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**On the Fermi Golden Rule:  
degenerate eigenvalues**

by

Arne Jensen and Gheorghe Nenciu

R-2006-17

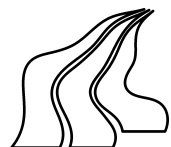
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# ON THE FERMI GOLDEN RULE: DEGENERATE EIGENVALUES

ARNE JENSEN AND GHEORGHE NENCIU

ABSTRACT. We review and further develop the framework in [10] of the stationary theory of resonances, arising by perturbation of either threshold, or embedded in the continuum, eigenvalues. While in [10] only non-degenerate eigenvalues were considered, here we add some results for the degenerate case.

## 1. INTRODUCTION

In this paper we consider the following question. Given a Schrödinger operator  $H$  on a Hilbert space  $\mathcal{H}$  with an eigenvalue either at a threshold or embedded in the continuum. We add a perturbation and consider the family  $H(\varepsilon) = H + \varepsilon W$  for  $\varepsilon$  small. We ask what happens to this eigenvalue. This question was considered in detail in [10] in the case, where the eigenvalue is non-degenerate. In this paper we consider the case of a degenerate eigenvalue.

We assume that the eigenvalue is located at  $E_0$ . We denote the projection onto the eigenspace for eigenvalue  $E_0$  of  $H$  by  $P_0$ . We assume  $\text{Rank } P_0 = N < \infty$ . We also use  $Q_0 = I - P_0$ . The problem we consider can be formulated as follows. We want to find an effective Hamiltonian  $h(\varepsilon)$  on  $P_0\mathcal{H}$  and an error term  $\delta(\varepsilon, t)$ , such that

$$P_0 e^{-itH(\varepsilon)} P_0 = e^{-ith(\varepsilon)} P_0 + \delta(\varepsilon, t). \quad (1.1)$$

Furthermore, we want to have an estimate uniform in time of the form

$$\sup_{t>0} \|\delta(\varepsilon, t)\| \leq C\varepsilon^p, \quad p > 0. \quad (1.2)$$

This time-dependent approach to resonance behavior of the time evolution, without analyticity assumptions, has its origin in the work by Orth [13]. See the remarks in the introduction in [10], the recent review [4], and the remarks at the end of this section.

We use a stationary approach to the problem, based on Stone's formula

$$P_0 e^{-itH(\varepsilon)} P_0 = \lim_{\eta \rightarrow 0} \frac{1}{\pi} \int_{\sigma(H(\varepsilon))} dx e^{-itx} \text{Im } P_0 (H(\varepsilon) - x - i\eta)^{-1} P_0. \quad (1.3)$$

A central idea is then to localize close to the energy  $E_0$ . We choose an interval  $I_\varepsilon = (e_0(\varepsilon) - d(\varepsilon), e_0(\varepsilon) + d(\varepsilon))$ , and take the characteristic function  $g_\varepsilon(x) = \chi_{I_\varepsilon}(x)$  as the cut-off function. In some cases one may prefer to take a smoothed out

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characteristic function instead. With such a choice one can obtain a refinement of (1.1) in the form

$$P_0 e^{-itH(\varepsilon)} P_0 = (I + A(\varepsilon)) e^{-ith(\varepsilon)} (I + A(\varepsilon)) + \delta(\varepsilon, t),$$

where  $A(\varepsilon) = \mathcal{O}(\varepsilon^p)$  for some  $p > 0$ , and  $\delta(\varepsilon, t)$  now exhibits decay in  $t$  for  $t$  large. However, our concern in this paper is with error estimates uniform in time, so we take just the characteristic function as our cut-off function.

A central point in our approach is to find the “right” location  $e_0(\varepsilon)$ , and the “right” size function  $d(\varepsilon)$ , such that energies in  $I_\varepsilon$  give the resonance behavior, and energies outside  $I_\varepsilon$  only contribute to the error term  $\delta(\varepsilon, t)$ , via a split in the integration domain in (1.3). This means that we consider first

$$P_0 e^{-itH(\varepsilon)} g_\varepsilon(H(\varepsilon)) P_0 = \lim_{\eta \rightarrow 0} \frac{1}{\pi} \int_{I_\varepsilon} dx e^{-itx} \operatorname{Im} P_0 (H(\varepsilon) - x - i\eta)^{-1} P_0. \quad (1.4)$$

Suppose that by a careful choice of  $I_\varepsilon$  one can prove that

$$P_0 e^{-itH(\varepsilon)} g_\varepsilon(H(\varepsilon)) P_0 = e^{-ith(\varepsilon)} + \delta(\varepsilon, t), \quad (1.5)$$

with  $\delta(\varepsilon, t)$  satisfying (1.2). Then by Hunziker’s trick (see [6] or the proof of Theorem 3.7 in [10]) one obtains (1.1) with  $C$  in (1.2) replaced by  $2C$ .

To deal with the localized part of the integral we use the Schur-Livsic-Feshbach-Grushin formula (SLFG formula for short). We briefly recall it from [10]. Let  $R_\varepsilon(z) = (H(\varepsilon) - z)^{-1}$ , and let  $R_{0,\varepsilon}(z)$  be the resolvent of  $Q_0 H(\varepsilon) Q_0$  as an operator in  $Q_0 \mathcal{H}$ . Then we have in the decomposed space  $\mathcal{H} = P_0 \mathcal{H} \oplus Q_0 \mathcal{H}$

$$R_\varepsilon(z) = \begin{bmatrix} R_{\text{eff}}(z) & -\varepsilon R_{\text{eff}}(z) P_0 W Q_0 R_{0,\varepsilon}(z) \\ -\varepsilon R_{0,\varepsilon}(z) Q_0 W P_0 R_{\text{eff}}(z) & R_{22} \end{bmatrix}, \quad (1.6)$$

with

$$R_{22} = R_{0,\varepsilon}(z) + \varepsilon^2 R_{0,\varepsilon}(z) Q_0 W P_0 R_{\text{eff}}(z) P_0 W Q_0 R_{0,\varepsilon}(z),$$

and

$$R_{\text{eff}}(z) = (P_0 H(\varepsilon) P_0 - \varepsilon^2 P_0 W Q_0 R_{0,\varepsilon}(z) Q_0 W P_0 - z P_0)^{-1},$$

It is convenient (especially for the case of threshold eigenvalues) to work with a factored perturbation, so we assume that we have a factorization

$$W = A^* D A \quad (1.7)$$

of  $W$  with  $D$  a self-adjoint involution. An example of such a factorization is the polar decomposition of  $W$ ,

$$W = |W|^{1/2} D |W|^{1/2}, \quad (1.8)$$

where we take  $D$  to be unitary by defining it to be the identity on  $\operatorname{Ker} W$ . We introduce the notation

$$G(z) = A Q_0 (H - z)^{-1} Q_0 A^*. \quad (1.9)$$

and (see [5])

$$P_0 (H - z)^{-1} P_0 = F(z, \varepsilon)^{-1}. \quad (1.10)$$

Then, using the factored version of the second resolvent equation, one can rewrite  $F(z, \varepsilon)$  as follows:

$$\begin{aligned}
F(z, \varepsilon) &= P_0 H(\varepsilon) P_0 - \varepsilon^2 P_0 W Q_0 R_{0, \varepsilon}(z) Q_0 W P_0 - z P_0 \\
&= E_0 P_0 + \varepsilon P_0 W P_0 - \varepsilon^2 P_0 A^* D G(z) D A P_0 \\
&\quad - \varepsilon^3 P_0 A^* D G(z) [D + \varepsilon G(z)]^{-1} G(z) D A P_0 - z P_0 \\
&\equiv E_0 P_0 + \varepsilon P_0 W P_0 - \varepsilon^2 S(z, \varepsilon) - z P_0.
\end{aligned} \tag{1.11}$$

The localized part of Stone's formula then takes the form

$$P_0 e^{-itH(\varepsilon)} g_\varepsilon(H(\varepsilon)) P_0 = \lim_{\eta \rightarrow 0} \frac{1}{\pi} \int_{I_\varepsilon} dx e^{-itx} \operatorname{Im} P_0 F(x + i\eta, \varepsilon)^{-1} P_0. \tag{1.12}$$

At this point the hard work starts. We need to rewrite  $F(z, \varepsilon)$ , show invertibility, separate the resonance term, and estimate the remainder. All that depends crucially on the smoothness properties of  $F(z, \varepsilon)$ . From (1.11) it is clear that  $F(z, \varepsilon)$  inherits the smoothness properties of  $G(z)$ , and this explains, why those appear in the formulation of the results below.

**1.1. Comments on the literature.** The reader may consult the paper [4] for an extensive review on eigenvalues, resonances, and the Fermi Golden Rule. We also refer to the introduction of [10] and the references given there. Here we comment on results related to those presented in the following section, and some new results, which appeared after the submission of [10].

With analyticity assumptions and for eigenvalues away from thresholds complete and optimal results were obtained by Hunziker [6]. In particular, it follows from [6] that with the choice of initial function  $\psi \in P_0 \mathcal{H}$  the optimal error estimate for the behavior of  $\langle \psi, e^{-itH(\varepsilon)} \psi \rangle$  is  $\mathcal{O}(\varepsilon^2)$ . The problem at hand is to extend, as much as possible, Hunziker's results to the non-analytic case, as well as to threshold eigenvalues.

For the case of a degenerate eigenvalue embedded in the continuum, the reduced Hamiltonian used in [12, 15] contains only the first three terms in our  $h(\varepsilon)$ , see (2.23), and they get an error estimate  $\mathcal{O}(\varepsilon)$ . Our proof of Theorem 4 below is a refinement of the argument given in [15]. One can apply our argument to case of time-periodic Schrödinger operators, studied in [15]. Under the assumption of the Fermi Golden Rule condition (2.21) an error estimate  $\mathcal{O}(\varepsilon^2)$  follows from the results in [3], in the non-degenerate case.

Concerning eigenvalues embedded at a threshold, then Theorem 5 gives a result on two channel Schrödinger operators in a specific set-up with a doubly degenerate eigenvalue, and a threshold resonance. Further results will be given elsewhere. Concerning two channel operators, we mention [11], where conditions are given that imply a degenerate threshold eigenvalue gives rise to negative discrete eigenvalues. Only off-diagonal perturbations are used, and resonances are not studied, in [11]. In the paper [14] both eigenvalues and resonances are studied for a two channel Schrödinger operator, under small off-diagonal perturbations. To study the location of resonances, dilation analyticity is assumed in [14]. The behavior

of  $e^{-itH(\varepsilon)}$  is not studied in [14], whereas here it is our main concern. See also Remark 6.

## 2. THE RESULTS

First we recall the main results in [10]. We start with a non-degenerate eigenvalue  $E_0$  embedded in the continuum. For  $a > 0$  we define

$$D_a(E_0) = \{z \in \mathbf{C} \mid |z - E_0| < a, \operatorname{Im} z > 0\}. \quad (2.1)$$

We denote by  $C^{n,\theta}(D_a(E_0))$  the functions in  $D_a(E_0)$  that are  $n$  times continuously norm-differentiable, with the  $n^{\text{th}}$  derivative satisfying a uniform Hölder condition in  $D_a(E_0)$ , of order  $\theta$ ,  $0 \leq \theta \leq 1$ . We assume that the derivatives also are uniformly bounded in  $D_a(E_0)$ . We need to assume that  $G(z) \in C^{n,\theta}(D_a(E_0))$ . Such conditions can be verified in an abstract setting, using the Mourre estimate and the multiple commutator technique, see e.g. [1, 2, 3] and references therein. Note that this implies that  $G(z)$  has boundary values  $G(x + i0)$ , which are in  $C^{n,\theta}([E_0 - a, E_0 + a])$ . For Schrödinger operators the smoothness of  $G(z)$  also follows, if the potential decays sufficiently fast at infinity.

**Theorem 1** ([10, Theorem 4.1]). *Assume  $G(z) \in C^{n,\theta}(D_a(E_0))$ . Assume  $N = 1$  and  $n + \theta > 0$ . Write  $F(x + i0, \varepsilon) = (R(x, \varepsilon) + iI(x, \varepsilon))P_0$ . Then for  $\varepsilon$  sufficiently small there exists a (unique for  $n + \theta \geq 1$ ) solution to  $R(x, \varepsilon) = 0$  in the interval  $(E_0 - a, E_0 + a)$ , denoted by  $x_0(\varepsilon)$ . Let  $\Gamma(\varepsilon) = -I(x_0(\varepsilon), \varepsilon)$ , write*

$$\lambda_\varepsilon = x_0(\varepsilon) - i\Gamma(\varepsilon), \quad (2.2)$$

and let  $\Psi_0$  denote a normalized eigenfunction for eigenvalue  $E_0$  of  $H$ . Then for  $\varepsilon$  sufficiently small, and for all  $t > 0$ , the following results hold true:

(i) Assume  $n = 0$ ,  $0 < \theta < 1$ , and

$$\Gamma(\varepsilon) \geq C\varepsilon^\gamma \quad \text{with } 2 \leq \gamma < \frac{2}{1-\theta}. \quad (2.3)$$

Then we have

$$|\langle \Psi_0, e^{-itH(\varepsilon)} \Psi_0 \rangle - e^{-it(x_0(\varepsilon) - i\Gamma(\varepsilon))}| \leq C \frac{1}{1-\theta} \varepsilon^\delta, \quad (2.4)$$

where

$$\delta = 2 - \gamma(1 - \theta) > 0. \quad (2.5)$$

(ii) For  $n + \theta \geq 1$  we have

$$|\langle \Psi_0, e^{-itH(\varepsilon)} \Psi_0 \rangle - e^{-it(x_0(\varepsilon) - i\Gamma(\varepsilon))}| \leq C \begin{cases} \varepsilon^2 |\ln \varepsilon| & \text{for } n = 0, \theta = 1, \\ \varepsilon^2 & \text{for } n + \theta > 1. \end{cases} \quad (2.6)$$

Consider now the case of a non-degenerate eigenvalue at the threshold  $E_0 = 0$ . The problem here is that the usual methods to prove the smoothness of  $G(z)$  do not work at thresholds, and actually it may not be smooth, or even blows up, in the neighborhood of the origin. The way out from this difficulty taken in [10] is to use the asymptotic expansion of  $G(z)$  around threshold. Let us stress that (see [10] and references therein) the asymptotic expansions of the resolvent around

thresholds are not universal; e.g. in the Schrödinger case the type of expansion depends on dimension and on the threshold spectral properties of the Hamiltonian. The asymptotic expansion in the assumption below (see [10, Section 3]) is modeled after Schrödinger and Dirac operators in odd dimensions.

**Assumption 2.** (A1) *There exists  $a > 0$ , such that  $(-a, 0) \subset \rho(H)$  and  $[0, a] \subset \sigma_{\text{ess}}(H)$ .*

(A2) *Assume that zero is a non-degenerate eigenvalue of  $H$ :  $H\Psi_0 = 0$ , with  $\|\Psi_0\| = 1$ , and there are no other eigenvalues in  $[0, a]$ . Let  $P_0 = |\Psi_0\rangle\langle\Psi_0|$  be the orthogonal projection onto the one-dimensional eigenspace.*

(A3) *Assume*

$$\langle\Psi_0, W\Psi_0\rangle = b > 0. \quad (2.7)$$

(A4) *For  $\text{Re } \kappa \geq 0$  and  $z \in \mathbf{C} \setminus [0, \infty)$  we let*

$$\kappa = -i\sqrt{z}, \quad z = -\kappa^2. \quad (2.8)$$

*There exist  $N_0 \in \mathbf{N}$  and  $\delta_0 > 0$ , such that for  $\kappa \in \{\kappa \in \mathbf{C} \mid 0 < |\kappa| < \delta_0, \text{Re } \kappa \geq 0\}$  we have*

$$G(z) = \sum_{j=-1}^{N_0} \tilde{G}_j \kappa^j + \kappa^{N_0+1} \tilde{G}_{N_0}(\kappa), \quad (2.9)$$

where

$$\tilde{G}_j \quad \text{are bounded and self-adjoint,} \quad (2.10)$$

$$\tilde{G}_{-1} \quad \text{is of finite rank and self-adjoint,} \quad (2.11)$$

$$\tilde{G}_{N_0}(\kappa) \quad \text{is uniformly bounded in } \kappa. \quad (2.12)$$

From (2.9) we get

$$\langle\Psi_0, A^* D G(z) D A \Psi_0\rangle = \sum_{j=-1}^{N_0} g_j \kappa^j + \kappa^{N_0+1} g_{N_0}(\kappa), \quad (2.13)$$

where

$$g_j = \langle\Psi_0, A^* D \tilde{G}_j D A \Psi_0\rangle, \quad (2.14)$$

$$g_{N_0}(\kappa) = \langle\Psi_0, A^* D \tilde{G}_{N_0}(\kappa) D A \Psi_0\rangle. \quad (2.15)$$

Notice that due to (2.10) we have

$$g_j = \bar{g}_j. \quad (2.16)$$

(A5) *There exists an odd integer,  $-1 \leq \nu \leq N_0$ , such that*

$$g_\nu \neq 0, \quad \tilde{G}_j = 0 \quad \text{for } j = -1, 1, \dots, \nu - 2. \quad (2.17)$$

The main (semi)-abstract result in [10] is as follows:

**Theorem 3** ([10, Theorem 3.7]). *Suppose (A1)–(A5) in Assumption 2 hold true. Then for sufficiently small  $\varepsilon > 0$  we have*

$$|\langle \Psi_0, e^{-itH(\varepsilon)} \Psi_0 \rangle - e^{-it(x_0(\varepsilon) - i\Gamma(\varepsilon))}| \leq C\varepsilon^{p(\nu)}. \quad (2.18)$$

Here  $p(\nu) = \min\{2, (2 + \nu)/2\}$ , and

$$\Gamma(\varepsilon) = -i\nu^{-1}g_\nu b^{\nu/2} \varepsilon^{2+\nu/2} (1 + \mathcal{O}(\varepsilon)), \quad (2.19)$$

$$x_0(\varepsilon) = b\varepsilon(1 + \mathcal{O}(\varepsilon)). \quad (2.20)$$

We send the reader to [10] for application of the above theorem to odd dimensional Schrödinger operators.

Next we present two new results for degenerate embedded eigenvalues. The first one concerns eigenvalues embedded in the continuum. The error estimate in the following result is optimal, when one considers  $P_0\mathcal{H}$ . By modifying this space one may obtain better results, see [6].

**Theorem 4.** *Assume  $N \geq 2$  and  $G(z) \in C^{n,\theta}(D_a(E_0))$  with  $n + \theta \geq 2$ . Assume there exists  $\gamma > 0$  such that*

$$\text{Im } P_0 A^* D G(E_0 + i0) D A P_0 \geq \gamma P_0. \quad (2.21)$$

Then there exists a function  $\delta(\varepsilon, t)$  satisfying (1.2) with  $p = 2$ , such that

$$P_0 e^{-itH(\varepsilon)} P_0 = e^{-it h(\varepsilon)} P_0 + \delta(\varepsilon, t). \quad (2.22)$$

Here  $h(\varepsilon)$  on  $P_0\mathcal{H}$  is given by

$$\begin{aligned} h(\varepsilon) = & E_0 P_0 + \varepsilon P_0 W P_0 - \varepsilon^2 P_0 W Q_0 (H - E_0 - i0)^{-1} Q_0 W P_0 \\ & - \varepsilon^3 \left\{ P_0 W Q_0 (H - E_0 - i0)^{-1} Q_0 W Q_0 (H - E_0 - i0)^{-1} Q_0 W P_0 \right. \\ & + \frac{1}{2} \left[ P_0 W P_0 W \frac{d}{dE} Q_0 (H - E - i0)^{-1} Q_0 \Big|_{E=E_0} W P_0 \right. \\ & \left. \left. + P_0 W \frac{d}{dE} Q_0 (H - E - i0)^{-1} Q_0 \Big|_{E=E_0} W P_0 W P_0 \right] \right\}. \quad (2.23) \end{aligned}$$

The condition (2.21) is the usual Fermi Golden Rule condition for an embedded eigenvalue.

We turn now to the case, when the Fermi Golden Rule (2.21) does not hold true. We believe that by refining the proof of Theorem 4 one can replace the Fermi Golden Rule condition (2.21) by a weaker one (see (1.11) for the definition of  $S(z, \varepsilon)$ ):

$$\text{Im } S(x + i0, \varepsilon) > 0, \quad (2.24)$$

$$\sup_{\substack{x \in (E_0 - a, E_0 + a) \\ |\varepsilon| \leq c_0}} \|\text{Im } S(x + i0, \varepsilon)\| \cdot \|(\text{Im } S(x + i0, \varepsilon))^{-1}\| < \infty. \quad (2.25)$$

Recall that  $\|\text{Im } S(x + i0, \varepsilon)\| \cdot \|(\text{Im } S(x + i0, \varepsilon))^{-1}\|$  is the condition number of the matrix  $\text{Im } S(x + i0, \varepsilon)$ .

Unfortunately (2.24) does not cover the case, when by perturbation of a degenerate eigenvalue one obtains both eigenvalues and resonances, which is the generic



case at threshold. However even in this case one can obtain partial results under additional conditions on the spectrum of  $P_0WP_0$ . Suppose that  $P_0WP_0$  (as an operator in  $P_0\mathcal{H}$ ) has a non-degenerate eigenvalue  $b_1$  with eigenfunction  $\Psi_1$ ,

$$\sigma(P_0WP_0) = \{b_1\} \cup \sigma_2, \quad \text{dist}(b_1, \sigma_2) = d > 0 \quad (2.26)$$

and consider  $\langle \Psi_1, e^{-itH(\varepsilon)} \Psi_1 \rangle$ . The idea is to reduce the problem to the non-degenerate case already studied. For, write  $F(z, \varepsilon)$  (see (1.11)) as

$$F(z, \varepsilon) = E_0P_0 + \varepsilon P_0WP_0 - \varepsilon^2 S(z, \varepsilon) - zP_0, \quad (2.27)$$

and apply once again the SLFG formula to obtain

$$\begin{aligned} \langle \Psi_1, (H(\varepsilon) - z)^{-1} \Psi_1 \rangle &= \frac{1}{F_1(z, \varepsilon)} \\ &= [E_0 - z + \varepsilon \langle \Psi_1, W \Psi_1 \rangle - \varepsilon^2 \langle \Psi_1, S(z, \varepsilon) \Psi_1 \rangle \\ &\quad - \varepsilon^4 \langle \Psi_1, S(z, \varepsilon) Q_1 (E_0 - z + \varepsilon Q_1 W Q_1 - \varepsilon^2 Q_1 S(z, \varepsilon) Q_1)^{-1} Q_1 S(z, \varepsilon) \Psi_1 \rangle]^{-1} \\ &\equiv [E_0 - z + \varepsilon \langle \Psi_1, W \Psi_1 \rangle - \varepsilon^2 S_1(z, \varepsilon)]^{-1}, \end{aligned} \quad (2.28)$$

where  $Q_1 = P_0 - |\Psi_1\rangle\langle\Psi_1|$ . The point of (2.28) is that as far as  $\text{dist}(z, \varepsilon\sigma_2) > C\varepsilon$ ,  $S_1(z, \varepsilon)$  inherits the smoothness properties of  $S(z, \varepsilon)$ , and then one can apply the methods in [10] to the problem at hand, both for threshold and embedded eigenvalues.

As an example we shall consider a doubly degenerate threshold eigenvalue in a two channel Schrödinger operator in three dimensions. The setting is the one described in [10]. In particular, in this case  $E_0 = 0$ . In the ‘‘open’’ channel we take an operator modeling Schrödinger operators in three dimensions with a non-degenerate bound state at threshold. As for the ‘‘closed’’ channel, since only the bound state in the closed channel is relevant in the forthcoming discussion, we shall take  $\mathbf{C}$  as the Hilbert space representing the closed channel, i.e.  $\mathcal{H} = L^2(\mathbf{R}^3) \oplus \mathbf{C}$ . As the unperturbed Hamiltonian we take

$$H = \begin{bmatrix} -\Delta + V & 0 \\ 0 & 0 \end{bmatrix}, \quad (2.29)$$

and as the perturbation we take

$$W = \begin{bmatrix} 0 & |W_{12}\rangle\langle 1| \\ |1\rangle\langle W_{12}| & b \end{bmatrix}, \quad (2.30)$$

which is a shorthand for

$$W \begin{bmatrix} f(\mathbf{x}) \\ \xi \end{bmatrix} = \begin{bmatrix} W_{12}(\mathbf{x})\xi \\ \int \overline{W_{12}(\mathbf{x})} f(\mathbf{x}) + b\xi \end{bmatrix}. \quad (2.31)$$

Here we assume

$$\langle \cdot \rangle^\beta V \in L^\infty(\mathbf{R}^3), \quad \langle \cdot \rangle^{\gamma/2} W_{12} \in L^\infty(\mathbf{R}^3) \quad (2.32)$$

with  $\beta > 9$  and  $\gamma > 5$ .

We use the following factorization of  $W$ . To simplify the notation below we introduce the weight function

$$\rho_\gamma = \langle \cdot \rangle^{-\gamma/2}. \quad (2.33)$$

Let

$$B = \begin{bmatrix} \rho_{-\gamma} & 0 \\ 0 & 1 \end{bmatrix}, \quad (2.34)$$

and

$$C = BWB = |C|^{1/2} D |C|^{1/2}, \quad (2.35)$$

where  $D$  is defined to be the identity on  $\text{Ker } C$ , such that  $D$  is self-adjoint with  $D^2 = I$ . The operator  $C$  is bounded and self-adjoint, and we take

$$A = |C|^{1/2} B^{-1}, \quad (2.36)$$

i.e.

$$W = B^{-1} |C|^{1/2} D |C|^{1/2} B^{-1}. \quad (2.37)$$

About  $-\Delta + V$  we suppose that it has a non-degenerate threshold eigenvalue

$$(-\Delta + V)\Psi_0 = 0, \quad \|\Psi_0\| = 1. \quad (2.38)$$

as well as a threshold resonance with canonical resonance function  $\Psi_c$  (for definition and further details see [10, Appendix A] for an approach based on [8, 9], or see [7]). We use the notation

$$\tilde{\Psi}_0 = \begin{bmatrix} \Psi_0 \\ 0 \end{bmatrix}, \quad \tilde{1} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad \tilde{\Psi}_c = \begin{bmatrix} \Psi_c \\ 0 \end{bmatrix}. \quad (2.39)$$

We have in this case

$$P_0 = |\tilde{\Psi}_0\rangle\langle\tilde{\Psi}_0| + |\tilde{1}\rangle\langle\tilde{1}| \quad (2.40)$$

and

$$G(z) = |C|^{1/2} \begin{bmatrix} \rho_\gamma Q_0(-\Delta + V + \kappa^2)^{-1} Q_0 \rho_\gamma & 0 \\ 0 & 0 \end{bmatrix} |C|^{1/2}. \quad (2.41)$$

As in the non-degenerate case at threshold, the smoothness of  $G(z)$  is replaced with its asymptotic expansion in  $\kappa = -i\sqrt{z}$ , and from (2.41) it follows that what is needed is the asymptotic expansion of (with a slight abuse of notation)  $\rho_\gamma Q_0(-\Delta + V + \kappa^2)^{-1} Q_0 \rho_\gamma$ , which has been written down in [10].

Consider now the spectrum of  $P_0 W P_0$ . In the basis  $\{\tilde{\Psi}_0, \tilde{1}\}$ :

$$P_0 W P_0 = \begin{bmatrix} 0 & c \\ \bar{c} & b \end{bmatrix}, \quad (2.42)$$

where

$$c = \int \Psi_0(\mathbf{x}) W_{12}(\mathbf{x}) d\mathbf{x} \quad (2.43)$$

is assumed to be different from zero. The eigenvalues are

$$\lambda_\pm = \frac{b \pm \sqrt{b^2 + 4|c|^2}}{2}, \quad (2.44)$$

and we denote by  $\Psi_\pm$  the corresponding normalized eigenfunctions. Notice that  $\lambda_+ > 0$  and  $\lambda_- < 0$ .

Under the above conditions the following holds true. Note that we do not need any condition on  $b$  except that it is real. This is in contrast to the case considered in [10], see also (2.7).

**Theorem 5.** *For sufficiently small  $\varepsilon > 0$  we have the following results:*

(i) *For  $t > 0$  we have*

$$|\langle \Psi_+, e^{-itH(\varepsilon)} \Psi_+ \rangle - e^{-it(x_+(\varepsilon) - i\Gamma(\varepsilon))}| \leq C\varepsilon^{1/2}. \quad (2.45)$$

*Here*

$$\Gamma(\varepsilon) = \frac{g_{-1}}{\lambda_+^{1/2}} \varepsilon^{3/2}, \quad (2.46)$$

$$x_+(\varepsilon) = \varepsilon\lambda_+, \quad (2.47)$$

*with*

$$g_{-1} = \frac{|\langle \Psi_+, W\tilde{\Psi}_0 \rangle|^2}{12\pi} |\mathbf{X}|^2 + |\langle \Psi_+, W\tilde{\Psi}_c \rangle|^2, \quad (2.48)$$

*where*

$$X_j = \int_{\mathbf{R}^3} \Psi_0(\mathbf{x}) V(\mathbf{x}) x_j d\mathbf{x}, \quad j = 1, 2, 3. \quad (2.49)$$

(ii) *We have*

$$|\langle \Psi_-, e^{-itH(\varepsilon)} \Psi_- \rangle - e^{-itx_-(\varepsilon)}| \leq C\varepsilon^{1/2}, \quad (2.50)$$

*where*

$$x_-(\varepsilon) = \overline{x_-(\varepsilon)} = \varepsilon\lambda_-(1 + \mathcal{O}(\varepsilon^{1/2})). \quad (2.51)$$

**Remark 6.** (i) If one computes the eigenfunction  $\Psi_+$  explicitly, then one finds after some calculations that we have

$$g_{-1} = \frac{\lambda_+^2}{\lambda_+^2 + |c|^2} \left( \frac{1}{12\pi} |\langle W_{12}, \Psi_0 \rangle|^2 |\mathbf{X}|^2 + |\langle W_{12}, \Psi_c \rangle|^2 \right). \quad (2.52)$$

(ii) Contrasting the above results with the results in [11, 14], one notices that the coupling constant dependence is different. For a purely off-diagonal perturbation and eigenvalue only in the closed channel (or only at the threshold), the coupling constant dependence for both discrete eigenvalues and resonances is  $\mathcal{O}(\varepsilon^2)$ , as shown in those papers.

### 3. OUTLINE OF PROOFS

We now outline the proof of Theorems 4 and 5, full details will appear elsewhere. We use the notation  $C$  for a positive constant, which may change from line to line in the computations. We also assume throughout that  $|\varepsilon| < c_0$  for some small constant, which is determined by the computations.

**3.1. Proof of Theorem 4.** From (1.11) and the smoothness assumption on  $G(z)$  it follows that  $S(z, \varepsilon)$  has an extension as a  $C^2$  function to the closure  $\overline{D_a(E_0)}$ . With a slight abuse of notation we write  $S(x, \varepsilon)$  instead of  $S(x + i0, \varepsilon)$  for  $x \in (E_0 - a, E_0 + a)$ . We write out the Taylor expansion with remainder as follows

$$S(x, \varepsilon) = S(E_0, \varepsilon) + S'(E_0, \varepsilon)(x - E_0) + \frac{1}{2}S''(\tilde{x}, \varepsilon)(x - E_0)^2. \quad (3.1)$$

Condition (2.21) implies, perhaps with a smaller  $a$ , that we have

$$\operatorname{Im} S(x, \varepsilon) \geq \frac{\gamma}{2}P_0, \quad x \in (E_0 - a, E_0 + a). \quad (3.2)$$

This estimate implies that

$$-\operatorname{Im} F(x, \varepsilon) \geq \frac{\gamma}{2}\varepsilon^2 P_0. \quad (3.3)$$

We also note that for  $x \in (E_0 - a, E_0 + a)$  we have

$$\|\operatorname{Im} F(x, \varepsilon)\| \leq C\varepsilon^2. \quad (3.4)$$

We need the following lemma.

**Lemma 7.** *For  $x \in (E_0 - a, E_0 + a)$  we have*

$$\|F(x, \varepsilon)^{-1}\| \leq \frac{C}{\max\{d(x, \varepsilon), \varepsilon^2\}}, \quad (3.5)$$

where

$$d(x, \varepsilon) = \operatorname{dist}(x, \sigma(E_0 + \varepsilon P_0 W P_0)). \quad (3.6)$$

*Proof.* Since  $F(z, \varepsilon)$  is an operator on the finite dimensional space  $P_0\mathcal{H}$ , it suffices to prove that for all  $u \in P_0\mathcal{H}$ ,  $\|u\| = 1$ , we have

$$\|F(z, \varepsilon)u\| \geq C \max\{d(x, \varepsilon), \varepsilon^2\}. \quad (3.7)$$

Now (3.3) implies that

$$\|F(z, \varepsilon)u\| \geq \frac{\gamma}{2}\varepsilon^2. \quad (3.8)$$

For  $x \in (E_0 - a, E_0 + a)$  with  $d(x, \varepsilon) \geq C\varepsilon^2$  the spectral theorem and (3.4) imply that

$$\|F(z, \varepsilon)u\| \geq \frac{d(x, \varepsilon)}{4}. \quad (3.9)$$

Combining these estimates we obtain the estimate (3.5).  $\square$

We introduce the operator

$$\tilde{L}(x, \varepsilon) = E_0 P_0 + \varepsilon P_0 W P_0 - \varepsilon^2 S(E_0, \varepsilon) - \varepsilon^2 S'(E_0, \varepsilon)(x - E_0) - x P_0. \quad (3.10)$$

As in [10] we estimate the error incurred by replacing  $F(x, \varepsilon)$  with  $\tilde{L}(x, \varepsilon)$  in the integral (1.12).

**Lemma 8.** *We have the following estimate*

$$\int_{E_0 - a}^{E_0 + a} \|F(x, \varepsilon)^{-1} - \tilde{L}(x, \varepsilon)^{-1}\| dx \leq C\varepsilon^2. \quad (3.11)$$

*Proof.* Note that  $F''(x, \varepsilon) = -\varepsilon^2 S''(x, \varepsilon) = \mathcal{O}(\varepsilon^2)$ . This result, and the definition of  $\tilde{L}(x, \varepsilon)$ , yield

$$\|F(x, \varepsilon) - \tilde{L}(x, \varepsilon)\| \leq C\varepsilon^2|x - E_0|^2. \quad (3.12)$$

and thus

$$\|\tilde{L}(x, \varepsilon)\| \geq \frac{1}{2}\|F(x, \varepsilon)\|. \quad (3.13)$$

Using the estimate (3.5) we then get

$$\begin{aligned} \int_{E_0-a}^{E_0+a} \|F(x, \varepsilon)^{-1} - \tilde{L}(x, \varepsilon)^{-1}\| dx &\leq C \int_{E_0-a}^{E_0+a} \frac{\varepsilon^2|x - E_0|^2}{[\max\{d(x, \varepsilon), \varepsilon^2\}]^2} dx \\ &\leq C\varepsilon^2 \int_{E_0-a}^{E_0+a} \frac{|x - E_0|^2}{d(x, \varepsilon)^2 + \varepsilon^4} dx. \end{aligned} \quad (3.14)$$

It remains to estimate the integral (3.14). Let  $\varepsilon$  be fixed. We then introduce the notation

$$\sigma(E_0P_0 + \varepsilon P_0WP_0) = \bigcup_{j=1}^n \{x_j\}, \quad I_j = \{x \in (E_0 - a, E_0 + a) \mid d(x, \varepsilon) = |x - x_j|\},$$

where the  $x_j$  are the  $n \leq N$  distinct eigenvalues. Note that  $|E_0 - x_j| \leq C\varepsilon$  by perturbation theory. We can assume all eigenvalues are in the interval  $(E_0 - a, E_0 + a)$ . Then the integral in (3.14) equals the sum of the integrals over the intervals  $I_j$ . We estimate one of them as follows.

$$\begin{aligned} \int_{I_j} \frac{|x - E_0|^2}{d(x, \varepsilon)^2 + \varepsilon^4} dx &= \int_{I_j} \frac{|(x - x_j) + (x_j - E_0)|^2}{d(x, \varepsilon)^2 + \varepsilon^4} dx \\ &\leq \int_{-2a}^{2a} \frac{y^2 + 2|y|\varepsilon + \varepsilon^2}{y^2 + \varepsilon^4} dy \leq C. \end{aligned}$$

□

Thus it remains to study the term

$$\int_{E_0-a}^{E_0+a} (\tilde{L}(x, \varepsilon)^{-1} - (\tilde{L}(x, \varepsilon)^*)^{-1}) e^{-itx} dx. \quad (3.15)$$

We introduce the operator

$$D(\varepsilon) = (P_0 + \varepsilon^2 S'(E_0, \varepsilon))^{1/2} = P_0 + \mathcal{O}(\varepsilon^2) \quad (3.16)$$

on  $P_0\mathcal{H}$ , and rewrite  $\tilde{L}(x, \varepsilon)$  as follows.

$$\begin{aligned} \tilde{L}(x, \varepsilon) &= D(\varepsilon) [D(\varepsilon)^{-1} (\varepsilon P_0WP_0 - \varepsilon^2 S(E_0, \varepsilon)) D(\varepsilon)^{-1} - (x - E_0)P_0] D(\varepsilon) \\ &= D(\varepsilon) (h_\varepsilon - (x - E_0)P_0) D(\varepsilon). \end{aligned}$$

This equation also defines  $h_\varepsilon$ . We note that

$$\|h_\varepsilon\| = \mathcal{O}(\varepsilon), \quad (3.17)$$

and that (2.21) implies

$$\operatorname{Im} h_\varepsilon < 0, \quad \|\operatorname{Im} h_\varepsilon\| = \mathcal{O}(\varepsilon^2). \quad (3.18)$$

It follows that  $(\tilde{L}(x, \varepsilon)^*)^{-1}$  has an analytic continuation across the real axis into the lower half plane, denoted by  $\tilde{L}_-(x, \varepsilon)^{-1}$ . The meromorphic continuation of  $\tilde{L}(x, \varepsilon)^{-1}$  into the lower half plane is denoted by  $\tilde{L}_+(x, \varepsilon)^{-1}$ . Due to (3.17) the poles of this continuation lie in an  $\varepsilon$ -neighborhood of  $E_0$ .

We now connect the points  $-a$  and  $a$  by a semi-circle in the lower half plane, denoted by  $\mathcal{C}$ . The positively oriented closed contour consisting of this semi-circle and the interval  $[-a, a]$  is denoted by  $\Gamma$ . This allows us to deform the integration contour in (3.15). We also change the variable to  $y = x - E_0$ . This leads to the following result.

$$\begin{aligned} & \int_{E_0-a}^{E_0+a} (\tilde{L}(x, \varepsilon)^{-1} - (\tilde{L}(x, \varepsilon)^*)^{-1}) e^{-itx} dx \\ &= e^{-itE_0} \int_{-a}^a (\tilde{L}_+(y + E_0, \varepsilon)^{-1} - (\tilde{L}_-(y + E_0, \varepsilon)^*)^{-1}) e^{-ity} dy \\ &= e^{-itE_0} \int_{\mathcal{C}} (\tilde{L}_+(z, \varepsilon)^{-1} - (\tilde{L}_-(z, \varepsilon)^*)^{-1}) e^{-itz} dz \end{aligned} \quad (3.19)$$

$$+ e^{-itE_0} \oint_{\Gamma} \tilde{L}_+(z, \varepsilon)^{-1} e^{-itz} dz. \quad (3.20)$$

We consider first the integral (3.19). We have  $\|\tilde{L}_{\pm}(z, \varepsilon)^{-1}\| \leq C$  for  $z \in \mathcal{C}$ . Using the properties of  $D(\varepsilon)$ , see (3.16), we get

$$\begin{aligned} & \int_{\mathcal{C}} (\tilde{L}_+(z, \varepsilon)^{-1} - (\tilde{L}_-(z, \varepsilon)^*)^{-1}) e^{-itz} dz \\ &= \int_{\mathcal{C}} ((h_{\varepsilon} - z)^{-1} - (h_{\varepsilon}^* - z)^{-1}) e^{-itz} dz + \mathcal{O}(\varepsilon^2) \\ &= -2i \int_{\mathcal{C}} (h_{\varepsilon} - z)^{-1} (\operatorname{Im} h_{\varepsilon}) (h_{\varepsilon}^* - z)^{-1} e^{-itz} dz + \mathcal{O}(\varepsilon^2) \\ &= \mathcal{O}(\varepsilon^2), \end{aligned}$$

due to (3.18) and  $\sup_{z \in \mathcal{C}} (\|(h_{\varepsilon} - z)^{-1}\| + \|(h_{\varepsilon}^* - z)^{-1}\|) \leq C < \infty$ . The residue theorem is now applied to the integral in (3.20). It leads to

$$\oint_{\Gamma} \tilde{L}_+(z, \varepsilon)^{-1} e^{-itz} dz = D(\varepsilon)^{-1} e^{-ith_{\varepsilon}} D(\varepsilon)^{-1} + \mathcal{O}(\varepsilon^2).$$

Compute the derivatives in the definition of  $h_{\varepsilon}$ . Then  $h_{\varepsilon} + E_0 P_0 = h(\varepsilon) + \mathcal{O}(\varepsilon^4)$ , with  $h(\varepsilon)$  as defined in (2.23). Using the Duhamel formula to estimate

$$\|e^{-ith_{\varepsilon}} - e^{-it(h(\varepsilon) - E_0 P_0)}\|,$$

one finds that this term is of order  $\mathcal{O}(\varepsilon^2)$ , uniformly in  $t > 0$ . Thus this term can be absorbed into the error term  $\delta(\varepsilon, t)$ . Putting everything together and using (3.16), we have shown that

$$P_0 e^{-itH(\varepsilon)} P_0 = e^{-itE_0} e^{-ith_{\varepsilon}} + \mathcal{O}(\varepsilon^2).$$

The error term is uniform in time  $t > 0$ . That concludes the proof of Theorem 4.

**3.2. Proof of Theorem 5.** We choose  $I_{+,\varepsilon} = [\varepsilon \frac{\lambda_+}{2}, 3\varepsilon \frac{\lambda_+}{2}]$  and  $I_{-,\varepsilon} = [3\varepsilon \frac{\lambda_-}{2}, \varepsilon \frac{\lambda_-}{2}]$ , respectively. Applying twice the SLFG formula (see the argument leading to (2.28) above) one obtains

$$\langle \Psi_{\pm}, e^{-itH(\varepsilon)} g_{\pm,\varepsilon}(H(\varepsilon)) \Psi_{\pm} \rangle = \lim_{\eta \rightarrow 0} \frac{1}{\pi} \int_{I_{\pm,\varepsilon}} dx e^{-itx} \operatorname{Im} F_{\pm}(x + i\eta, \varepsilon)^{-1}. \quad (3.21)$$

where (see (2.28), (1.11) and take into account that  $Q_0 W Q_0 = 0$  giving  $S(z, \varepsilon) = P_0 A^* DG(z) D A P_0$ ):

$$\begin{aligned} F_{\pm}(z, \varepsilon) &= -z + \varepsilon \langle \Psi_{\pm}, W \Psi_{\pm} \rangle - \varepsilon^2 \langle \Psi_{\pm}, A^* DG(z) D A \Psi_{\pm} \rangle \\ &\quad - \varepsilon^4 \langle \Psi_{\pm}, A^* DG(z) D A \Psi_{\mp} \rangle \\ &\quad \times \left( -z + \varepsilon \langle \Psi_{\mp}, W \Psi_{\mp} \rangle - \varepsilon^2 \langle \Psi_{\mp}, A^* DG(z) D A \Psi_{\mp} \rangle \right)^{-1} \\ &\quad \times \langle \Psi_{\mp}, A^* DG(z) D A \Psi_{\pm} \rangle. \end{aligned} \quad (3.22)$$

Consider first  $\langle \Psi_{+}, e^{-itH(\varepsilon)} g_{+,\varepsilon}(H(\varepsilon)) \Psi_{+} \rangle$ . Notice that on the set

$$D_{\varepsilon,+} = \{z \in \mathbf{C} \mid |z - \varepsilon \lambda_+| < \frac{\varepsilon \lambda_+}{2}, \operatorname{Im} z > 0\},$$

for  $\varepsilon$  sufficiently small:

$$|(-z + \varepsilon \langle \Psi_{-}, W \Psi_{-} \rangle - \varepsilon^2 \langle \Psi_{-}, A^* DG(z) D A \Psi_{-} \rangle)^{-1}| \leq C/\varepsilon. \quad (3.23)$$

It follows that on  $D_{\varepsilon,+}$  the last term in  $F_{\pm}(z, \varepsilon)$  is bounded by  $\mathcal{O}(\varepsilon^2)$  and then, since  $\nu = -1$ , it can be absorbed in the error term (see the proof of Lemma 3.7 in [10]). The remaining terms are precisely those appearing in the proof of Theorem 3.7 in [10]. Application of Theorem 3 (Theorem 3.7 in [10]) together with the computation of  $g_{-1}$  finishes the proof of Theorem 5(i).

Consider now  $\langle \Psi_{-}, e^{-itH(\varepsilon)} g_{-,\varepsilon}(H(\varepsilon)) \Psi_{-} \rangle$ . Due to the assumption (2.32) the negative spectrum of  $-\Delta + V$  does not accumulate at zero. Thus, for  $\varepsilon$  small enough,  $F_{-}(z, \varepsilon)$  is analytic in a complex neighborhood of  $I_{-,\varepsilon}$  and real on  $I_{-,\varepsilon}$ . Moreover, by inspection, on  $I_{-,\varepsilon}$ :

$$\frac{d}{dx} F_{-}(x, \varepsilon) = -1 + \mathcal{O}(\varepsilon^{1/2}). \quad (3.24)$$

Since by Cauchy-Riemann equations,  $\operatorname{Im} F_{-}(x + i\eta, \varepsilon) \neq 0$  for sufficiently small  $\eta \neq 0$  and  $x \in I_{-,\varepsilon}$  it follows that in a complex neighborhood of  $I_{-,\varepsilon}$  has a unique real simple zero

$$x_{-}(\varepsilon) = \varepsilon \lambda_{-} (1 + \mathcal{O}(\varepsilon^{1/2})). \quad (3.25)$$

Then by the residue theorem and (3.24):

$$\langle \Psi_{-}, e^{-itH(\varepsilon)} g_{-,\varepsilon}(H(\varepsilon)) \Psi_{-} \rangle = -e^{-ix_{-}(\varepsilon)t} \frac{d}{dx} F_{-}(x_{-}(\varepsilon), \varepsilon) = e^{-ix_{-}(\varepsilon)t} + \mathcal{O}(\varepsilon^{1/2}), \quad (3.26)$$

and applying once again Hunziker's trick (see [10, Theorem 3.7]) one obtains (2.50).

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