Gauge Transformations, the Galileo Invariance of the Modified Kramers Equation for Waves Processes in the Phase Space and Quantum Mechanic

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Цель исследований, о которых будет говориться в докладе

- Поиск примера математической модели, дающей, возможно, более точное описание квантовых процессов, чем уравнение Шредингера (с учетом, например, процессов декогеренции).
- Исследование полученной модели и поиск эффектов, не укладывающихся в стандартные модели квантовых процессов.

Общие предположения и уточнение цели

- Квантовую систему нельзя изолировать от взаимодействия с окружением.
- Хорошо бы научиться моделировать квантовые процессы, учитывающие влияние среды на систему с тем, чтобы описывался процесс перехода от чистого состояния к смешанным (декогеренция).
- Построить математическую модель квантового процесса, сохраняя базовый принцип волны-частицы (движущейся частицы с изменяющимся вектором внутреннего состояния), но не в конфигурационном пространстве, а в фазовом, сохраняя принцип суперпозиции волн и правило вычисления распределения вероятностей нахождения частицы.

Presuppositions of the model

We consider certain mathematical model of a process whose state at each moment of time t is given by a (complex valued) wave function $\varphi(x,p,t)$ on the phase space R^6, where (x,p) *in* R^6.

Suppose that:

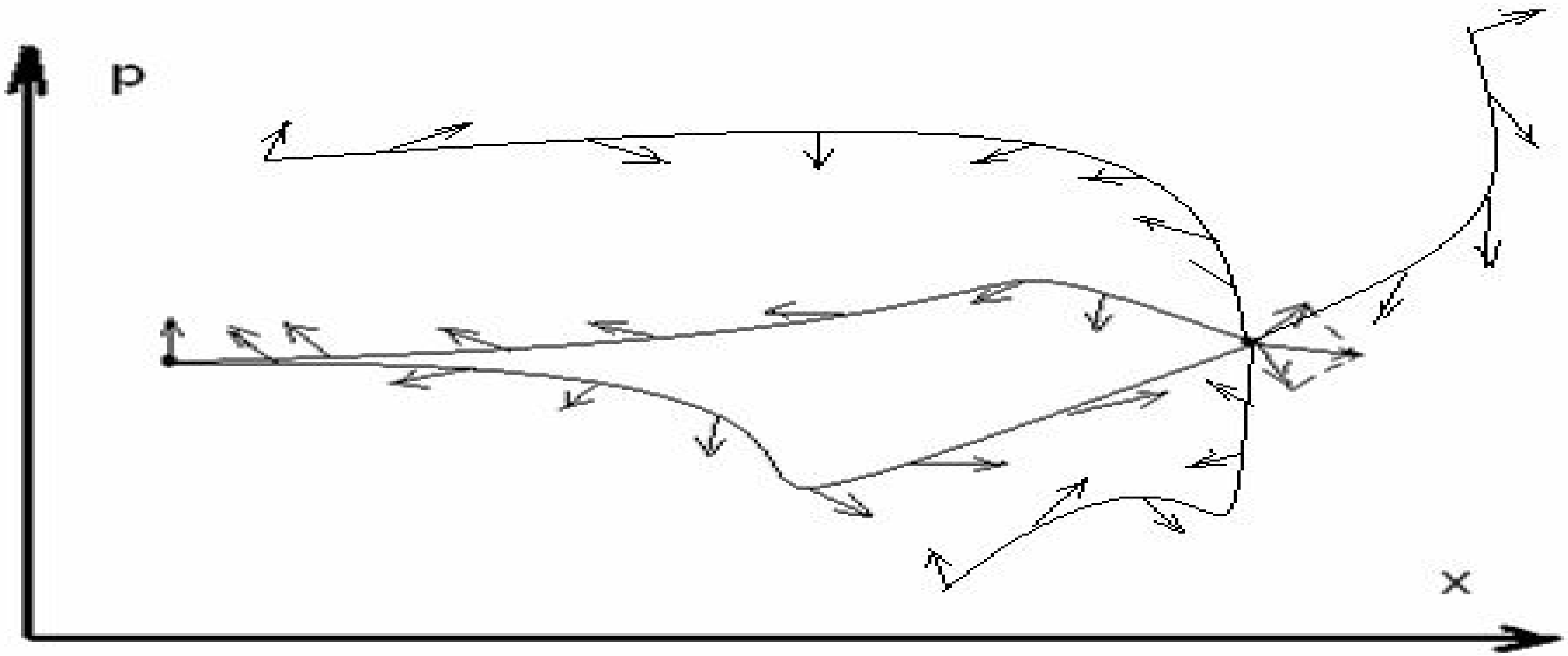
- wave functions obey the superposition principle on the phase space;
- the density of probability $\rho_D(x,p)$ in a bounded domain of the phase space $(x,p) \in D \subseteq R^6$ is given by the standard formula

$$\rho_D(x,p) = |\varphi(x,p)|^2 \Big/ \int_D |\varphi(x,p)|^2 \, dxdp$$

It is assumed that each complex vector of the wave function φ is simultaneously in 2 motions:

- values $\varphi(x,p)$ of the wave function move along the random trajectories given by the classical Kramers equation describing the diffusion motion of a particle in the phase space under action of external forces defined by the potential function $V(x)$ and the heat medium with temperature T, and the medium resistance per unit of mass γ.
- the phase of the wave function at the point (x, p) changes with constant angular velocity $\omega = mc^2/\hbar$ in the coordinate system related with this point, where m is the mass of the particle, c is the light velocity, $\hbar$ is the Planck constant.

Основная идея вывода уравнения процесса



Картинка Фейнмана в фазовом пространстве

- **Частица движется по случайной траектории. При этом вектор внутреннего состояния этой частицы, меняется с некоторой постоянной скоростью угловой скоростью $\omega = mc^2/\hbar$ в движущейся системе координат.**
- **Нужно рассмотреть интеграл по вероятностной мере на траекториях, определенной диффузионным (броуновским) процессом.**
- **Начальное распределение комплексных векторов φ(x,p,0) считать произвольным.**
- **Определить распределение векторов φ(x,p,t) в момент t.**

The classical Kramers equation

The diffusion process (the heat Brownian motion) is given by the Kramers equation:

$$\frac{\partial f}{\partial t} = \sum_{j=1}^{3}\left(\frac{\partial V}{\partial x_j}\frac{\partial f}{\partial p_j} - \frac{p_j}{m}\frac{\partial f}{\partial x_j}\right) + \gamma\sum_{j=1}^{3}\frac{\partial}{\partial p_j}\left(p_j f + kTm\frac{\partial f}{\partial p_j}\right),$$

where

f (x,p,t) is the density of probability distribution of the particle in the phase space at the moment of time *t*;

V(x) is the potential function of the external forces acting on the particle;

m is the mass of the particle;

γ=β/m is the resistance coefficient of the medium per unit of mass;

k is the Boltzmann constant;

T is the temperature of the medium.

About the change of the wave phase

- We suppose that the phase of the wave function at the point *(x, p)* changes with constant angular velocity $\omega = mc^2/\hbar$ in the proper time τ. This velocity is very big and we have need of calculation effects of the theory of relativity.
- By the theory of relativity : $\tau = (Et - xp)/(mc^2)$
  and $\varphi(x, p, t) = \varphi_0 \exp(-i\omega\tau) = \varphi_0 \exp\left(-(i/\hbar)(Et - xp)\right)$.
- That is why the shift of the wave function with respect to coordinate x on Δx with conservation of the proper time at the point *(x, p)* yields the phase shift in the oscillation of the function $\varphi(x,p,t)$ on $-i\Delta xp/\hbar$.
- This also gives that the operator of infinitesimal shift $\partial/\partial x_j$ is replaced by the operator $\partial/\partial x_j - ip_j/\hbar$.
- Respectively, if one multiplies this operator by $i\hbar$, then one obtains the operator $p_j + i\hbar\partial/\partial x_j$.

The modified Kramers equation

Consider the following equation for the wave function *φ(x,p,t):*

$$\frac{\partial\varphi}{\partial t}=\sum_{j=1}^{3}\left(\frac{\partial V}{\partial x_j}\frac{\partial\varphi}{\partial p_j}-\frac{p_j}{m}\left(\frac{\partial}{\partial x_j}-\frac{ip_j}{\hbar}\right)\varphi\right)-\frac{i}{\hbar}\left(mc^2+\sum_{j=1}^{3}\frac{p_j^2}{2m}+V\right)\varphi+\gamma B\varphi,$$

where

$$B\varphi=\sum_{j=1}^{3}\frac{\partial}{\partial p_j}\left(\left(p_j+i\hbar\frac{\partial}{\partial x_j}\right)\varphi+kTm\frac{\partial\varphi}{\partial p_j}\right). \qquad (1)$$

Let us proceed to the study of this equation (1).

It is the Kramers equation:

$$\frac{\partial f}{\partial t}=\sum_{j=1}^{3}\left(\frac{\partial V}{\partial x_j}\frac{\partial f}{\partial p_j}-\frac{p_j}{m}\frac{\partial f}{\partial x_j}\right)+\gamma\sum_{j=1}^{3}\frac{\partial}{\partial p_j}\left(p_j f+kTm\frac{\partial f}{\partial p_j}\right).$$

An analogue of our task in statistical physics:

The Fokker-Planck equation

$$\frac{\partial P(x,t)}{\partial t} = \sum_{j=1}^{3}\left(\frac{1}{\gamma m}\frac{\partial}{\partial x_j}\left(\frac{V(x)}{\partial x_j}P(x,t)\right) + \frac{kT}{\gamma m}\frac{\partial^2 P(x,t)}{\partial x_j^2}\right) + O(\gamma^{-2}),$$

is derived from the Kramers equation

$$\frac{\partial f}{\partial t} = \sum_{j=1}^{3}\left(\frac{\partial V}{\partial x_j}\frac{\partial f}{\partial p_j} - \frac{p_j}{m}\frac{\partial f}{\partial x_j}\right) + \gamma \sum_{j=1}^{3}\frac{\partial}{\partial p_j}\left(p_j f + kTm\frac{\partial f}{\partial p_j}\right),$$

where *P(x,t)* is the density of probability distribution of the particle in the configuration space and *f (x,p,t)* is the density of probability distribution of the particle in the phase space at the moment of time *t;*

V(x) is the potential function of the external forces acting on the particle;

m is the mass of the particle;

γ=β/m is the resistance coefficient of the medium per unit of mass;

k is the Boltzmann constant;

T is the temperature of the medium.

Let be a process is described by the equation of the Kramers in the phase space . Then the Fokker-Planck equation is an approximation describing of this process in the configuration space through about 1/γ.

The results obtained earlier

Theorem. *The motion described by equation 1 asymptotically ($\gamma \to \infty$) splits into rapid and slow motion.*

1) After rapid motion the arbitrary wave function $\varphi(x,p,0)$ goes, in time of order $1/\gamma$, to a function which after normalization has the form:

$$\varphi(x,p) = \frac{1}{(2\pi\hbar)^{3/2}} \int_{R^3} \psi(y)\chi(x-y)e^{-i(y-x)p/\hbar}\,dy,$$

where $\psi(y) = \int_{R^3} \varphi(y,p,0)\,dp$ *and* $\chi(x-y) = \left(\frac{kTm}{\pi\hbar^2}\right)^{3/4} e^{-\frac{kTm(x-y)^2}{2\hbar^2}}.$

2) The slow motion starting from the wave function of this form with nonzero function $\psi(y)$, goes inside the subspace and is parameterized by the wave function $\psi(y)$ depending on time. The function $\psi(y,t)$ satisfies the Schrodinger equation of the form $i\hbar\partial\psi/\partial t = \hat{H}\psi$, where

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\sum_{j=1}^{3}\frac{\partial^2}{\partial y_j}\right) + V(y) + mc^2 - \frac{3kT}{2} + O(\gamma^{-1})$$

Более точный результат, полученный в последней работе

Заметим, что в этой теореме дается уравнение, приближенно описывающее медленный процесс с точностью до γ^0. В этом уравнении не учитываются диссипативные члены. Метод Ван Кампена позволяет строить приближенные уравнения по степеням γ^{-1}.

Используя этот метод, получена следующая теорема.

- Теорема. *Медленный процесс, о котором говорится в предыдущей теореме, более точно описывается уравнением* $i\hbar\partial\psi/\partial t = \hat{H}_1\psi$, *где*

$$\hat{H}_1 = -\frac{\hbar^2}{2m}\left(\sum_{j=1}^{3}\frac{\partial^2}{\partial y_j}\right) + V(y) + mc^2 - \frac{3kT}{2} +$$

$$+\frac{i\gamma^{-1}}{4}\left(\sum_{j=1}^{3}\frac{\hbar}{m}\frac{\partial^2 V}{\partial y_j^2} - \frac{3(kT)^2}{\hbar}\right) + O(\gamma^{-2}).$$

The decoherence of quantum states

- Further, dissipation of the process (1) leads to decoherence, and any superposition of states goes to one of eigenstates of the Hamilton operator.
- At the last stage, the mixed state of heat equilibrium (the Gibbs state) arises due to the heat influence of the medium and the random transitions among the eigenstates of the Hamilton operator.
- Besides that, it is shown that, on the contrary, if the resistance of the medium per unit of mass of particles small, then in the considered model, the density of distribution of probability satisfies the standard Liouville equation, as in classical statistical mechanics.

Задача исследования обобщенного уравнения Крамерса при малых γ

$$\frac{\partial\varphi}{\partial t}=\sum_{j=1}^{3}\left(\frac{\partial V}{\partial x_j}\frac{\partial\varphi}{\partial p_j}-\frac{p_j}{m}\left(\frac{\partial}{\partial x_j}-\frac{ip_j}{\hbar}\right)\varphi\right)-\frac{i}{\hbar}\left(mc^2+\sum_{j=1}^{3}\frac{p_j^2}{2m}+V\right)\varphi+\gamma B\varphi,$$

где

$$B\varphi=\sum_{j=1}^{3}\frac{\partial}{\partial p_j}\left(\left(p_j+i\hbar\frac{\partial}{\partial x_j}\right)\varphi+kTm\frac{\partial\varphi}{\partial p_j}\right).$$

- Это задача определение поправки к уравнению классического движения с учетом малого γ.
- Задача прохождение почти классической частицы через две щели и явление дифракции.

Gauge transformations of wave functions

- The density of probability distribution $\rho(x, p, t)$ of a quantum particle whose state at the moment of time t is given by the wave function $\varphi(x,p,t)$, is proportional to $|\varphi|^2 = \varphi \varphi^*$.

  This implies that the replacement of a wave function φ by the wave function of the form $\exp(ig/\hbar)\cdot\varphi$, where $g=g(x,p,t)$ is an arbitrary real valued function, does not change the density of the probability distribution $\rho(x, p, t)$. Such transformation of wave function is usually called a **gauge transformation**.
- Let us look how equation (1) changes under this gauge transformation.

Gauge transformations of equation 1

- Equation 1 takes the form:

$$D_0^x\varphi = \sum_{j=1}^{3}\left(\frac{\partial H}{\partial x_j}D_j^p\varphi - \frac{\partial H}{\partial p_j}D_j^x\varphi\right) + \gamma\sum_{j=1}^{3}D_j^p\left(i\hbar D_j^x\varphi + kTmD_j^p\varphi\right),$$

where

$$D_0^x = \partial/\partial t + iA_0/\hbar, \qquad D_j^x = \partial/\partial x_j + iA_j/\hbar, \qquad D_j^p = \partial/\partial p_j + iB_j/\hbar,$$

$$\mathrm{j} = 1,2,3 \text{ and in our case } A_0 = H = mc^2 + p^2/2m + V, \quad A_j = -p_j, \; B_j = 0.$$

- A gauge transform of this equation:

$$\varphi \mapsto \varphi' = \exp(-ig/\hbar)\varphi; \quad A_0 \mapsto A_0^{'} = A_0 + (\partial g/\partial t); \quad A_j \mapsto A_j^{'} = A_j + (\partial g/\partial x_j);$$

$$B_j \mapsto B_j^{'} = B_j + (\partial g/\partial p_j); \qquad \mathrm{j} = 1,2,3.$$

The Galileo invariance

- The Kramers diffusion equation is not invariant with respect to Galilean transformations.
- By definition of Galilean transformations, the new coordinate system is expressed through the old one by the following formulas: $t' = t; \quad x' = x - ut; \quad p' = p - mu;$

$$\text{and} \quad E' = p'^2/2m = E - pu + (mu^2/2),$$

where *u* is the velocity of the new coordinate system.

- Theorem. Substituting these expressions into equation 1 and then after the gauge transformation with *g*= *mux'+mut'/2* we obtain the equation 1 for φ' *(x', p', t').*

Thus, we have proved the Galileo invariance of our model.

Conclusion

- We consider the process of diffusion scattering of a wave function given on the phase space. In this process the heat diffusion is considered only along momenta. We write the modified Kramers equation describing this situation.
- In this model, the usual quantum description arises as asymptotics of this process for large values of resistance of the medium per unit of mass of particle. It is shown that in this case the process passes several stages:

1. During the first short stage, the wave function goes to one of “stationary” values.
2. At the second long stage, the wave function varies in the subspace of “stationary” states according to the Schrodinger equation.
3. Further, dissipation of the process leads to decoherence, and any superposition of states goes to one of eigenstates of the Hamilton operator. At the last stage, the mixed state of heat equilibrium (the Gibbs state) arises due to the heat influence of the medium and the random transitions among the eigenstates of the Hamilton operator.

- The model is invariant with respect to Galilean transformations.

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