Quantum mechanics on compact manifolds and nanosystems: uncertainty relations, coherent states and semiclassical limit*

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Abstract

Quantum mechanics on a compact manifold, in particular, on a bounded domain is discussed. The work is motivated by modern investigations of nanosystems and a gas model proposed by Poincaré which is related to the fundamental irreversibility problem.

We construct an analogue of coherent states (quasicoherent states) for the bounded domain. We prove that, as with the coherent states on the line, there are quasicoherent states with arbitrarily small value of the dispersion of the position and a finite dispersion of the momentum, and vise versa.

The numerical estimations are obtained: there are quasicoherent wave packets with the standard deviation of the position of order 10^{-10} m and the standard deviation of the momentum of order 10^{-10} kg*m/sec on the segment with the length of 1 m. As the segment length approaches to infinity, the quasicoherent states on the segment tend to the usual coherent states on the line.

The semiclassical limit is performed: dispersions of both the position and momentum tend to zero, as $\hbar$ tends to zero. So, the wave packet tends to the classical particle with well defined both position and momentum.

1. Introduction

Quantum mechanics is usually formulated for the case of the particle (or a system of particles) in the unbounded space $\mathbb{R}^n$. Modern investigations in gas models, solid-state physics etc. require a quantum theory on a compact manifold and on a manifold with a boundary. Quantum mechanics on a

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compact manifold has some significant differences with the usual quantum mechanics on $\mathbb{R}^n$.

For example, there is the famous Heisenberg uncertainty relation

$$\Delta x \Delta p \geq \hbar/2. \tag{1}$$

But this relation is valid only for the case of unbounded space. For compact manifolds we have the states with the relation

$$\Delta x \Delta p = 0. \tag{2}$$

This is possible, since Δx cannot be infinite (the manifold is compact!), but Δp can be equal to zero (the momentum spectrum is discrete, and there are states with well-defined momentum).

2. Quantum mechanics on Riemannian manifolds

Let M be a manifold with or without a boundary, and g be a metrics on M (i.e., a symmetric nonsingular positive definite covariant tensor of rank 2).

In order to specify a quantum mechanical system on manifold M, we must define a Hilbert space and operators of the main physical observables: energy, momentum and position.

Define a Hilbert space

$$L_2(M,g) = \{\psi : M \to \mathbb{C} | \int_M |\psi(x)|^2 \sqrt{g(x)}\, dx < \infty\}$$

with an inner product

$$(\psi, \varphi) = \int_M \overline{\psi(x)} \varphi(x) \sqrt{g(x)}\, dx,$$

where $g(x) = \det(g_{ij}(x))$ (since we have a volume element $\sqrt{g(x)}\, dx$ on M, we can integrate over M).

The Hamilton (energy) operator is defined as

$$\hat{H} = -\frac{\hbar^2}{2m} \Delta_g + V(x),$$

where $\Delta_g = \frac{1}{\sqrt{g}} \partial_i (\sqrt{g} g^{ij} \partial_j)$ is the Beltrami–Laplace operator. $V = 0$ for a free particle.

It is supposed that the operator $\hat{H}$ is self-adjoint on some domain $D(\hat{H})$. Then one can define a unitary dynamics by

$$\psi(t) = U(t)\psi_0, \quad U(t) = e^{-\frac{i}{\hbar} t \hat{H}}$$

for any $\psi_0 \in L_2(M,g)$ and $t \in \mathbb{R}$.

We can define the momentum operator as

$$\hat{p}_j = -i\hbar\nabla_j,$$

where ∇_j is the covariant derivative ($\nabla_j\nabla^j = \Delta_g$).

As for the position operator, we don't know a universal definition for an arbitrary manifold. Any function $f : M \to \mathbb{R}^n$, where $n = \dim M$, can be chosen as a position operator.

3. A special case: a segment

Consider the case of a segment: $M = [-l, l]$ (the metrics is standard: $g_{11}(x) \equiv 1$), the Hilbert space is $L_2(-l, l)$. Depending on the Hamiltonian, this case corresponds to the particle in an infinite well or the particle on a circle.

The position operator x acts on a function $\psi(x) \in L_2(-l, l)$ just as $x\psi(x)$. In contrast to the case of $L_2(\mathbb{R})$, the position operator is bounded here, and its domain is $D(x) = L_2(-l, l)$.

The momentum operator is $p = -i\hbar\frac{d}{dx}$ with the domain

$$D(\hat{p}) = \{\psi \in AC(-l, l) \,|\, \psi(-l) = \psi(l)\},$$

where $AC(-l, l)$ is a set of absolutely continuous functions with derivatives from $L_2(-l, l)$. Its eigenvalues and eigenfunctions are

$$p_k = \frac{\pi}{l}\hbar k, \quad \varphi_k = \frac{1}{\sqrt{2l}}\, e^{i\frac{\pi}{l}kx}, \quad k = 0, \pm 1, \pm 2, \dots .$$

Any function $\psi(x) \in L_2(-l, l)$ can be represented as

$$\psi(x) = \frac{1}{\sqrt{2l}} \sum_{k=-\infty}^{+\infty} a_k\, e^{i\frac{\pi}{l}kx} = \frac{1}{\sqrt{2l}} \sum_{k=-\infty}^{+\infty} a_k \frac{1}{\sqrt{2l}}\, e^{i\frac{p_k}{\hbar}x}.$$

Define the mean values of position and momentum

$$\overline{x} = \int_{-l}^{l} x|\psi(x)|^2\, dx, \qquad \overline{p} = \sum_{k=-\infty}^{+\infty} p_k|a_k|^2, \tag{3}$$

dispersions and standard deviations of position and momentum

$$\Delta x^2 = \int_{-l}^{l} (x - \overline{x})^2|\psi(x)|^2\, dx, \quad \Delta x = \sqrt{\Delta x^2}, \tag{4}$$

$$\Delta p^2 = \sum_{k=-\infty}^{+\infty} (p_k - \overline{p})^2|a_k|^2, \quad \Delta p = \sqrt{\Delta p^2}. \tag{5}$$

For any momentum eigenstate φ_k the relations $\Delta x = l/\sqrt{3}$, $\Delta p = 0$, and $\Delta x \Delta p = 0$ are satisfied.

So, relation (1) is not valid here. There are some other mathematical expressions of the uncertainty principle for this case (see, e.g., [1]).

4. Problem formulation

We consider the following two problems.

- Whether exists a family of wave functions $\psi_\alpha(x) \in L_2(-l,l)$, $\alpha \in (0,\infty)$, such that $\Delta x_\alpha \to 0$, as $\alpha \to \infty$, and Δp_α is finite for any α. Here Δx_α and Δp_α are the standard deviations of position and momentum defined by (4), (5) for the function $\psi_\alpha(x)$.

  In other words, whether Δx can be reduced to an arbitrary small value, while Δp is finite for any fixed state (just in the previous section we saw that the converse assertion is trivially satisfied with $\Delta p = 0$ and finite Δx).
- Whether exists some α that the wave packet $\psi_\alpha(x)$ from our family has small both Δx and Δp. Such quantum wave packet could be associated with a classical particle with well-defined position and momentum.

  In addition, we demand the mean values $\overline{x}_\alpha$ and $\overline{p}_\alpha$ (see (3) of the wave functions $\psi_\alpha(x)$ to be close to some given values x^* and p^*.

In fact, we search for an analogue of the well-known coherent states for $L_2(\mathbb{R})$ [2]:

$$\widetilde{\psi}(p) = \frac{1}{\sqrt[4]{2\pi\beta^2}} e^{-\frac{(p-p^*)^2}{4\beta^2} - \frac{ipx^*}{\hbar}}, \tag{6}$$

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \widetilde{\psi}(p) e^{\frac{ipx}{\hbar}}\, dp, \tag{7}$$

where $x^*, p^* \in \mathbb{R}$, $\beta > 0$ are parameters. One can prove that x^* and p^* are the mean values of position and momentum, β is the standard deviation of momentum Δp, and

$$\Delta x \Delta p = \hbar/2,$$

where Δx is the standard deviation of position. So, the coherent states (the gaussian wave packets) minimize the uncertainty relation. In this sense the coherent quantum states are the nearest to classical states. The parameters x^* and p^* are associated with the momentum and position of a classical particle [2, 3].

5. Quasicoherent states for $L_2(-l,l)$ and the main theorem

Now we construct the family $\psi_\alpha(x) \in L_2(-l,l)$, $\alpha \in (0,\infty)$, for arbitrary given given $x^* \in (-l,l)$ and $p^* \in \mathbb{R}$. Denote $k^* = \frac{l}{\pi}\frac{p^*}{\hbar}$.

Let $\varphi_\alpha(k)$ be the gaussian probability density function with the standard deviation α:

$$\varphi_\alpha(k) = \frac{1}{\sqrt{2\pi\alpha^2}} e^{-\frac{(k-\overline{k})^2}{2\alpha^2}},$$

where $\overline{k}$ is the nearest integer to k^*. Denote $\overline{p} = \frac{\pi}{l}\hbar\overline{k}$. Then $|\overline{p} - p^*| \le \frac{\pi}{l}\hbar$.

In fact, we can take any probability density function with a finite second moment and some additional properties (satisfied for the gaussian function) as $\varphi_\alpha(k)$. But for simplicity we consider only the most interesting case of the gaussian function.

Now let us define

$$a_k^{(\alpha)} = \left[\int_{\frac{\pi}{l}(k-\frac{1}{2})}^{\frac{\pi}{l}(k+\frac{1}{2})} \varphi_\alpha(\tilde{k})\, d\tilde{k}\right]^{\frac{1}{2}},$$

$k = 0, \pm 1, \pm 2, \ldots$ (the dimensionality of k is length^{-1}), and

$$\psi_\alpha(x) = \frac{1}{\sqrt{2l}} \sum_{k=-\infty}^{+\infty} a_k^{(\alpha)}\, e^{i\frac{\pi}{l}k(x-x^*)}, \tag{8}$$

We will call the functions $\psi_\alpha(x)$ quasicoherent states in $L_2(-l,l)$, because they have been constructed based on the usual coherent states (6)–(7) in $L_2(\mathbb{R})$. Momentum coefficients $\{a_k^\alpha\}$ are some kind of discretization of (6) with the appropriate parameters and sum (8) is an analogue of integral (7).

Let us denote the mean values and the standard deviations of ψ_α as $\overline{x}_\alpha$, $\overline{p}_\alpha$, Δx_α, and Δp_α.

Define also

$$\Delta_* x_\alpha^2 = \int_{-l}^{l} (x - x^*)^2 |\psi_\alpha(x)|^2\, dx.$$

One can easily see that

$$\Delta_* x_\alpha^2 = \Delta x_\alpha^2 + (\overline{x}_\alpha - x^*)^2.$$

So, the smallness of Δx_α follows from the smallness of $\Delta_* x_\alpha$. The inverse is also true, if $\overline{x}$ is close to x^*.

Theorem 1. *The following bounds are satisfied:*

$$1)\ \ \Delta_* x_\alpha \le \left[\frac{9\pi\varphi(\overline{k})l}{2\alpha} \int_{-1}^{1} \frac{(y - \frac{x^*}{l})^2}{\sin^2 \frac{\pi}{2}(y - \frac{x^*}{l})}\, dy\right]^{\frac{1}{2}} \to 0, \quad \alpha \to \infty; \tag{9}$$

$$2)\ \ \lim_{\alpha\to\infty} \frac{\Delta p_\alpha}{\alpha} = C \ne 0; \tag{10}$$

$$3)\ \ |\overline{x}_\alpha - x^*| \leq \frac{x^*}{\alpha l} \frac{18\pi\varphi(\overline{k})}{\cos^2\frac{\pi x^*}{2l}} \to 0, \quad \alpha \to \infty, \tag{11}$$

$$\overline{p}_\alpha = \frac{\pi}{l}\hbar\overline{k} \equiv \overline{p}. \tag{12}$$

For $l = 1$ m (a macroscale), $x^* = 0$, arbitrarily p^*, $\alpha = 10^{33}$ m^{-1} one can show that $\Delta x \leq 10^{-11}$ m and $\Delta p \leq 10^{-11}$ kg*m/sec. So, the sizes of this wave packet are less than the nanoscale. Even a nanodevice will not detect a scattering of this wave packet and will consider it as a well localized particle.

We can perform a semiclassical limit: $\hbar \to 0$, $\alpha \to \infty$ such that $\hbar\alpha \to 0$. Then we see that $\overline{x}_\alpha \to x^*$, $\overline{p}_\alpha \to p^*$, $\Delta x_\alpha \to 0$, $\Delta p_\alpha \to 0$. So, in the limit we have a classical particle with well defined and predefined values of position and momentum.

If we perform the limit $l \to \infty$, we can show that in the limit we get the usual coherent states in $L_2(\mathbb{R})$ (6)–(7).

6. Conclusions

In this paper a family of quasicoherent states in $L_2(-l, l)$ is constructed and a theorem about estimations of $\overline{x}$, $\overline{p}$, Δx, and Δp is proved. In particular, theorem states that $\Delta x \to 0$, if $\Delta p \to \infty$;

As a corollary from the theorem, it is shown that the wave packets with the following estimations are exist for $l = 1\ m$: $\Delta x \leq 10^{-10}$ m, $\Delta p \leq 10^{-10}$ kg*m/sec.

So, there exist wave packets with small both Δx and Δp (less than nanoscale), and for the macroscopic mass (1 kg) a particle can be described by the well-defined position and momentum variables.

References

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