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On the adiabatic behaviour for a Wigner–Weisskopf atom

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Abstract

In this research announcement we present some recent results of the authors on the adiabatic theorem for a system without a spectral gap [4].

Keywords: Adiabatic theorem without spectral gap, Feshbach method, time-dependent Schrödinger equation, Heisenberg time evolution

Introduction. Consider a quantum mechanical system consisting of a quantum dot coupled to a reservoir. The dot energy varies adiabatically in time starting in a bound state. Assuming that the energy of the bound state stays away from the continuous spectrum for all times, the survival probability of the bound state is one by the standard adiabatic theorem, i.e. the one for systems with a spectral gap.

In [4] we study the case where the bound state dives into the continuous spectrum for a macroscopic time during the adiabatic variation of the dot energy which returns to its initial value at the end. The gapless adiabatic theorem [1, 8, 9] yields that the survival probability is also one if the bound state exists all the time and its spectral projection is twice differentiable. However, the survival probability should be zero if the bound state becomes a resonance at some point. This conjecture is based on heuristics and related to the adiabatic pair creation [7] and memory effects in quantum mesoscopic transport [2, 3]. Except for some rather technical and/or restrictive results [3, 6, 7], these heuristics have not been proven rigorously.

In the following section we will outline some new results on the adiabatic theorem for a Wigner–Weisskopf atom recently obtained in [4]. The main result states that the survival probability vanishes in the adiabatic limit, i.e. the adiabatic theorem breaks down for a large class of couplings between the quantum dot and the reservoir when the bound state dives into the continuous spectrum during the adiabatic tuning of the dot energy. In addition, a detailed spectral analysis of the model is given and a 'threshold adiabatic theorem' is proved. Admittedly the considered setting is much simpler than most physically interesting models [3, 6, 7]. However, we believe that the methods used in [4] have the potential to work in the case of many Schrödinger and Dirac operators as well.

Model and results. We consider a simple model of a one-level atom coupled to a reservoir, a Wigner–Weisskopf model of an atom. On the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3) \oplus \mathbb{C}$

we define the Hamiltonian

$$H_\tau(E) = \begin{bmatrix} -\Delta & 0 \\ 0 & E \end{bmatrix} + \tau \begin{bmatrix} 0 & |\varphi\rangle \\ \langle\varphi| & 0 \end{bmatrix}.$$

It represents a quantum dot with dot energy $E \in \mathbb{R}$ coupled to the reservoir $\mathbb{R}^3$. The coupling between both systems is controlled by the parameter $\tau \in \mathbb{R}$ and the normalized coupling function $\varphi \in L^2(\mathbb{R}^3)$. In the uncoupled case, $\tau = 0$, the particle can either sit in the quantum dot with energy E or move freely in the reservoir.

In the following we always assume that the coupling function φ satisfies $\int_{\mathbb{R}^3}(1+x^2)^w|\varphi(x)|^2dx < \infty$ for all $w \in \mathbb{R}$ and that there is $\nu \in \mathbb{N}$ such that $|k|^{-\nu}\widehat{\varphi}(k)$ is continuous at $k = 0$. Here $\widehat{\varphi}$ denotes the usual Fourier transform of φ. Note that the second condition implies that all derivatives of $\widehat{\varphi}$ with degree less than ν are zero at $k = 0$. In particular, we always have $\widehat{\varphi}(0) = 0$.

In [4, Section 2] we analyze the spectrum of the instantaneous operator $H_\tau(E)$. Obviously, $[0,\infty[$ is the essential spectrum of $H_\tau(E)$. We show that for any value of $\tau \neq 0$ there exists a critical value $E_c > 0$ such that the operator $H_\tau(E)$ has exactly one simple negative eigenvalue for every $E < E_c$. Moreover, $H_\tau(E_c)$ has the eigenvalue 0 embedded at the threshold. If the operator $H_\tau(E)$ has an eigenvalue $\lambda(E)$, $P(E)$ denotes the corresponding eigenprojection and $\Psi(E)$ a corresponding normalized eigenfunction.

We study the Heisenberg time-evolution of the bound state for $\tau \neq 0$ when the dot energy E varies adiabatically in time. The time-evolution operator for $H_\tau(E(\eta t))$ is determined by the time-dependent Schrödinger equation

$$i\frac{\partial}{\partial t}U_\eta(t,t_0) = H_\tau(E(\eta t))U_\eta(t,t_0), \quad U_\eta(t_0,t_0) = \mathrm{Id},$$

for $t, t_0 \in \mathbb{R}$. To model an adiabatic switching, E is made time-dependent, $t \mapsto E(\eta t)$, with a parameter $\eta > 0$. Then the adiabatic limit is $\eta \downarrow 0$. Initially the atom is assumed to be in a bound state and the following conditions on the function $E(\cdot)$ hold: $E(\cdot)\colon [-1,0] \to \mathbb{R}$ is $C^2([-1,0])$. There exists $s_m \in (-1,0)$ such that $E(\cdot)$ is strictly increasing on $[-1,s_m]$ and strictly decreasing on $[s_m,0]$. Its maximal value $E_m = E(s_m)$ is positive while $E(-1) = E(0) < 0$. Moreover, given any intermediate value $E \in (E(-1),E_m)$, there exist exactly two points $s < s_m < s'$ such that $E(s) = E(s') = E$.

The main result [4, Theorem 1.3] is summarized as follows:

Theorem 1. *Let φ and $E(\cdot)$ fulfill the assumptions stated above and $\tau > 0$ small enough.*

(i) There is a critical dot energy $E_c \in (0,E_m)$ such that $\lambda(E_c) = 0$ is an embedded simple eigenvalue of $H_\tau(E_c)$ with corresponding eigenprojection $P(E_c)$. For every $E < E_c$ there exists a unique discrete negative eigenvalue $\lambda(E)$ corresponding to a smooth eigenprojection $P(E)$ with

$$\|P'(E)\| \leq \frac{C}{(E_c - E)^{3/4}} \quad \textit{and} \quad \lim_{E\uparrow E_c}\|P(E) - P(E_c)\| = 0. \tag{1}$$

(ii) There exists a class of functions φ for which the instantaneous Hamiltonian $H_\tau(E)$ has purely absolutely continuous spectrum when $E_c < E \leq E_m$, and

$$\lim_{\eta\downarrow 0}|\langle\Psi(E(0))|U_\eta(0,-1/\eta)\Psi(E(-1))\rangle|^2 = 0. \tag{2}$$

In other words, the survival probability goes to zero if the instantaneous bound state becomes a resonance during the adiabatic tuning of $E(\cdot)$. Examples of allowed functions are those that satisfy $\nabla\widehat{\varphi}(0) \neq 0$ or $\widehat{\varphi}(k) = e^{-|k|^{-2}}$ near $k = 0$.

(iii) Assume that $\widehat{\varphi}(k) = 0$ on $B_\delta(0)$ for some $\delta > 0$ and that $0 < E_m < \delta^2$. Then $H_\tau(E(s))$ has a simple eigenvalue $\lambda(E(s))$ for every $s \in [-1, 0]$. The eigenvalue is discrete and negative outside $[s_c, s_c']$ and embedded in the continuous spectrum inside $[s_c, s_c']$. Moreover,

$$\lim_{\eta \downarrow 0} |\langle \Psi(E(0)) | U_\eta(0, -1/\eta) \Psi(E(-1)) \rangle|^2 = 1. \tag{3}$$

So the adiabatic theorem holds in this case.

(iv) Fix $\alpha > 0$. There exist $K > 0$, independent of α, and $\eta_0(\alpha) > 0$ such that for every $\eta < \eta_0(\alpha)$ and $s \in (s_c, s_c')$ with $|s - s_c| \leq \alpha \eta^{\frac{4}{2\nu+7}}$,

$$|\langle \Psi(E_c) | U_\eta(s/\eta, s_c/\eta) \Psi(E_c) \rangle|^2 \geq 1 - \alpha K. \tag{4}$$

Ergo, the critical eigenvector survives in the supercritical regime for small microscopic times of order $\eta^{\frac{4}{2\nu+7}}$.

The assumptions have to ensure that there is an (embedded) bound state at the spectral threshold. The problem is still open if the bound state turns into a resonance at the threshold.

Important ingredients in the spectral analysis are a Feshbach formula for the resolvent of $H_\tau(E)$ [4, Equation (2.6)] and an asymptotic expansion of the free resolvent $(-\Delta - z)^{-1}$ at the threshold $z = 0$ as presented in [5]. In particular, they yield the spectral projections of the bound state via the Riesz resolvent formula. Other steps are the decomposition of the Heisenberg time evolution using the Dyson equation [4, Subsection 4.1] and an enhanced propagation estimate [4, Proposition 4.2]

$$\langle \zeta | \mathrm{e}^{-\mathrm{i}tH_\tau(E_a)} \zeta \rangle \leq \text{const} \, (1 + |t|)^{-5/2} \tag{5}$$

for $E_a > E_c$ where $\zeta = \left[\begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right]$ is the basis vector in the quantum dot. As part of the proofs of (ii) and (iii) we show that the instantaneous bound state is a good approximation to the 'true' Heisenberg time evolution up to the threshold [4, Theorem 1.3(ii)].

The results above easily extent to a quantum dot with N energy levels and hence $\mathcal{H} = L^2(\mathbb{R}^3) \oplus \mathbb{C}^N$. Suppose that initially the system has N discrete eigenvalues and only one of them dives into the continuum during the adiabatic tuning. Then a particle in the diving state scatters away while the $N - 1$ other eigenvalues stay away from the continuum and therefore their states remain.

Moreover, we may allow for any odd dimension d in the reservoir. Then the conditions on $\widehat{\varphi}$ can be relaxed for $d \geq 5$ or must be more restrictive for $d = 1$. The crucial point here is that the propagation estimate (5) holds in $d \geq 5$ for any Hamiltonian, while in $d = 1$ and 3 the estimate, normally with exponent $-3/2$ resp. $-1/2$, has to be enhanced which is ensured by the behavior of $\widehat{\varphi}$ at $k = 0$.

Despite the fact that the overall survival probability goes to zero in the adiabatic limit according to (ii) the critical eigenfunction may survive for a long microscopic time $t = \eta s$

in the supercritical regime. An extreme example is φ with $\widehat{\varphi}(k) = \exp(-|k|^2)$ near $k = 0$. Then (4) holds for any $\nu \geq 1$. Nevertheless the survival probability at the terminal point is zero in the adiabatic limit.

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