Proceedings of the Estonian Academy of Sciences,
2010, **59**, 4, 290–293
doi: 10.3176/proc.2010.4.06
Available online at www.eap.ee/proceedings

MATHEMATICS

A global, dynamical formulation of quantum confined systems

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Received 19 May 2009, accepted 12 December 2009

Abstract. A brief review of some recent results on the global self-adjoint formulation of systems with boundaries is presented. We concentrate on the 1-dimensional case and obtain a dynamical formulation of quantum confinement.

Key words: self-adjoint extensions, boundary interactions, dynamical confinement.

1. INTRODUCTION

Let $H_0 : \mathscr{D}(H_0) \subset L^2(\mathbb{R}^d) \longrightarrow L^2(\mathbb{R}^d)$ be a self-adjoint (s.a.) Hamiltonian operator defined on the domain $\mathscr{D}(H_0)$ and describing the dynamics of a d-dimensional quantum system. Let us also consider the decomposition $\mathbb{R}^d = \Omega \cup \Omega^c$, where Ω is an open set and $\Gamma = \overline{\Omega} \cap \Omega^c$ is the common boundary of the two open sets $\Omega_1 = \Omega$ and $\Omega_2 = \overline{\Omega}^c$.

To obtain a confined version (for instance, to Ω_1) of the system described by H_0, the standard approach is to determine the s.a. realizations of the operator H_0 in $L^2(\Omega_1)$. It is well known, however, that this formulation displays several inconsistencies [1–3], the main issues being the ambiguities besetting the physical predictions (when there are several possible s.a. realizations of H_0 in $L^2(\Omega_1)$), the lack of s.a. formulations of some important observables in $L^2(\Omega_1)$, and the difficulties in translating this approach to other (non-local) formulations of quantum mechanics, like the deformation formulation [4]. These problems are well illustrated by textbook examples [1,4,5].

Our aim here is to present an alternative approach to quantum confinement. This formulation consists in determining all s.a. Hamiltonian operators $H : \mathscr{D}(H) \subset L^2(\mathbb{R}^d) \longrightarrow L^2(\mathbb{R}^d)$, defined on a dense subspace $\mathscr{D}(H)$ of the global Hilbert space $L^2(\mathbb{R}^d)$, which dynamically confine the system to Ω_1 (or Ω_2) while reproducing the action of H_0 in an appropriate subdomain. More precisely, let P_{Ω_k} be the projector operator onto Ω_k, $k = 1,2$, i.e.

$$P_{\Omega_k}\psi = \chi_{\Omega_k}\psi, \quad \psi \in L^2(\mathbb{R}^d), \tag{1}$$

where χ_{Ω_k} is the characteristic function of Ω_k: $\chi_{\Omega_k}(x) = 1$ if $x \in \Omega_k$ and $\chi_{\Omega_k}(x) = 0$, otherwise. Our aim is to determine all linear operators $H : \mathscr{D}(H) \subset L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$ that satisfy the following three properties:

(i) H is s.a. on $L^2(\mathbb{R}^d)$;

(ii) if $\psi \in \mathscr{D}(H)$, then $P_{\Omega_k}\psi \in \mathscr{D}(H)$ and $[P_{\Omega_k}, H]\psi = 0$, $k = 1,2$;

(iii) $H\psi = H_0\psi$ if $\psi \in \mathscr{D}(H_0)$ is an eigenstate of P_{Ω_k}.

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Moreover, for the 1-dimensional case, we want to recast the operators H in the form $H = H_0 + B^{BC}$, where B^{BC} is a distributional boundary potential (that may depend on the particular boundary conditions satisfied by the domain of H) and H is s.a. on its maximal domain. This formulation is global, because the system is defined in $L^2(\mathbb{R}^d)$, and the confinement is dynamical, i.e. it is a consequence of the initial state and of the Hamiltonian H. Indeed, from (i) and (ii) it follows that P_{Ω_k} commutes with all the spectral projectors of H and so also with the operator $\exp\{iHt\}$ for $t \in \mathbb{R}$. Hence, if ψ is an eigenstate of P_{Ω_k}, it will evolve to $\exp\{iHt\}\psi$, which is again an eigenstate of P_{Ω_k} with the same eigenvalue. In other words, P_{Ω_k} is a constant of motion and a wave function confined to Ω_1 (or to Ω_2) will stay so forever.

The problem of determining a dynamical formulation of quantum confinement can be addressed from the point of view of the study of s.a. extensions of symmetric restrictions [1,6–8] and is closely related with the subjects of point interaction Hamiltonians [7,9–11] and surface interactions [12]. Our results may be useful in this last context as well as for the deformation quantization of systems with boundaries [4].

In this paper we shall provide a concise review of the solutions to the above problems. The reader should refer to [13] for a detailed presentation, including proofs of the main theorems, the extension of the boundary potential formulation to higher dimensions, and some applications to particular systems.

2. CONFINING HAMILTONIANS DEFINED ON $L^2(\mathbb{R}^d)$

We start by introducing some relevant notation. Let $X, Y \subset V$ be two subspaces of a vector space V such that $X \cap Y = \{0\}$, then their direct sum is denoted by $X \oplus Y$. Let now A, B be two linear operators with domains $\mathscr{D}(A), \mathscr{D}(B) \subset L^2(\mathbb{R}^d)$ such that $\mathscr{D}(A) \cap \mathscr{D}(B) = \{0\}$, then the operator $A \oplus B$ is defined by:

$$A \oplus B : \begin{cases} \mathscr{D}(A \oplus B) = \mathscr{D}(A) \oplus \mathscr{D}(B) = \{\psi \in L^2(\mathbb{R}^d) : \psi = \psi_1 + \psi_2,\ \psi_1 \in \mathscr{D}(A),\ \psi_2 \in \mathscr{D}(B)\} \\ \\ (A \oplus B)\,\psi = A\psi_1 + B\psi_2, \forall \psi \in \mathscr{D}(A \oplus B). \end{cases} \tag{2}$$

For simplicity let us assume that $\mathscr{D}(\Omega_k) \subset L^2(\Omega_k) \cap \mathscr{D}(H_0)$, $k = 1,2$ (where $\mathscr{D}(\Omega_k)$ is the space of infinitely smooth functions $t : \mathbb{R}^d \to \mathbb{C}$ with support on a compact subset of Ω_k) and let us define the operators:

$$H_k^S : \mathscr{D}(\Omega_k) \longrightarrow L^2(\Omega_k), \quad \phi \longrightarrow H_k^S \phi = H_0 \phi, \quad k = 1,2, \tag{3}$$

which are symmetric. Let also $H_k^{S^\dagger}$ be the adjoint of H_k^S.

Our main result characterizes the operators $H : \mathscr{D}(H) \subset L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$, associated to a s.a. H_0, and satisfying properties (i)–(iii).

Theorem 1. *Let H_0 be s.a. on $L^2(\mathbb{R}^d)$ and such that $\mathscr{D}(H_0) \supset \mathscr{D}(\Omega_1) \cup \mathscr{D}(\Omega_2)$ and $[H_0, P_{\Omega_k}]\psi = 0$, $k = 1,2$, $\forall \psi \in \mathscr{D}(\Omega_1) \cup \mathscr{D}(\Omega_2)$. An operator H satisfies the defining properties* (i)–(iii) *iff it can be written in the form $H_1 \oplus H_2$ for some H_1, H_2 s.a. extensions of the restrictions* (3)*. Moreover, all operators H are s.a. extensions of $H_1^S \oplus H_2^S$ and s.a. restrictions of $H_1^{S^\dagger} \oplus H_2^{S^\dagger}$.*

The condition (stated in the theorem) that $[H_0, P_{\Omega_k}]\psi = 0$, $\forall \psi \in \mathscr{D}(\Omega_1) \cup \mathscr{D}(\Omega_2)$, and the assumption that H_1^S and H_2^S have s.a. extensions are the minimal requirements for the existence of operators H satisfying (i)–(iii). Proofs of these results are given in [13].

We now focus on the case where $d = 1$, $\Omega_1 = \mathbb{R}^-$ and

$$H_0 = -\frac{d^2}{dx^2} + V(x), \quad \mathscr{D}(H_0) = \{\psi \in L^2(\mathbb{R}) : \psi, \psi' \in AC(\mathbb{R}); H_0\psi \in L^2(\mathbb{R})\}, \tag{4}$$

where $AC(\mathbb{R})$ is the set of absolutely continuous functions on $\mathbb{R}$ and $V(x)$ is a regular potential. We shall assume it to be i) real, ii) locally integrable and satisfying iii) $V(x) > -kx^2$, $k > 0$ for sufficiently large $|x|$. The conditions on $V(x)$ are such that $H_0 : \mathscr{D}(H_0) \subset L^2(\mathbb{R}) \to L^2(\mathbb{R})$ is the unique s.a. realization of the differential expression $-\frac{d^2}{dx^2}+V(x)$ on $L^2(\mathbb{R})$ [14] and ensure that all s.a. realizations of $-\frac{d^2}{dx^2}+V(x)$ on the semi-axes $]-\infty,0]$ and $[0,+\infty[$ are determined by boundary conditions at $x=0$ only.

For H_0 of the kind (4) the s.a. operators $H=H_1\oplus H_2$ are all of the form [13,14]:

$$H^{\lambda_1,\lambda_2}=H_1^{\lambda_1}\oplus H_2^{\lambda_2}:\begin{cases}\mathscr{D}(H^{\lambda_1,\lambda_2})=\mathscr{D}(H_1^{\lambda_1})\oplus\mathscr{D}(H_2^{\lambda_2})\\ \\ H^{\lambda_1,\lambda_2}\psi=H^{S^\dagger}\psi,\end{cases}\tag{5}$$

where

$$\mathscr{D}(H_k^{\lambda_k})=\{\psi_k=\chi_{\Omega_k}\phi_k:\ \phi_k\in\mathscr{D}(H_0)\wedge\phi_k'(0)=\lambda_k\phi_k(0)\},\tag{6}$$

$\lambda_k\in\mathbb{R}\cup\{\infty\}$, $k=1,2$ and the case $\lambda_k=\infty$ corresponds to Dirichlet boundary conditions. Moreover,

$$H^{S^\dagger}=H_1^{S^\dagger}\oplus H_2^{S^\dagger}:\begin{cases}\mathscr{D}(H^{S^\dagger})=\{\psi=\chi_{\Omega_1}\phi_1+\chi_{\Omega_2}\phi_2:\ \phi_1,\phi_2\in\mathscr{D}(H_0)\}\\ \\ H^{S^\dagger}\psi=\chi_{\Omega_1}H_0\phi_1+\chi_{\Omega_2}H_0\phi_2.\end{cases}\tag{7}$$

Hence, all s.a. confining Hamiltonians of the form $H_1\oplus H_2$ are s.a. restrictions of $H^{S^\dagger}$. To proceed, let us define the operators ($k=1,2$ and $n=0,1$):

$$\hat{\delta}_k^{(n)}(x):\mathscr{D}(H^{S^\dagger})\longrightarrow\mathscr{D}'(\mathbb{R});\ \psi=\chi_{\Omega_1}\phi_1+\chi_{\Omega_2}\phi_2\longrightarrow\hat{\delta}_k^{(n)}(x)\psi=\delta^{(n)}(x)\phi_k(x),\tag{8}$$

where $\mathscr{D}'(\mathbb{R})$ is the space of Schwartz distributions on $\mathbb{R}$ and $\delta^{(0)}(x)=\delta(x)$ and $\delta^{(1)}(x)=\delta'(x)$ are the Dirac measure and its first distributional derivative. We can now recast the operators (5) in the additive form $H=H_0+B^{BC}$:

Theorem 2. *The s.a. Hamiltonian H^{λ_1,λ_2} given by Eq.* (5) *act as*

$$H^{\lambda_1,\lambda_2}\psi=\left\{H_0-B_1^{\lambda_1}+B_2^{\lambda_2}\right\}\psi,\quad\forall\psi\in\mathscr{D}(H^{\lambda_1,\lambda_2}),\tag{9}$$

where now H_0 is the extension to the space of distributions of the original Hamiltonian given in (4), *$H_0:\mathscr{D}'(\mathbb{R})\longrightarrow\mathscr{D}'(\mathbb{R})$, and*

$$B_k^\lambda\equiv\begin{cases}-\hat{\delta}_k'(x)+(-1)^k\hat{\delta}_k(x),\quad\lambda=\infty\\ \\ \hat{\delta}_k'(x)+2\lambda\hat{\delta}_k(x)+(-1)^k\frac{d}{dx}\left[\hat{\delta}_k(x)\left(\frac{d}{dx}-\lambda\right)\right],\quad\lambda\neq\infty\end{cases}\qquad k=1,2.\tag{10}$$

Moreover, the maximal domain of the expression (9,10) *coincides with $\mathscr{D}(H^{\lambda_1,\lambda_2})$* (5), *i.e.*

$$\mathscr{D}_{\max}(H^{\lambda_1,\lambda_2})\equiv\{\psi\in L^2(\mathbb{R}):\ H^{\lambda_1,\lambda_2}\psi\in L^2(\mathbb{R})\}=\mathscr{D}(H^{\lambda_1,\lambda_2}).\tag{11}$$

The proof is given in [13].

ACKNOWLEDGEMENTS

We thank A. Posilicano and P. Garbaczewski for several discussions. This work was partially supported by grants POCTI/0208/2003 and PTDC/MAT/69635/2006 of the Portuguese Science Foundation.

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Tõkestatud kvantsüsteemide globaalne dünaamiline formuleering

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On antud lühiülevaade matemaatilistest probleemidest, mis tekivad ruumiliselt tõkestatud kvantsüsteemide globaalse omaduaalse formuleeringu korral. Lähemalt on vaadeldud ühemõõtmelist juhtu ja näidatud, et teatud distributsioone sisaldavad omaduaalsed hamiltoniaanid lubavad kirjeldada kvantsüsteemi ruumilist tõkestatust dünaamiliselt.