Geometry of Lagrangian manifolds in thermodynamics

V.P. Maslov, A.S. Mishchenko (Moscow)

Abstract

It is considered, that the classical thermodynamic properties of substance are defined by relations connecting volume, pressure, temperature, entropy and energy of the given substance. Generally substance is characterized by some number of magnitudes, which half is intensive, and half — by extensive magnitudes. From this point of view pressure and temperature are considered as intensive magnitudes, and volume and entropy - extensive magnitudes. The modern point of view consists that in a condition of a thermodynamic equilibrium the substance should be characterized by a point in the space $R^{2n+1}(p,q,\Phi)$, where coordinates $q=(q_1,q_2,\ldots,q_n)$ are intensive magnitudes, first two of which are pressure and temperature ($q_1 = P, \quad q_2=-T$), and coordinate $p_1,p_2,\ldots,p_n$) are extensive coordinates first two from which are volume and entropy ($p_1=V, \quad p_2=S$). First four coordinates (P,V,T,S) describe, so to tell, variables of a mechanical nature for homogeneous substances. generally follows to consider heterogeneous (i.e. multicomponent) systems, and also variables not mechanical nature (for example, electromagnetic properties). In any case, the space $R^{2n+1}(p,q,\Phi)$ is supplied by a contact structure, i.e. differential 1-form $\omega = d\Phi - pdq$, and the set of thermodynamic equilibrium states of substance is represented by a submanifold $L\subset R^{2n+1}(p,q,\Phi)$, such that $\omega=0$. Hence tha projection $L_0\subset R^{2n}(p,q)$ is a Lagrangian submanifold in symplectic space $R^{2n}(p,q)$ with the symplectic form $\Omega = dp\wedge dq$. Function Φ is function of action on Lagrangian manifold L_0, $d\Phi = pdq$. For classical thermodynamics it coincides with a thermodynamic potential ($\Phi = E+PV-TS$).

By Gibbs ([1]) the energy E is a function of variables (V,S), as, however, and all remaining thermodynamic magnitudes. It hence, that Lagrangian manifold L_0 bijectively is projected on a domain in the space $R^2(P,S)$, i.e. the manifold L is defined by the graph of function $E=E(V,S)$.

Implicitly Gibbs actually assumed, that the surface $E=E(V,S)$, being noncompact, its any plane of support has by property, that touches a surface in each common point. This condition ensures realization of the following statement: from minimization thermodynamic potential at fixed P and T the positiveness of Hessian of function $E=E(V,S)$, $\mathrm{Hess}_{(V,S)}E(V,S)>0$ follows. By Maslov ([3]) such condition are called essential. Then in essential condition are fulfilled local thermodynamic inequalities ([2]). Let's consider function

$$\tilde{\Phi}^L(q) = \min_{q(x)=q;x\in L}\Phi(x),$$

under condition of existence of the minimum in question. Consider a symplectic transformation φ of symplectic spaces

$$\varphi : R^{2n}(p,q)\longrightarrow R^{2n}(P,Q)$$

and Lagrangian manifold

$\Gamma_\varphi \subset R_{4n}(P,p,Q,q)$, which is the graph of transformations φ. Let S - be function of action on Lagrangian manifold Γ_φ, $dS = PdQ - pdq$. Let's assume, that manifold Γ_φ is uniquely projected on the space $R^{2n}(Q,q)$. Then function S can be understood as function of variables (Q,q), $S = S(Q,q)$. In this case the function S is called generating function of transformation φ.

contact

be defined similar to manifold L_1.

Theorem 1. *At an approaching choice of boundary conditions on manifold L and transformation φ the following formula takes place*

$$\tilde{\Phi}^{L_1}(Q) = \min_q \left(S(Q,q) + \tilde{\Phi}^L(q) \right).$$

Similar, if $\varphi_1, \varphi_2, \ldots, \varphi_n$ is a sequence of symplectic transformations which admit generating functions

$$S_1(Q,q_1), S_2(q_1,q_2), \ldots, S_n(q_{n-1},q_n),$$

and $L_1 = \tilde{\varphi}_1\tilde{\varphi}_2 \cdots \tilde{\varphi}_n(L)$, then

$$\tilde{\Phi}^{L_1}(Q) = \min_{q_1,q_2,\ldots,q_n} \left(S_1(Q,q_1) + S_2(q_1,q_2) + \cdots + S_n(q_{n-1},q_n) + \tilde{\Phi}^L(q_n) \right).$$

The choice of boundary conditions should supply existence of a minimum at an evaluation of $\tilde{\Phi}^{L_1}$. The theorem 1 supplies the map of insignificant points of manifold L into insignificant points of manifold L_1 (compare [3]).

the Lagrangian L.

Theorem 2. *Assume that the Lagrangian $L(q,\dot{q})$ satisfies the conditions that the index of inertia of $Hess_{q,\dot{q}}L$ equals to (n,n). Let $S(Q,q,t)$ be the generating function of transformation induced by Lagrangian L. Assume that there is a minimum*

$$\tilde{\Phi}^{L_1}(Q) = \min_q \left(S(Q,q) + \tilde{\Phi}^L(q) \right).$$

Then

$$Hess_Q \tilde{\Phi}^{L_1}(Q) < 0.$$

The theorem 2 ensures realization local thermodynamic inequalities in essential points of Lagrange manifold L_1.

Theorem 3. *Let L be a Lagrange manifold which uniquely projected onto $p-$ coordinates. Then at an approaching choice of boundary conditions in essential points the local thermodynamic inequalities are fulfilled, i.e.*

$$Hess_q \Phi^L(q) < 0.$$

As approaching boundary conditions for the theorem 3 the following condition can serve: **Condition 1.** *The function $E(p)$, $dE = -qdp$, $E = \Phi^L(p) - pq$ is locally convex upwards in all domain of definition $G(p) \subset R^n(p)$ behind elimination of some compact set $K \subset G(p)$.*

The condition 1 is fulfilled for the majority of modelling examples of gases (ideal gas, Van der Waals gas , degenerated Fermi gas).

The theorems 1 and 2 allow to construct such Lagrangian manifolds, which are not projected uniquely on p - coordinate, but in all essential points satisfie to local thermodynamic inequalities..

References

[1] J.W.Gibbs, *A method of geometrical representation of the thermodynamic properties of substatnces by mean of surfaces,* Trans. Connect. Acad., 1873, II, Dec., p. 382-404.

[2] L.D.Landau, E.M.Lifshitz, *Statistical Physics,* – "Nauka", Moscow., 1964.

[3] V.P.Maslov, *On a class of Lagrangian manifolds corresponding to variational problrms, problems of control theory an thermodynamics*(in Russian)// Funct. Analysis and applications, Vol. 32, No 2., 1998