{1}{2m}p^2+\frac{1}{2}kx^2$

哈密顿正则方程

$$\begin{cases}kx=-\dot p\\ \frac{1}{m}p=\dot x \Rightarrow \frac{1}{m}\dot p=\ddot x\end{cases} \rightarrow m\ddot x=-kx$$

$x=C\cos\left(\sqrt{\frac{k}{m}}t+\theta\right)$

$p=m\dot x=-C\sqrt{km}\sin\theta\left(\sqrt{\frac{k}{m}}t+\theta\right)$

where $C=\sqrt{\frac{2E}{k}}$

对于s个自由度的力学系统，把 q_α & p_α 构成的2s空间叫做相空间.

对于大数目粒子的集合，考虑处于给定约束条件下许多性质完全相同的力学系统(系综)；各种可能的代表点则对应于系综中所有力学系统的状况，各种可能的相轨道则对应于系综的演变.

定义相空间中代表点的密度 ρ：在相空间体积元 dv 中，代表点的个数为 dN.

有 $dN=\rho dv$，其中 $dv=dq_1 dq_2\cdots dq_s\, dp_1 dp_2\cdots dp_s$

dv 必须充分大，以包含大数目的代表点，才谈得上密度；又必须充分小，才可以把 ρ 看作相空间的连续函数.

随着时间的推移，系综的所有代表点各沿着互不相交的相轨道从相空间的一个区域转移到另一个区域.

$$\frac{d\rho}{dt}=\frac{\partial\rho}{\partial t}+\sum_{\alpha=1}^{s}\left(\frac{\partial\rho}{\partial p_\alpha}\dot p_\alpha+\frac{\partial\rho}{\partial q_\alpha}\dot q_\alpha\right)$$

研究通过 dv 的一对曲面 q_1, q_1+dq_1 进出的 dv 的代表点数

$dv=dA_1 dq_1$ 其中 $dA_1=dq_2\cdots dq_s dp_1\cdots dp_s$

代表点数的净增量

$$\frac{\partial N_1}{\partial t}=[\rho\dot q_1 dA_1]|_{q_1}-[\rho\dot q_1 dA_1]|_{q_1+dq_1}$$

$$=-\left[\frac{\partial}{\partial q_1}(\rho\dot q_1)dq_1\right]dA_1=-\frac{\partial}{\partial q_1}(\rho\dot q_1)dv$$

从而密度的净增量

$$\frac{\partial\rho_1}{\partial t}=\frac{1}{dv}\frac{\partial N_1}{\partial t}=-\frac{\partial}{\partial q_1}(\rho\dot q_1)$$

通过其他曲面进出 dv 的代表点数可用类似办法

$$\frac{\partial\rho}{\partial t}=-\sum_{\alpha=1}^{s}\left[\frac{\partial}{\partial q_\alpha}(\rho\dot q_\alpha)+\frac{\partial}{\partial p_\alpha}(\rho\dot p_\alpha)\right]$$

$$=-\sum_{\alpha=1}^{s}\left(\frac{\partial\rho}{\partial q_\alpha}\dot q_\alpha+\rho\frac{\partial\dot q_\alpha}{\partial q_\alpha}+\frac{\partial\rho}{\partial p_\alpha}\dot p_\alpha+\rho\frac{\partial\dot p_\alpha}{\partial p_\alpha}\right)$$

代入 $\frac{d\rho}{dt}$ 式得

$$\frac{d\rho}{dt}=-\sum_{\alpha=1}^{s}\rho\left(\frac{\partial\dot q_\alpha}{\partial q_\alpha}+\frac{\partial\dot p_\alpha}{\partial p_\alpha}\right)$$

代入哈密顿正则方程

$$\frac{d\rho}{dt}=-\sum_{\alpha=1}^{s}\rho\left(\frac{\partial^2 H}{\partial q_\alpha\partial p_\alpha}-\frac{\partial^2 H}{\partial p_\alpha\partial q_\alpha}\right)=0$$

刘维尔定理：代表点在相空间运动时，密度 ρ 不变.

统计力学的基本定理，是2s维的相空间中的定理. 在统计力学中讨论系综时需要运用哈密顿动力学而非拉格朗日动力学.

力学量 $\varphi(p,q,t)$ 的时间变化率

$$\frac{d\varphi}{dt}=\frac{\partial\varphi}{\partial t}+\sum_{\alpha=1}^{s}\left(\frac{\partial\varphi}{\partial q_\alpha}\dot q_\alpha+\frac{\partial\varphi}{\partial p_\alpha}\dot p_\alpha\right)$$

$$=\frac{\partial\varphi}{\partial t}+\sum_{\alpha=1}^{s}\left(\frac{\partial\varphi}{\partial q_\alpha}\frac{\partial H}{\partial p_\alpha}-\frac{\partial\varphi}{\partial p_\alpha}\frac{\partial H}{\partial q_\alpha}\right)$$

定义两个力学量的泊松括号

$$[\varphi,\psi]=\sum_{\alpha=1}^{s}\left(\frac{\partial\varphi}{\partial q_\alpha}\frac{\partial\psi}{\partial p_\alpha}-\frac{\partial\varphi}{\partial p_\alpha}\frac{\partial\psi}{\partial q_\alpha}\right)$$

则 $\frac{d\varphi}{dt}$ 可表为 $\frac{d\varphi}{dt}=\frac{\partial\varphi}{\partial t}+[\varphi,H]$

哈密顿正则方程可表为 $\begin{cases}\dot p_\beta=[p_\beta,H]\\ \dot q_\beta=[q_\beta,H]\end{cases}$

基本泊松括号 $[q_\alpha,q_\beta]=0$ $[p_\alpha,p_\beta]=0$ $[q_\alpha,p_\beta]=\delta_{\alpha\beta}$

从经典力学到量子力学的过渡是通过正则量子化完成的.

即经典力学中的力学量(如X和Y等)在量子力学中是用算符或矩阵(如 $\hat X$ 和 $\hat Y$ 等)表示的，而两个力学量的泊松括号用量子泊松括号(对易子)代替，即

$$[X,Y]\rightarrow\frac{1}{i\hbar}[\hat X,\hat Y]=\frac{1}{i\hbar}(\hat X\hat Y-\hat Y\hat X)$$

量子力学中的两个力学量 $\hat X$ 和 $\hat Y$ 是否可以同时具有确定的值就看它们的量子泊松括号 $\frac{1}{i\hbar}(\hat X\hat Y-\hat Y\hat X)$ 是否为零.