STEKLOV MATHEMATICAL INSTITUTE,

RUSSIAN ACADEMY OF SCIENCES

Valery V. Kozlov

On Gibbs Distribution for Quantum Systems

2011

The Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = \widehat{H}\psi$$

in Hilbert space $\mathcal{H}$. ψ is the wave function, $\widehat{H}$ is the Hamilton operator; $i^2 = -1$, $\hbar$ is the Plank constant.

The quantization of classical systems

$$\dot{x} = \frac{\partial H}{\partial p}, \qquad \dot{p} = -\frac{\partial H}{\partial x}$$

$$H = \frac{1}{2}(p,p) + V(x) = \frac{1}{2}\sum p_j^2 + V(x_1,\dots,x_n) \tag{1.1}$$

$\mathbb{T}^n = \{x_1,\dots,x_n \mod 2\pi\}$ is the configuration space

The standard procedure of quantization

$$x \mapsto \widehat{x}, \quad p \mapsto -i\hbar\frac{\partial}{\partial x}, \quad H \mapsto \widehat{H}$$

$$\widehat{H} = -\frac{\hbar^2\Delta}{2} + \widehat{V}(x) \tag{1.2}$$

Δ is the Laplace operator; $\mathcal{H} = L_2(\mathbb{T}^n)$,

$|\psi|^2$ is the probability density function.

A is an observable value, a Hermitian operator in $\mathcal{H}$,

$$\langle A\rangle_\psi = \langle A\psi, \psi\rangle \ \text{ is its average value in a state } \psi, \tag{1.3}$$

$\langle\cdot,\cdot\rangle$ is the Hermitian scalar product in $\mathcal{H}$.
$\langle A\rangle_\psi$ does not change with t if and only if $[A, \widehat{H}] = 0$.

$$\langle A\rangle_\psi = \operatorname{tr}(AP_\psi) = \operatorname{tr}(P_\psi A) \tag{1.4}$$

$P_\psi\colon \varphi \mapsto \langle\varphi,\psi\rangle\psi$ is the projection onto the unit vector $\psi \in \mathcal{H}$
P_ψ is a Hermitian operator and $\operatorname{tr} P_\psi = 1$
P_ψ **is called the density operator.**
$i\hbar \dfrac{\partial P_\psi}{\partial t} = [\widehat{H}, P_\psi]$ is the quantum Liouville equation

The Gibbs operator

$$\frac{e^{-\beta\widehat{H}}}{\operatorname{tr} e^{-\beta\widehat{H}}}, \qquad \beta \in \mathbb{R}_+.$$

This is a Hermitian operator and its trace is equal to 1.

$$(1.4) \quad \Longleftrightarrow \quad \langle A\rangle = \frac{\operatorname{tr}(Ae^{-\beta\widehat{H}})}{\operatorname{tr} e^{-\beta\widehat{H}}}.$$

The Fauler–Darwin approach

$$A^{(N)} = \frac{1}{N}\sum_{j=1}^{N} A_j \quad \text{— the 'summators'}$$

The Landau approach (introduce a thermostat)

The third approach

Polynomial conservation laws

$$\widehat{P} = \sum a_\mu(x)(-i\hbar\partial)^\mu, \qquad \mu \in \mathbb{Z}_+^n \tag{2.1}$$

$$\partial = (\partial_1, \dots, \partial_n), \quad \partial_j = \frac{\partial}{\partial x_j}; \quad \partial^\mu = \partial_1^{\mu_1} \dots \partial_n^{\mu_n}; \qquad a_\mu : \mathbb{T}^n \to \mathbb{C}$$

Definition. **The symbol of (2.1) is a formal series**

$$\operatorname{symb} \widehat{P} = P = \sum a_\mu(x) p^\mu, \tag{2.2}$$

$$p = (p_1, \dots, p_n), \quad p^\mu = p_1^{\mu_1} \cdots p_n^{\mu_n}.$$

Obviously, $\operatorname{symb} \widehat{H} = H$.

Definition. **The operators** $\widehat{P}$ **and** $\widehat{H}$ **are independent if their symbols are independent.**

Conjecture **1. If there is a nontrivial uniform differential operator which commutes with the Hamilton operator, then there is a nontrivial uniform operator commuting with $\widehat{H}$ and polynomial with respect to differentiations.**

Example. $V \mapsto \varepsilon V$, ε **is a small parameter.**

Proposition **1. If there is a nontrivial uniform operator in the form of a series $\widehat{P}_0 + \varepsilon \widehat{P}_1 + \varepsilon^2 \widehat{P}_2 + \cdots$ which commutes with $\widehat{H} = -\frac{\hbar^2}{2}\Delta + \varepsilon \widehat{V}(x)$, then Conjecture 1 holds.**

Let

$V(x) = \sum V_m e^{i(m,x)}$, $m \in \mathbb{Z}^n$, $(m,x) = m_1 x_1 + \cdots + m_n x_n$,

be the Fourier series for the potential V,

$S = \{m \in \mathbb{Z}^n : V_m \neq 0\}$ **be the spectrum of the function V.**

S **is invariant with respect to the involution $m \mapsto -m$.**

Let $\mathbb{R}^n = W_1 \oplus W_2$,

$W_1 \perp W_2$ with respect to $(\cdot\,,\cdot)$, and $S \subset (W_1 \cup W_2)$.

Then the classical system with Hamiltonian (1.1)

breaks into two independent subsystems.

Of course, we suppose $0 < \dim W_j < n$.

Definition. If such a representation is not possible, then the system is called connected.

In the quantum case $\mathcal{H}_1$ and $\mathcal{H}_2$ are generated by the wave functions $\psi_j = \sum c_k e^{i(k,x)}$, $k \in W_j$, $\sum |c_k|^2 = 1$.

At the same time, $\mathcal{H} = L_2(\mathbb{T}^2)$, and

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2. \tag{2.3}$$

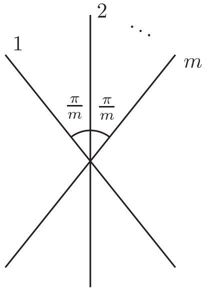
Theorem 1. *Suppose that* $V\colon \mathbb{T}^n \to \mathbb{R}$ *is a trigonometric polynom. Then a nontrivial polynomial operator which commutes with* $\widehat{H}$ *exists if and only if the quantum system is not connected.*

See: V. Kozlov and D. Treschev. *Theoret. and Math. Phys.* 2004, v. 140, no. 3, p. 1283–1298.

***Conjecture* 2. Theorem 1 holds in the general case (when the spectrum S is not finite).**

For the classical Hamiltonian systems with two degrees of freedom this conjecture is discussed in the papers:

M. Bialy, *Func. Anal. Appl.* 1987, v. 21, no. 4, p. 64–65;
V. Kozlov and D. Treschev. *Math. USSR-Sb.* 1989, v. 63, no. 1, p. 121–139;
V. Kozlov and N. Denisova. *Sb. Math.* 2000, v. 191, no. 2, p. 189–208.

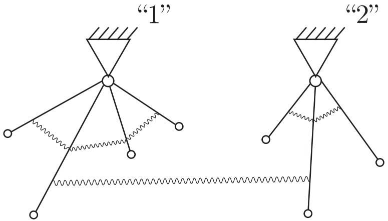


Gibbs distribution

Two independent quantum systems "1" and "2"
with the Hamiltonian operators $\widehat{H}_1$ and $\widehat{H}_2$
$\varepsilon W_{1,2}$ is the potential energy of interaction

$$\widehat{H} = \widehat{H}_1 + \widehat{H}_2 + \varepsilon W_{1,2}. \tag{3.1}$$

Example.



$$\widehat{P} = f(\widehat{H}, \varepsilon);\ \varepsilon \to 0 \quad \Longrightarrow \quad \widehat{P} = f_0(\widehat{H}_1 + \widehat{H}_2). \tag{3.2}$$

Let $\widehat{P}_1$ and $\widehat{P}_2$ be the density operators for subsystems.
***Hypothesis*. If $\varepsilon \to 0$, then**

$$\widehat{P}_0 = \widehat{P}_1 \otimes \widehat{P}_2. \tag{3.3}$$

This is the Gibbs hypothesis about thermodynamical equilibrium, when interaction disappears.

$$\widehat{P}_1 = f_1(\widehat{H}_1), \qquad \widehat{P}_2 = f_2(\widehat{H}_2). \tag{3.4}$$

Taking (3.2) and (3.4) into account, we rewrite (3.3) in the following form:

$$f_0(\widehat{H}_1 + \widehat{H}_2) = f_1(\widehat{H}_1) \otimes f_2(\widehat{H}_2),$$
$$f_k(z) = c_k e^{-\beta z}; \quad k = 1, 2;$$
$$\operatorname{tr} \widehat{P}_k = 1 \quad \Longrightarrow \quad c_k = \left[\operatorname{tr} e^{-\beta \widehat{P}_k}\right]^{-1}.$$

Theorem 2. *Suppose that Conjecture 1 and the Gibbs hypothesis hold. Then for $\varepsilon \to 0$ the density operators of the noninteracting subsystems take the form of the canonical Gibbs distribution.*

$$\beta = \frac{1}{kT},$$

T is an absolute temperature, k is the Boltzmann constant.

The Supplement: Some results and problems about the polynomial conservation laws

A. $M = \{x_1, \ldots, x_n\}$ is a compact real-analytic manifold, and

$$\sum g_{ij}(x)\, dx_i\, dx_j \tag{4.1}$$

is the Riemann metric on M.

$$\mathcal{H} = L_2(M, d\mu), \quad d\mu = g^{-1/2}\, d^n x, \quad g = \det \|g_{ij}\|.$$

The Hamilton operator

$$\widehat{H} = \frac{\hbar^2}{2}\,\Delta, \tag{4.2}$$

where

$$\Delta = -\frac{1}{\sqrt{g}} \sum \frac{\partial}{\partial x_j}\left(\sqrt{g}\, g^{kj} \frac{\partial}{\partial x_k}\right)$$

is the Laplace–Beltrami operator.

Theorem 3. *Let* $n = 2$ *and* $\chi(M) < 0$. *Then operator integrals do not exist.*

See: V. Kozlov. *Doklady Math.* 2005, v. 71, no. 2, p. 300–302.

Definition. **The principal symbol of a polynomial differentional operator $\widehat{P}$, $\deg \widehat{P} = m$, is the homogeneous polynomial in momenta**

$$\sum_{|\mu|=m} a_\mu(x) p^\mu.$$

***Proposition* 2. If two polynomial operators commute, then their principal symbols commute in the symplectic sense (their Poisson bracket is zero).**

B. ***Definition.*** **The polynomial oprator integral $\widehat{P}$ is called irreducible, if there is no polynomial integral $\widehat{Q}$ with $\deg \widehat{Q} < \deg \widehat{P}$.**

$$\frac{a\,dx^2 + 2b\,dx\,dy + c\,dy^2}{g(x,y)}; \quad a > 0,\ b^2 - ac < 0,$$

$g\colon \mathbb{T}^2 \to \mathbb{R}$ is an analytic function.

C. The local aspect of this problem.

See: V. Kozlov. *Symmetries, Topology and Resonances in Hamiltonian Mechanics*. Springer-Verlag. 1996.