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Study on the Phenomena of the System of Free Particles on the View Point of Natural Statistical Physics

By

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Abstract

In this paper, we study the phenomena of the system of free particles on the view point of natural statistical physics.

Thereby we derive the Schrödinger equation of this physical system and solve the initial value problem of this Schrödinger equation.

Thereby we obtain the structure of this physical system at the stationary state. Thus we obtain the information of the natural statistical distribution of the position variable and the momentum variable of this physical system.

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Introduction

In this paper, we study the phenomena of the system of free particles on the view point of natural statistical physics.

The mathematical model of this physical phenomena is the system of microparticles moving freely with constant velocity in the space $\boldsymbol{R} = (-\infty,\ \infty)$.

We derive the Schrödinger equation of this physical system and solve the initial value problem of this Schrödinger equation.

Thereby we obtain the structure of the physical system at the stationary state. Thus we obtain the information of the natural statistical distribution of the position variable and the momentum variable of this physical system. Thus we obtain the energy expectation

$$\overline{E} = \int_{-\infty}^{\infty} \frac{p^2}{2m} |c(p)|^2 dp$$

of the total system. Here $c(p) \in L^2$ is the Fourier transform of the L^2-density $\psi(x)$ which determines an initial distribution.

At last, we obtain the fact that this physical system is decomposed as follows:

$$\begin{aligned} \Omega &= \bigcup_{-\infty<p<\infty} \Omega_p, \ \text{(direct sum)}, \\ \Omega_p &= \{\rho \in \Omega;\ p(\rho) = p\},\ (-\infty < p < \infty), \\ P(\Omega_p) &= |c(p)|^2,\ (-\infty < p < \infty). \end{aligned}$$

As for these symbols, we refer to section 4 in this paper. As for the related works, we refer to Ito [8], [16], chapter 7, Ito [20], [26], [27], [28], [40], [44], [55] and Ito-Uddin [63].

Here I show my heartfelt gratitude to my wife Mutuko for her help of typesetting this manuscript.

1 Setting of the problem

In this section, we give the setting of the problem. We say that a particle moving freely in one dimensional space $\boldsymbol{R}$ is a **free particle**.

Therefore, any force does not acts on a free particle. Therefore each free particle with mass m moves by virtue of Newtonian equation of motion

$$m\frac{d^2x}{dt^2} = 0.$$

Here x is the variable representing the coordinate of the position of the free particle. It is the purpose to study the natural statistical phenomena of this system.

Although each free particle moves with constant velocity, the various natural statistical phenomena appear according to the initial conditions on the natural probability distributions of the position and momentum.

Really all natural existences move by virtue of the mutual interaction of forces.

Therefore the system of free particles is an idealized physical system.

Nevertheless the system of free particles is really used as an approximating model for the physical model for the ideal gas. Thus it is clarified that there are many concrete physical phenomena behind the system of free particles which is considered as a mathematical model only for the calculation until now.

2 Setting of mathematical model

In this section, we give the mathematical model of the natural statistical phenomenon of the system of free particles.

We assume that the physical system $\Omega = \Omega(\mathcal{B},\ P)$ of free particles in one dimensional space $\boldsymbol{R}$ is a probability space. An elementary event in Ω is composed of only one free particle.

Then $x = x(\rho)$ denotes the position variable of a free particle ρ and $p = p(\rho)$ denotes its momentum variable.

Here the variable x moves in the space $\boldsymbol{R}^1 = \boldsymbol{R}$ and the variable p moves in the dual space $\boldsymbol{R}_1$.

Because the space $\boldsymbol{R}^1 = \boldsymbol{R}$ is self-dual, we identify the dual space $\boldsymbol{R}_1$ with the space $\boldsymbol{R}^1$. Thus we denote the self-dual space $\boldsymbol{R}^1 = \boldsymbol{R}_1$ as the same symbol $\boldsymbol{R}$.

Assume that each free particle ρ has the mass $m > 0$. Then the total energy of the free particle ρ is equal to

$$\frac{1}{2m}p(\rho)^2$$

by virtue of the classical mechanics.

This energy variable is considered as a **generalized natural random variable**.

In this case, because the Schrödinger operator of the system of free particles will have the continuous spectrum, we must consider the generalized natural statistical state.

This is ruled by the law II in Ito [44].

Namely, the law of the natural probability distribution of $x(\rho)$ is determined by a L^2_{loc}-density $\psi(x)$ and the law of the natural probability distribution of $p(\rho)$ is determined by its Fourier transform $\hat{\psi}(p)$.

Then the local expectation $\overline{E}_S$ of the energy variable can be calculated by virtue of the fundamental statistical formulas in the law II in Ito [44]. Here S is an arbitrary compact set in $\boldsymbol{R}$ such that the condition

$$\int_S |\psi(x)|^2 dx > 0$$

is satisfied. Further using the indicator function $\chi_S(x)$ of S, we put $\psi_S(x) = \chi_S(x)\psi(x)$. Then the fundamental statistical formulas are given in the following:

$$P(\{\rho \in \Omega;\ x(\rho) \in A \cap S\}) = \frac{\displaystyle\int_{A\cap S} |\psi_S(x)|^2 dx}{\displaystyle\int_S |\psi_S(x)|^2 dx},$$

$$P(\{\rho \in \Omega;\ x(\rho) \in S,\ p(\rho) \in B\}) = \frac{\displaystyle\int_B |\hat{\psi}_S(p)|^2 dp}{\displaystyle\int_{-\infty}^{\infty} |\hat{\psi}_S(p)|^2 dp}.$$

Here S is an arbitrary compact set in $\boldsymbol{R}$ as in the above. A and B are two Lebesgue measurable sets in $\boldsymbol{R}$.

Then the local energy expectation $\overline{E}_S$ is equal to

$$\overline{E}_S = E_S[\frac{1}{2m}p(\rho)^2] = \frac{\displaystyle\int_{-\infty}^{\infty} \frac{p^2}{2m}|\hat{\psi}_S(p)|^2 dp}{\displaystyle\int_{-\infty}^{\infty} |\hat{\psi}_S(p)|^2 dp}$$

$$= \frac{\displaystyle\int_S \frac{\hbar^2}{2m}|\frac{d\psi_S(x)}{dx}|^2 dx}{\displaystyle\int_S |\psi_S(x)|^2 dx}.$$

Here we used the Plancherel formula for Fourier transformation.

Then we denote the local energy expectation as

$$J_S[\psi_S] = \frac{\displaystyle\int_S \frac{\hbar^2}{2m}|\frac{d\psi_S(x)}{dx}|^2 dx}{\displaystyle\int_S |\psi_S(x)|^2 dx}$$

and we say that $J_S[\psi_S]$ is the **local energy functional**.

Then we postulate the following principle.

Principle I (Local variational principle) When the Schrödinger operator for the physical system has the continuous spectrum, a stationary state is realized as the state where the energy functional considered locally for the physical system takes its stationary value.

By using this principle, we choose the L^2_{loc}-density realized physically in the practice among all admissible L^2_{loc}-densities for this physical system.

Therefore we consider the following problem.

Problem I (Local variational problem) Let $\{K_j\}$ be an increasing sequence of nonempty compact sets exhausting $\boldsymbol{R}$. Namely it satisfies the following conditions (i) and (ii):

(i) $K_1 \subset K_2 \subset \cdots \subset K_j \subset \cdots \subset \boldsymbol{R}$.

(ii) $\displaystyle\bigcup_{j=1}^{\infty} K_j = \boldsymbol{R}$.

Then, for an arbitrary nonnegative real number $\mathcal{E} \geq 0$, determine the locally square integrable function $\psi^{(\mathcal{E})}(x)(\neq 0)$ such that it satisfies the following conditions (1)$\sim$(4):

(1) $\psi^{(\mathcal{E})}|_{K_j} = \psi_j,\ (j = 1,\ 2,\ \cdots)$.

(2) $\psi_{j+1}|_{K_j} = \psi_j,\ (j = 1,\ 2,\ \cdots)$.

(3) $\displaystyle\int_{K_j} |\psi^{(\mathcal{E})}(x)|dx > 0$ for some $j > 0$.

(4) For $j \geq 1$ such that the condition (3) is satisfied, the functional

$$J_j[\psi_j] = \frac{\displaystyle\int_{K_j} (\frac{\hbar^2}{2m}|\frac{\psi_j(x)}{dx}|^2)dx}{\displaystyle\int_{K_j} |\psi_j(x)|^2 dx}$$

has its stationary value.

3 Mathematical analysis

By solving the local variational problem in section 2, we obtain the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_j(x)}{dx^2} = \mathcal{E}\psi_j(x),\ (x \in K_j;\ j = 1,\ 2,\ \cdots)$$

as the Euler equation. Here $\mathcal{E}$ denotes Lagrange's unknown constant.

By virtue of the conditions (1)$\sim$(4) of the problem I in section 2, we can choose the L^2_{loc}-densities $\psi^{(\mathcal{E})}(x)$ so that, for $\mathcal{E} \geq 0$, the conditions

$$\psi^{(\mathcal{E})}(x) = \psi_j(x),\ (x \in K_j;\ j = 1,\ 2,\ \cdots)$$

are satisfied.

Then $\psi^{(\mathcal{E})}(x)$ satisfies the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi^{(\mathcal{E})}(x)}{dx^2} = \mathcal{E}\psi^{(\mathcal{E})}(x),\ (-\infty < x < \infty).$$

Here $\mathcal{E}$ is the Lagrange's unknown constant.

Thus we have the following generalized eigenfunctions

$$\psi_{\pm}^{(\mathcal{E})}(x) = c(\mathcal{E})\exp\left(\pm\frac{i}{\hbar}x\sqrt{2m\mathcal{E}}\right)$$

for $\mathcal{E} \geq 0$ as the solutions of the generalized eigenvalue problem in the above.

For every $\mathcal{E} > 0$, there are two linearly independent generalized eigenfunctions. Therefore each spectrum $\mathcal{E} > 0$ is degenerate.

Here we exchange the parameter $\mathcal{E}$ for the normalization.

Namely, for $\mathcal{E} \geq 0$, we put

$$k^2 = \frac{2m\mathcal{E}}{\hbar^2},\ (-\infty < k < \infty).$$

Then we have

$$\psi^{(k)}(x) = \frac{1}{\sqrt{2\pi}}e^{ikx},\ (-\infty < k < \infty).$$

Thus we have the equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi^{(k)}(x)}{dx^2} = \mathcal{E}\psi^{(k)}(x),\ (\mathcal{E} = \frac{\hbar^2k^2}{2m}),\ (-\infty < x < \infty).$$

For this system of generalized eigenfunctions, the following normalization condition and the completeness condition are satisfied.

Theorem 3.1 *We use the above notation. Then we have the following* (1) *and* (2):

(1) (Normalization condition) *We have the equality*

$$\int_{-\infty}^{\infty}\psi^{(k')}(x)^*\psi^{(k)}(x)dx = \delta(k'-k),\ (-\infty < k,\ k' < \infty).$$

(2) (Completeness condition) *We have the equality*

$$\int_{-\infty}^{\infty}\psi^{(k)}(x')^*\psi^{(k)}(x)dk = \delta(x'-x),\ (-\infty < x,\ x' < \infty).$$

Here we denote the complex conjugate of a complex number c as c^*.

Here, by using the parameter

$$p = \hbar k,$$

we have

$$\psi^{(p)}(x) = \frac{1}{\sqrt{\hbar}}\psi^{(k)}(x),\ (p = \hbar k).$$

Then we have

$$\psi^{(p)}(x) = \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar},\ (\mathcal{E} = \frac{p^2}{2m}).$$

Thus we have the equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi^{(p)}(x)}{dx^2} = \mathcal{E}\psi^{(p)}(x),\ (\mathcal{E} = \frac{p^2}{2m}).$$

Namely $\psi^{(p)}(x)$ is the generalized eigenfunction.
Then we have the following theorem.

Theorem 3.2 *We use the above notation. Then we have the following* (1) *and* (2):

(1) (Normalization condition) *We have the equality*

$$\int_{-\infty}^{\infty}\psi^{(p')}(x)^*\psi^{(p)}(x)dx = \delta(p' - p),\ (-\infty < p,\ p' < \infty).$$

(2) (Completeness condition) *We have the equality*

$$\int_{-\infty}^{\infty}\psi^{(p)}(x')^*\psi^{(p)}(x)dp = \delta(x' - x),\ (-\infty < x,\ x' < \infty).$$

Now we put

$$\psi^{(p)}|_{K_j} = \psi_j,\ (j = 1,\ 2,\ \cdots).$$

Then we have

$$J_j[\psi_j] = \frac{\frac{\mathcal{E}}{2\pi\hbar}\int_{K_j}1dx}{\frac{1}{2\pi\hbar}\int_{K_j}1dx} = \mathcal{E},\ (\mathcal{E} = \frac{p^2}{2m}),\ (j = 1,\ 2).$$

Hence $\psi^{(p)}(x)$ is the solution of the problem I in section 2.

In the above, L^2_{loc}-densities $\psi^{(\mathcal{E})}_{\pm}(x)$, $\psi^{(k)}(x)$ and $\psi^{(p)}(x)$ are the different expressions of the solutions of the problem I in section 2 and only their normalization conditions are different. But, by virtue of the formulation of the laws of natural statistical physics, it is better to use $\psi^{(p)}(x)$ as the solutions.

Then, by virtue of the theory of Fourier transformation, there exists $c(p) \in L^2$ such that we have the relations

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} c(p) e^{ipx/\hbar} dp,$$

$$c(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x) e^{-ipx/\hbar} dx$$

for an arbitrary $\psi(x) \in L^2$.

The physical state of the total physical system Ω is determined by the initial natural probability distribution determined by a L^2-density $\psi(x)$. Then we have the generalized eigenfunction expansion

$$\psi(x) = \int_{-\infty}^{\infty} c(p) \psi^{(p)}(x) dp,$$

$$c(p) = \int_{-\infty}^{\infty} \psi^{(p)}(x)^* \psi(x) dx.$$

Then the energy expectation is given by the relation

$$\overline{E} = J[\psi] = \int_{-\infty}^{\infty} \frac{p^2}{2m} |\hat{\psi}(p)| dp = \int_{-\infty}^{\infty} \frac{p^2}{2m} |c(p)|^2 dp.$$

Further, because we have

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

by virtue of the condition of the L^2-density $\psi(x)$, we have the relation

$$\int_{-\infty}^{\infty} |c(p)|^2 dp = 1.$$

Then, because the relation

$$\frac{p^2}{2m} = \mathcal{E}$$

holds, we have the equality

$$\overline{E} = J(\psi) = \int_{-\infty}^{0} \frac{p^2}{2m} |c(p)|^2 dp + \int_{0}^{\infty} \frac{p^2}{2m} |c(p)|^2 dp$$

$$= \frac{1}{2}\int_0^\infty \mathcal{E}\sqrt{\frac{2m}{\mathcal{E}}}|c(-\sqrt{2m\mathcal{E}})|^2 d\mathcal{E} + \frac{1}{2}\int_0^\infty \mathcal{E}\sqrt{\frac{2m}{\mathcal{E}}}|c(\sqrt{2m\mathcal{E}})|^2 d\mathcal{E}$$

$$= \frac{1}{2}\int_0^\infty \mathcal{E}\sqrt{\frac{2m}{\mathcal{E}}}\left(\, |c(-\sqrt{2m\mathcal{E}})|^2 + |c(\sqrt{2m\mathcal{E}})|^2 \,\right) d\mathcal{E}.$$

Now, by putting

$$I(\mathcal{E}) = \frac{1}{2}\sqrt{\frac{2m}{\mathcal{E}}}\left(\, |c(-\sqrt{2m\mathcal{E}})|^2 + |c(\sqrt{2m\mathcal{E}})|^2 \,\right),\ (\mathcal{E} > 0),$$

we have the relations

$$\int_0^\infty I(\mathcal{E})d\mathcal{E} = \int_{-\infty}^\infty |c(p)|^2 dp = 1.$$

Therefore we have the equality

$$\overline{E} = J[\psi] = \int_0^\infty \mathcal{E}I(\mathcal{E})d\mathcal{E}.$$

Here we consider the inverse process of the method of separation of variables. At first, we consider the function

$$\psi^{(p)}(x,\ t) = \psi^{(p)}(x)\exp[-i\frac{\mathcal{E}}{\hbar}t].$$

By differentiating partially this function with respect to the time variable t, we have the equality

$$i\hbar\frac{\partial\psi^{(p)}(x,\ t)}{\partial t} = \mathcal{E}\psi^{(p)}(x)\exp[-i\frac{\mathcal{E}}{\hbar}t].$$

Here we denote the Schrödinger operator for the stationary state as

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}.$$

Then we have the equality

$$H\psi^{(p)}(x) = \mathcal{E}\psi^{(p)}(x),\ (\mathcal{E} = \frac{p^2}{2m}).$$

Hence we have the equality

$$i\hbar\frac{\partial\psi^{(p)}(x,\ t)}{\partial t} = \{H\psi^{(p)}(x)\}\exp[-i\frac{\mathcal{E}}{\hbar}t] = H\psi^{(p)}(x,\ t).$$

Therefore, by putting

$$\psi(x,\ t) = \int_{-\infty}^\infty c(p)\psi^{(p)}(x,\ t)dp,$$

we have the equality

$$i\hbar\frac{\partial\psi(x,\ t)}{\partial t} = H\psi(x,\ t).$$

Namely we have the equality

$$i\hbar\frac{\partial\psi(x,\ t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,\ t)}{\partial x^2}.$$

This is the time-evolving Schrödinger equation for the total physical system Ω.

Here, by using the completeness condition, we have the relation

$$\int_{-\infty}^{\infty} |\psi(x,\ t)|^2 dx = \int_{-\infty}^{\infty} |c(p)|^2 dp = 1,\ (-\infty < t < \infty).$$

By virtue of the law of conservation of probability, the time-evolving Schrödinger equation has no other form than that obtained in the above in order that the L^2-density $\psi(x,\ t)$ satisfies the normalization condition.

4 Natural statistical phenomena of free particles

By the study until now, we clarify that the physical system $\Omega = \Omega(\mathcal{B},\ P)$ of free particles has the following structure in the stationary state.

Namely, in the stationary state, Ω is decomposed as follows;

$$\Omega = \bigcup_{-\infty<p<\infty} \Omega_p,\ \text{(direct sum)},$$

$$\Omega_p = \{\rho \in \Omega;\ p(\rho) = p\},\ (-\infty < p < \infty),$$
$$P(\Omega_p) = |c(p)|^2,\ (-\infty < p < \infty).$$

Then, for $A \in \mathcal{B}$, we have the equality

$$P(A) = \int_{-\infty}^{\infty} P(A|p)|c(p)|^2 dp.$$

Here $P(A|p)$ denotes the conditional probability. Then, for p, $(-\infty < p < \infty)$, we say that the probability space $\Omega_p = \Omega_p(\mathcal{B}\cap\Omega_p,\ P(\cdot|p))$ is the **generalized proper physical system**.

Then, by virtue of the calculations until now, we determine $c(p)$ so that it satisfies the following conditions. Namely, when we put

$$I(\mathcal{E}) = \frac{1}{2}\sqrt{\frac{2m}{\mathcal{E}}}\ \left(\ |c(-\sqrt{2m\mathcal{E}})|^2 + |c(\sqrt{2m\mathcal{E}})|^2\ \right),\ (\mathcal{E} > 0),$$

$$I(0) = 0, \ (p^2 = 2m\mathcal{E})$$

for p, $(-\infty < p < \infty)$, we assume that the equality

$$\int_0^\infty I(\mathcal{E}) d\mathcal{E} = 1$$

holds.

Then, by virtue of the law of natural statistical physics, we have the following:

$$P(\Omega_p | p) = 1,$$

$$P\Big(\{\rho \in \Omega_p; \ x(\rho) \in A\} | p \Big) = \frac{\displaystyle\int_{A \cap S} |\psi_S^{(p)}(x)|^2 dx}{\displaystyle\int_S |\psi_S^{(p)}(x)|^2 dx},$$

$$P\Big(\{\rho \in \Omega_p; \ x(\rho) \in S, \ p(\rho) \in B\} | p \Big) = \frac{\displaystyle\int_B |\hat{\psi}_S^{(p)}(p)|^2 dp}{\displaystyle\int_{-\infty}^{\infty} |\hat{\psi}_S^{(p)}(p)|^2 dp}.$$

Thereby the conditional energy expectation $\overline{E}_p$ of the generalized proper physical system Ω_p is equal to

$$\overline{E}_p = \lim_{j \to \infty} J_{K_j}[\psi_{K_j}^{(p)}] = \mathcal{E} = \frac{p^2}{2m}.$$

Thus, by virtue of the relation among the total physical system and the generalized proper physical systems, we have the equality:

$$\overline{E} = E\left[\frac{1}{2m} p(\rho)^2 \right] = \int_{-\infty}^{\infty} \overline{E}_p |c(p)|^2 dp$$

$$= \int_{-\infty}^{\infty} \frac{p^2}{2m} |c(p)|^2 = \int_0^\infty \mathcal{E} I(\mathcal{E}) d\mathcal{E}, \ (p^2 = 2m\mathcal{E}).$$

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