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ON A MODEL OF SPONTANEOUS SYMMETRY BREAKING IN QUANTUM MECHANICS

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Our goal is to find a model for the phenomenon of spontaneous symmetry breaking arising in one dimensional quantum mechanical problems. For this purpose we consider boundary value problems related with two interior points of the real line, symmetric with respect to the origin. This approach can be treated as a presence of singular potentials containing shifted Dirac delta functions and their derivatives. From mathematical point of view we use a technique of selfadjoint extensions applied to a symmetric differential operator which has a domain containing smooth functions vanishing in two mentioned above points. We calculate the resolvent of corresponding extension and investigate its behavior if the interior points change their positions. The domain of these extensions can contain some functions that have non differentiability or discontinuity at the points mentioned above, the latter can be interpreted as an appearance of singular potentials centered at the same points. Next, broken-symmetry bound states are discovered. More precisely, for a particular entanglement of boundary conditions, there is a ground state, generating a spontaneous symmetry breaking, stable under the phenomenon of decoherence provoked from external fluctuations. We discuss the model in the context of the "chiral" broken-symmetry states of molecules like NH_3. We show that within a Hilbert space approach a spontaneous symmetry breaking disappears if the distance between the mentioned above interior points tends to zero.

Keywords: operator theory; resolvent; solution of wave equation: bound states; spontaneous and radiative symmetry breaking.

Introduction

We introduce in this paper a new mechanism for spontaneous symmetry breaking, with applications to molecular physics. We discuss it on one dimensional quantum problems. It is based on nontrivial boundary conditions which we describe as an "entanglement of boundary conditions". The motivation for our proposal is on the study of symmetric potentials, under parity, where the stable quantum ground state is not symmetric, but it is right or left-handed. This situation occurs in many molecules with symmetric configurations of the nuclei of the atoms, where the ground state is right or left-handed. Moreover, the ground state is even not an eigenstate of the Hamiltonian. A typical example is the molecule NH3. Its quantum potential contains two symmetric attractive minima with a repulsive barrier between them. The ground state is non-degenerate and right or left-handed. The main point is that a non-degenerate eigenstate of a symmetric Hamiltonian must either be symmetric or antisymmetric under parity transformations. However, external perturbations change the phase of a symmetric or antisymmetric state giving rise to an unstable incoherent mixture of both. This effect is known as decoherence, see [1] and for a review [2]. On the other side, a state concentrated only on one side of the repulsive barrier would be stable under external perturbations, but not necessary an eigenstate. In that case it is unstable under the time evolution dictated by the Schrodinger equation. It would evolve from a right-handed to a left-handed state and vice versa, since it is not an eigenstate, becoming unstable after a period of time. Nevertheless, if the repulsive barrier is high enough this scenario occurs after so large time that approximately the state of the molecule is concentrated on the right or left side of the repulsive barrier with a very large decaying process. This argument explains the existence of right or left-handed states in nature. In this paper we present a nonlocal interaction described by an entanglement of boundary conditions such that the corresponding symmetric Hamiltonian, for a particular value of the parameters describing the interaction, has a degenerate ground state. It is a linear combination of a right and a left-handed eigenstate. In addition, when we consider the phenomenon of decoherence the only stable eigenstate under external fluctuations corresponds to the left-handed or right-handed states. In distinction to our previous argument the stable ground state is now an exact eigenstate. So, our proposal fulfils both stability criteria. It is stable under external perturbations, since it is a left or right-handed state concentrated on one side of the barrier and stable under time evolution, since it is an eigenstate of the Hamiltonian. Our model describes the barrier in terms of the Dirac delta distribution, more precisely in terms of the derivative of it. The use of the Dirac delta distribution has been used with success in order to describe approximate potentials, see [3–11]. In our proposal the potential is modeled by two derivatives of the Dirac delta separated a distance 2h among them. The coefficients of each derivative of the delta depends on the boundary condition on the wave function at the other derivative of the delta. It is an entanglement of boundary conditions. The Hamiltonian we introduce is then symmetric under parity transformations and self-adjoint. Its ground state is an exact eigenstate concentrated on one side of the repulsive barrier. It is an interesting case of spontaneous symmetry breaking. The mathematical approach we will follow in our construction is a method of selfadjoint extensions of a symmetric operator.

Section 1 contains some known results concerning singular potentials in terms of the delta function and a small discursion on the subject. In particular, we mention a Hamiltonian whose ground state is degenerate, with two eigenfunctions, nevertheless, there is no symmetry breaking in this case. Further, in Section 2 and 3 we present the key contribution of the paper by introducing local and non-local potentials and discuss their quantum properties. In particular, the existence of spontaneous symmetry breaking is demonstrated in Section 2. In Section 3 we show that within a Hilbert space approach a spontaneous symmetry breaking disappears if $h \to 0$. Finally, we give our closing remarks in Section 4.

1. Preliminary Remarks

Let us consider a well known case of a boundary value problem at the unique interior point coinciding with the origin. So, let $D = -d^2 \cdot /dx^2$ be the differential operator on the set

$$\mathcal{D}(D) = \{y(x)|\ y(x), y'(x), y''(x) \in L^2(\mathbb{R}),\ y(0) = y'(0) = 0\}.$$

Its adjoint one D^* is the differential operator on the set

$$\mathcal{D}(D^*) = \{y(x)|\ y(x), y'(x), y''(x)|_{\mathbb{R}_+} \in L^2(\mathbb{R}_+),\ y(x), y'(x), y''(x)|_{\mathbb{R}_-} \in L^2(\mathbb{R}_-)\},$$

where $\mathbb{R}_+ = \{x|\ x \geq 0\}$ and $\mathbb{R}_- = \{x|\ x \leq 0\}$.

For any selfadjoint extension $\widetilde{D}$ of D the relation $D \subset D^*$ holds. Thus, $D \subset \widetilde{D} \subset D^*$ and any extension of D can be treated as a restriction of D^*. Direct calculations bring $(D^*y, z) = -y'(-0)\bar{z}(-0) + y'(+0)\bar{z}(+0) + y(-0)\bar{z}'(-0) - y(+0)\bar{z}'(+0) + (y, D^*z)$.

The latter yields

$$y'(-0)\bar{z}(-0) - y'(+0)\bar{z}(+0) - y(-0)\bar{z}'(-0) + y(+0)\bar{z}'(+0) = 0 \tag{1}$$

as a condition for the self-adjointness of the corresponding restriction. Since here boundary values form a four-dimensional space, any selfadjoint restriction can be given by two linear homogenous equations. In particular, the conditions (the same for y and z) $y(-0) = y(+0)$ and $\frac{y'(+0)-y'(0)}{y(0)} = 2c = const$ are suitable. Under these conditions the first derivative of $y(t)$ has a jump at zero. Therefore the second one treated as a distribution has a singularity like the delta-function and the corresponding extension $\widetilde{D}$ accepts a natural representation $\widetilde{D}y(x) = -y''(x) + 2c \cdot y(0)\delta(x) = -y''(x) + 2c \cdot y(x)\delta(x)$. For $c < 0$ the operator $\widetilde{D}$ has the negative eigenvalue $\lambda = -c^2$ and the corresponding eigenfunction $y(t) = e^{c|x|}$. These facts are well known (see the monograph [12]). In the same book one can find a study on singular potentials like shifted delta functions or their first derivative in finitely many points, but this study touches only local boundary conditions.

The present work deals with a generalization of the described above scheme for a non-local boundary problem at two points $-h, h$ and a behavior of the corresponding operator with two eigenfunctions if $h \to 0$. We show that the process $h \to 0$ eliminates one of these eigenfunctions.

As it is well known, even for the one-point problem there are some selfadjoint extensions with one or two negative eigenvalues wich involve naturally not only the delta-function but its first derivative: the boundary conditions ($\alpha > 0,\ \beta > 0$)

$$\begin{aligned} \alpha\big(y(+0) + y(-0)\big) &= \big(-y'(+0) + y'(-0)\big), \\ \beta\big(y(+0) - y(-0)\big) &= -\big(y'(+0) + y'(-0)\big), \end{aligned} \tag{2}$$

where $\int\limits_{-\infty}^{-0} (|y(x)|^2 + |y(x)'|^2 + |y(x)''|^2)dx + \int\limits_{+0}^{+\infty} (|y(x)|^2 + |y(x)'|^2 + |y(x)''|^2)dx < \infty$, satisfy Conditions (1), so the corresponding extension is selfadjoint. This case was analyzed in [13]. The extension $\widetilde{D}$ under discussion has two eigenvalues $-\alpha^2$ and $-\beta^2$, their corresponding eigenfunctions are $e^{-\alpha|x|}$ and $\mathrm{Sgn}\,(x)e^{-\beta|x|}$ respectively, $\mathrm{Sgn}\,(x) = 1$ for $x > 0$ and $\mathrm{Sgn}\,(x) = -1$ for $x < 0$, $\widetilde{D}$ is the selfadjoint Hamiltonian with Representation

$$\widetilde{D}y(x) = -y''(x) - \frac{1}{\beta} \cdot \delta'(x)\left(y'(-0) + y'(+0)\right) - \alpha \cdot \delta(x)\left(y(-0) + y(+0)\right).$$

Our principal interest leads to the case $\alpha = \beta$. Indeed, the latter yields that $-\alpha^2$ is the unique negative eigenvalue and has two non symmetric eigenfunctions $y_1(x) =$