Problems with variable Hilbert space in quantum mechanics

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Abstract

The general problem is studied on a simple example. A quantum particle in an infinite one-dimensional well potential is considered. Let the boundaries of well changes in a finite time $T$. The standard methods for calculating probability of transition from an initial to the final state are in general inapplicable since the states of different wells belong to different Hilbert spaces.

If the final well covers only a part of the initial well (and, possibly, some outer part of the configuration space), the total probability of the transition from any stationary state of the initial well into all possible states of the final well is less than 1 at $T \to 0$. If the problem is regularized with a finite-height potential well, this missing probability can be understood as a non-zero probability of transitions into the continuous spectrum, despite the fact that this spectrum disappears at the removal of regularization. This phenomenon (“transition to nowhere”) can result new phenomena in some fundamental problems, in particular at description of earlier Universe.

We discuss also how to calculate the probabilities of discussed transitions at final $T$ for some ranges of parameters.

Keywords: quantum well, Hilbert space, probability

1. INTRODUCTION

The paper combines the solution of two problems, motivated by common source, described in the sect. 2.

In the sect. 3 we discuss a new phenomenon caused by a change of the Hilbert space.

In the sect. 4 we discuss technical problem of useful methods of calculations in a certain range of parameters.

The discussions of obtained results are presented in each section 3, 4 separately.

2. FORMULATION OF THE PROBLEM

Quantum particle in the infinite well $U$ is the standard entry-level problem in many quantum mechanics textbooks (see e.g. [1-3])

\[ \hat{H} = \frac{p^2}{2m} + U_i(x), \]
\[ U_i(x) = \begin{cases} \infty : & x \in (-\infty, 0), (b, \infty), \\ 0 : & x \in [0, b]. \end{cases} \] (1)

The stationary states of this problem are $|n\rangle_i \equiv |n; (0, b)\rangle$ (the subscript $i$ means initial) with

\[ |n\rangle_i \to \psi_{n,i} = \begin{cases} 0 : & x \in (-\infty, 0), \\ \sqrt{\frac{2}{\pi}} \sin \frac{\pi nx}{b} : & x \in [0, b], \\ 0 : & x \in (b, \infty); \end{cases} \] (2)

\[ E_n = \frac{(\pi \hbar n)^2}{2mb^2}, \quad n = 1, 2, \ldots \]

These states form a basis for the Hilbert space $\mathcal{H}_i \equiv \mathcal{H}(0, b)$ of continuous square-integrable functions defined on the support $[0, b]$ and vanishing at its endpoints.

The stationary states for another (final) well $f$ with boundaries

\[ [0, b] \to [a, a + ba] \]

are described by equations (2) with the change

\[ x \to x - a, \quad b \to ba, \]

e.g. $|n\rangle_f \equiv |n; (a, a + ba)\rangle$. They form a basis for another Hilbert space $\mathcal{H}_f \equiv \mathcal{H}(a, a + ba)$, defined on the support $[a, a + ba]$. (Spaces $\mathcal{H}_f$ and $\mathcal{H}_i$ are isomorphic but do not coincide).

To simplify the presentation, we set in calculations $a = 0$ almost everywhere.

- The following problem is easily solved:

Let the width of the well changes instantly, $b \to ba$.

Find the probability $W_{nk}^{bf}$ of the transition $|n\rangle_i \to |k\rangle_f$. \hspace{1cm} (4)

The result is obtained from eq. (2). In particular, for the shrinking well ($a < 1$):

\[ W_{nk}^{bf} \equiv |M_{nk}^{bf}|^2, \quad |M_{nk}^{bf}| = \frac{2k\sqrt{\pi}}{\pi} \cdot \frac{\sin(\pi nx)}{k^2 - (na)^2}. \] (5)

- A “natural” modification of this problem is

Find the similar probability $W_{nk}^{bf}$ in the case when width changes as $b \to ba(t)$ over a finite time $T$.

This problem is non-trivial. The difficulties that have arisen persist even with a more general view of transitions at $T \to 0$.

From the formal point of view this problem is described by the Schrödinger equation

\[ i\hbar \frac{d\psi(x, t)}{dt} = \hat{H}\psi(x, t) = \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U_i(x) + \hat{V}_p(x, t) \right) \psi(x, t). \] (7a)
The change of the well is described by the change from those of initial well at

\[ V \] and out of wells (where these eigenfunctions are equal 0). (sect. 3).

The infinite height wells are replaced by the wells is closer to reality: 

\[ \text{of large height } V, \text{ which is not changed when the well width varies} \]

The regularized problem (\( \alpha > 1 \)) has 

\[ W(n; i|f) = \int dx \psi_{n,i}(x)\psi_{n,f}(x) = 1 \text{ (normalization).} \]

In other words, function \( |n\rangle_f \), normalized on the initial interval, keeps the normalization in the Hilbert state with the expanded support.

\[ \int \psi_{n,i}(x)\psi_{n,f}(x) = 1. \]

The summation of individual probabilities naturally gives the same result:

\[ W(n; i|f) = \sum_b |\psi_{n,i}(x)\psi_{n,f}(x)|^2 = \sum_{\alpha} \left( \frac{\pi \alpha}{b} \right)^2 \sum_{k=1}^{\infty} \frac{k^2 \sin^2(\pi \alpha \kappa)}{(k^2 - \pi^2 \alpha^2)^2} < 1. \]

3.3. Disappearance of probability

According to (10), at \( \alpha < 1 \) some fraction of probability disappears. In the discussed regularization picture it means that some part of the initial state goes over into the continuous spectrum, despite the fact that this spectrum disappears when the regularization is removed. It is clear that this phenomenon takes place also in the more general case of moving boundaries if the final well does not cover the initial one, for example, at the shift of boundaries with \( a > 0 \) for both \( a + b < b \) and \( a + b < b \).

Therefore, we find that the description in terms of only initial and final wells appears incomplete. It should be supplemented by

\[ O \subset L_2 \supset H_i, H_f. \]

Our problem corresponds to the limit \( V \to \infty \) (removal of regularization).

With this regularization, the standard type calculations with some improvements becomes consistent but, unfortunately, very bulky.

\[ \text{3.2. Total probability of transitions} \]

We study the essential feature of relation between the Hilbert spaces through analysis of the instantly changing well boundary. Let us consider the probability for the transition of some state of the initial well \( |n\rangle_i \) into the any state of the final well \( |k\rangle_f \), forgetting the regularization. This probability is

\[ W(n; i|f) = \sum_k |M_{nk}|^2 = \langle n_i | \sum_k |k\rangle_f \langle k|_f |n\rangle_i. \]

Here we define the operator \( I_f = \sum |k\rangle_f \langle k| \). It acts as the unit operator in the space \( H_f \). Eq. (9) determines, in fact, how this operator acts in the other space \( H_i \) for our problem. It can be understood by two ways, giving coinciding results. First of all, one can summarize probabilities of individual transitions.

Second, we use definition of the operator \( I_f \) as the projector to the segment \((0, b\alpha)\). (We denote \( \alpha_x = \alpha \).

• For the expanding well \( \alpha > 1 \) we have

\[ W(n; i|f) = \int dx \psi_{n,i}(x)\psi_{n,f}(x) = 1 \text{ (normalization).} \]

• For the shrinking well \( \alpha < 1 \) the initial normalization integral lost the interval \((b\alpha, b)\), so that we have

\[ W(n; i|f) = \int dx \psi_{n,i}(x)\psi_{n,f}(x) < 1. \]

The summation of individual probabilities naturally gives the same result:

\[ W(n; i|f) = \sum_{\alpha} \left( \frac{\pi \alpha}{b} \right)^2 \sum_{k=1}^{\infty} \frac{k^2 \sin^2(\pi \alpha \kappa)}{(k^2 - \pi^2 \alpha^2)^2} < 1. \]

3. PROBLEMS WITH HILBERT SPACES

3.1. Regularization

It should be noted that in the calculations of transition probabilities we used the eigenfunctions, defined both within wells and out of wells (where these eigenfunctions are equal 0). It can be treated as the fact that we consider the Hilbert spaces \( H(0, b), H(0, b\alpha) \) and that these spaces are subspaces of entire Hilbert space \( L_2 \) of continuous square-integrable functions defined on real axis \((\infty, \infty)\), i.e. \( H(0, b), H(0, b\alpha) \subset L_2 \).

In reality, the infinite well potential is only an approximation which is useful for calculations. The regularized problem is closer to reality: The infinite height wells are replaced by the wells of large height \( V \), which is not changed when the well width varies. One considers the same Schrödinger equation with the following regularized potential (for the initial well)

\[ U_{reg}^{(1)}(x) = \begin{cases} 
V: & x \in (-\infty, 0), \\
0: & x \in [0, b), \\
V: & x \in (b, \infty). 
\end{cases} \]

The change of the well is described by the change \( b \to b\alpha \).

At this regularization properties of \( n \)-th state differs weakly from those of initial well at

\[ \xi_n = E_n/V = (\pi n \hbar)^2/(2mb^2 V) \ll 1. \]

At approaching \( \xi_n \) to 1 the regularized picture becomes different from non-regularized one.

In this approach both initial and final situations are described by functions belonging to the equipped Hilbert space
information about a big system embracing both these wells. In the considered toy example properties of this big system are sufficiently clear.

3.4. Possible value of probability disappearance

The situation with the change of Hilbert space is realized in the Nature at phase transitions.

In the standard description of phase transitions in quantum systems both initial and final Hilbert spaces are described often by corresponding sets of elementary excitations. The discussed "loss of probability" means that a complete description may require the inclusion of normally skipped degrees of freedom of some embraced system.

For the phase transitions in the matter the properties of this big system are usually almost evident. The most interesting problems with the change of the Hilbert space are those in fact, similar opportunity was discussed recently with respect to "the discreteness of Universe at the Planck scale (naturally expected to arise from quantum gravity)" [4].

4. METHODS FOR CALCULATION

Now we consider more technical problems - we present a regular methods for calculation of the transition probabilities, which would allow one to use some known approximate methods in the cases when it looks natural. This problem was discussed by many authors for different particular laws of boundary motion (see e. g. 2, 3, 5, 7). In this section we don’t pretend for new results but present brief review of developed methods, allowing news only in some details.

We note that the main parameter of the problem for the evolution of n-th state is the time of motion of walls \( T \sim 1/\alpha \), in its relation to the characteristic time of life \( \tau_n = h/E_n \).

4.1. Slow motion of wells. Adiabatic case

If the walls move slowly (\( T > \tau_n \)), the adiabatic approximation looks reasonable [1, 3]. In this approximation, the evolution of the system is considered as a sequence of stationary states of the infinite well with new width. The previous state in this sequence is the starting one for the subsequent one. In the main approximation, the probability of \( n \to n \) transition is close to 1 (even at big \( \alpha \) or \( 1/\alpha \)), other probabilities are small [1].

4.2. Fast motion of wells. 1

If the condition \( T > \tau_n \) is violated, the calculations without enormously large intermediate quantities can be based on the mapping of time dependent well to the initial well [2, 3]. We present here some variant of this approach. At \( T < \tau_n \) this approach allows to apply method which is similar to the standard perturbation theory.

The mapping by itself is the rescaling of the coordinate \( y = x/\alpha(t) \). In this new variable, the potential keeps form \( U_i(y) \) at all times. However, the form of the kinetic term is modified, \( d/dx \to \alpha^{-1} dx/dy + y^{-1} dy/dx \). Besides, the transformation of the wave function and the scale of time are useful:

\[
(A) : \quad y = x/\alpha(t),
\]
\[
(B) : \quad \psi = \sqrt{\gamma(\chi)}, \quad (C) : \quad \tau = \int_0^t dt/\alpha^2(t).
\]

Now the Schrödinger equation is transformed to the form

\[
-ih\frac{d\chi}{dt} = (\hat{H}_1 + \hat{\gamma}) \chi;
\]
\[
\hat{H}_1 = -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial y^2} - \frac{3}{4y^2} \right) + U_i(y),
\]
\[
\hat{\gamma} = -\frac{\hbar^2}{2m\alpha^2} \left( \alpha^2 \frac{\partial^2}{\partial \alpha^2} + 2\alpha \frac{d^2}{d\alpha^2} \right).
\]

The eq. (11 (C)) can be treated as that for obtaining dependence \( a(t) \) which allows to transform differentiation with respect to \( a(t) \) to the differentiation with respect to \( \tau \).

We treat \( \hat{H}_1 \) as the new non-perturbed Hamiltonian and term \( \hat{\gamma} \) as the perturbation.

The eigenstates \( \chi_n^{w}(y, \tau) \) of the Hamiltonian \( \hat{H}_1 \) are continuous functions vanishing at the boundaries of well (superscript \( ^w \) marks these states). They are expressed in terms of the Bessel function (see Table 1 below).

We find useful to express zeroes of the Bessel function in the form of more refined regularization procedure.

\[\int_0^{\chi_n^{w}(y, \tau)} \chi_m^{w}(y, \tau) dy = \delta_{mn}.\]

We find useful to express zeroes of the Bessel function in the special form \( z_n = \pi n \mu_n \) with factor \( \mu_n \) which is close to 1:

| \( n \) | 1 | 2 | 3 | ... | \( n \) |
|---|---|---|---|---|---|
| \( u_n - 1 \) | 0.22 | 0.116 | 0.08 | ... | \(< (1/4n)\) |

**TABLE 1:** Values \( u_n - 1 \) for different \( n \).

This closeness means that eigenvalues and eigenfunctions of \( \hat{H}_1 \) are close to those for the initial problem [2].

4.3. Fast motion of wells. 2. Perturbation

Note that the factor \( 1/y^2 \) in \( \hat{\gamma} \) do not obstruct the convergence of matrix elements \( V_{nk}^{w} \) since \( \chi_n(y) \to Ay^{-\frac{3}{2}} \) at \( y \to 0 \).

Main features of solution are seen well in the simplest example with the linear dependence \( a(t) = 1 + \alpha(t) \), where

\[\frac{1}{\alpha(t)} \neq 0 \quad \text{one can use the mapping } y = (x - a(t))/\alpha(t).\]
\[ \alpha' = (a - 1)/T. \] In this case the integration of (11) results in
\[ \tau = \frac{1}{\alpha'} \left( 1 - \frac{1}{\alpha} \right) \Rightarrow \alpha = \frac{1}{1 - \alpha' \tau}, \quad \tau = \frac{t}{\alpha(t)}. \quad (14) \]

After that the perturbation operator is transformed to the form
\[ \hat{V} = -\frac{\hbar^2}{2m \alpha^2} \frac{\partial^2}{\partial \tau^2} - \frac{2 \partial}{\alpha \alpha'} \frac{\partial}{\partial \tau} + \frac{2y}{\alpha \alpha'} \frac{\partial^2}{\partial y \partial \tau}. \quad (15) \]

To estimate conditions for applicability of the standard type perturbation theory to the discussed problem, we note that in the matrix element \( V_{nm} \) the operator \( \partial/\partial \tau \) gives factor \( (E_{nm} - E_{wn})/\hbar \). Hence, for this transition the expansion parameter is \( \delta = (E_{nm} - E_{wn})/(\hbar \alpha') \sim T/\tau_{nm} \) (at \( |\alpha(a - 1)| \sim 1 \) we have \( T \sim T \)). The perturbation theory works at \( \delta \ll 1 \), i.e. in the case when a time of motion of walls, \( T < \tau_{nm} \). Note that if this condition is valid for the states with moderate \( n \), it is violated for the states with very large \( n \) (typical situation for validity of perturbation theory for high lying levels in quantum mechanics).

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