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Interchannel Resonances at a Threshold

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Abstract

Fermi's Golden Rule, the perturbation theoretic formula for calculating the half width of a resonance, is not applicable to the case of a transition from a bound state into an open channel, when the energy of the bound state is exactly at the threshold of the continuum. We study solvable models of this phenomenon. The exact results coincide in leading order with the formulas found by modifying Fermi's Golden Rule.

1 Introduction

An interchannel resonance in quantum mechanical scattering is considered as arising by a perturbation of a bound state in a closed channel, with the bound state energy lying in a region where other channels are open [1]. In the case of a small perturbation the half–width of the resonance is in general calculated with **Fermi's Golden Rule**, FGR [2, 3, 4]. If the unpertubed Hamiltonian H_0 (which is the kinetic energy plus interchannel potentials) with a bound state $|\varphi\rangle$ in the closed channel and continuum wave functions ψ_k in the open channel (we will consider only one open channel) is perturbed by αV, then FGR gives the imaginary part of the resonance energy as a product of:

1. α^2,
2. the absolute square of the transition matrix element $\langle\varphi|V\psi_k\rangle$,
3. the spectral density in the open channel, and
4. the constant π.

A mathematical treatment, using complex scaling [5], confirms Fermi's Golden Rule as the contribution to perturbation theory in second order, with the exception of *the case, where the energy of the bound state does coincide with the threshold of the continuous spectrum in the open channel.* When trying to apply FGR to such a case one observes the following facts:

a) The transition matrix element is zero in general; only in the case of an open s–channel with a zero–energy inner–channel resonance may it be nonvanishing at the threshold.

b) The spectral density at the threshold is infinite.

So FGR gives either infinity or an undecided value of zero times infinity; up to now we don't know for sure whether the bound state turns into a resonance, and, in case it should do so, we don't have a perturbation–theoretic formula for its lifetime.

Such cases actually do occur with atoms [6]. In principle they could also appear with nuclei or in solid state physics, where the channels are the bands of electron states, and where a bound state is located at an impurity. For semiconductors just the resonances near a band edge (= threshold) are of particular importance [7].

In this paper we study simple solvable models: First a one–dimensional lattice model with two bands. Then we make a comparison with a simplified model, which keeps only the barest essentials. This serves as an argument for the validity of the solvable continuum models with a separable potential for coupling of the channels. The continuum models are one–dimensional or the radial parts of a rotation–invariant three–dimensional system.

The leading term in an expansion of the lifetime turns out to be proportional to a half–integer–exponentiated coupling constant. We end up with a conjecture how to modify FGR to get a generally valid formula for the imaginary part of the resonance energy.

2 A one–dimensional lattice model

We consider a one–dimensional lattice $\mathbf{Z}$, carrying two channels, which would be translation invariant, if there were not an impurity at the point denoted by $n = 0$. We consider only a local action of the impurity, so we can restrict the Hilbert space for each channel to the space of even functions. (The odd functions are zero at $n = 0$ and are not affected by the impurity.) So it is enough to consider the half space with points $n \geq 0$, and the even wave functions can be represented by elements of the Hilbert space $\ell^2(\mathbf{N})$ with the norm for $\psi = (\psi_n) \in \ell^2(\mathbf{N})$ given by

$$\|\psi\|^2 = |\psi_0|^2 + 2\sum_{n=1}^{\infty} |\psi_n|^2. \tag{1}$$

In each channel there is a kinetic energy K:

$$(K\psi)_n = \begin{cases} 2\psi_n - \psi_{n-1} - \psi_{n+1} & n \geq 1 \\ 2\psi_0 - 2\psi_1 & n = 0. \end{cases}$$

The complete system with two bands is modelled in the Hilbert space $\ell^2(\mathbf{N}) \oplus \ell^2(\mathbf{N})$. One channel gives a band shifted by a positive energy b, so, without impurity, the Hamiltonian would be $(K + b\mathbf{1}) \oplus K$. The impurity is represented by a negative local inner–channel potential $(-w\delta_{n,0}) \oplus (-v\delta_{n,0})$, where w is positive.

We are interested in the bound state in the upper band. It has the wave function

$$\varphi_n = ce^{-n\gamma_0}, \qquad c = (\coth\gamma_0)^{-1/2} \tag{2}$$

where

$$2\sinh\gamma_0 = w \tag{3}$$

and a binding energy which we consider as exactly equal to the relative shift of the bands:

$$b = 2\cosh\gamma_0 - 2. \tag{4}$$

Now we collect all these contributions as the unperturbed Hamiltonian H_0. In matrix notation

$$H_0 = \begin{pmatrix} b\mathbf{1} + K - w\delta_{n,0} & 0 \\ 0 & K - v\delta_{n,0} \end{pmatrix} \tag{5}$$

it has the bound state $\begin{pmatrix} \varphi_n \\ 0 \end{pmatrix}$ with energy zero, which equals the lower band edge of the lower channel.

Next we add a perturbation αV by an impurity at the point $n = 0$, which introduces a coupling of the channels. For explanations see the discussion in part 3. We define

$$H_\alpha = H_0 + \alpha V, \qquad V = \delta_{n,0}\begin{pmatrix} \mathbf{1} & t^* \\ t & u \end{pmatrix}, \qquad t \in \mathbf{C}, \qquad u \in \mathbf{R}. \tag{6}$$

In the open channel the resonance state should behave like a Gamow function [8], so, to solve the equation, we make the ansatz

$$\psi_n = \begin{pmatrix} e^{-n\gamma} \\ a \cdot e^{ikn} \end{pmatrix} \tag{7}$$

$$(H_\alpha - E)\psi = 0 \tag{8}$$

and search for solutions with Im $(k) < 0$, $E \to 0$, $a \to 0$ and $\gamma \to \gamma_0$ as $\alpha \to 0$.

Inserting (7) into (8) gives for the components $((H_\alpha - E)\psi)_n$ for $n \geq 1$ the equations

$$E = 2 - 2\cosh\gamma + b = 2 - 2\cos k, \tag{9}$$

$$\begin{aligned} b + 2 - 2e^{-\gamma} - w - E + \alpha(1 + t^* a) &= 0, \\ (2 - 2e^{ik} - v - E)a + \alpha(ua + t) &= 0. \end{aligned} \tag{10}$$

Expressing E by the appropriate parts of (9) we transform (10) to

$$a = \frac{-\alpha t}{\alpha u - v - 2i\sin k} = \frac{\alpha - w + 2\sinh\gamma}{-t^*\alpha} \tag{11}$$

and

$$\alpha^2(t^*t - u) + \alpha(f + ug) - fg = 0 \tag{12}$$

where we have introduced

$$\begin{aligned} f &:= v + 2i\sin k \\ g &:= w - 2\sinh\gamma. \end{aligned} \tag{13}$$

Considering, by way of equ. (9), E, γ, f, g as analytic functions of the uniformizing complex variable k:

$$\gamma = \gamma(k) = \text{ar cosh } (b/2 + \cos k) \tag{14}$$

with

$$\lim_{k\to 0} \gamma(k) = \gamma_0 > 0,$$

we will be mainly interested in the behaviour of these functions of k near zero. The expansions are:

$$\begin{aligned} E &= k^2 - \frac{k^4}{12} + O(k^6) \\ f &= v + 2ik - \frac{i}{3}k^3 + O(k^5) \\ g &= k^2\coth\gamma_0 + \left(\frac{1}{w} + \frac{2}{w^3} - \frac{\sqrt{w^2+4}}{12w}\right)k^4 + O(k^6) =: c^{-2}k^2 + dk^4 + O(k^6). \end{aligned} \tag{15}$$

The goal is to get E as a function of real α by way of k. Using equation (12) it seems easier first to consider α as a complex valued function of k, and then to invert this to a function $k(\alpha)$. Four different cases have to be treated separately:

a) If $t^*t - u = 0$:

$$\alpha = \frac{f \cdot g}{f + ug} \begin{cases} (c^{-2}k^2 + dk^4)\left(1 - \frac{t^*t}{c^2 v}k^2 + i\frac{2t^*t}{c^2 v}k^3\right) + O(k^6) & \text{if } v \neq 0 \\ (c^{-2}k^2 + dk^4)\left(1 + i\frac{t^*t}{2c^2}\right) k + O(k^5) & \text{if } v = 0. \end{cases}$$

b) If $t^*t - u \neq 0$, the solution of the quadratic equation with $\alpha \to 0$ as $k \to 0$ has to be chosen:

$$\begin{aligned} \alpha &= \frac{f + ug}{2(t^*t - u)} \left(\sqrt{1 + \frac{4fg(t^*t - u)}{(f + ug)^2}} - 1 \right) = \\ &= \begin{cases} (c^{-2}k^2 + dk^4)\left(1 - \frac{t^*t}{c^2 v}k^2 + 2it^*t\frac{c^{-2}}{v^2}k^3\right) + O(k^6) & \text{if } v \neq 0 \\ (c^{-2}k^2 + dk^4)\left(1 + i\frac{t^*t}{2c^2}k\right) + O(k^4) & \text{if } v = 0. \end{cases} \end{aligned} \tag{16}$$

The leading contributions to the power series for the case b are independent of u and identical to the power series in case a, where we may replace u by t^*t. But the distinction between absence and presence of an impurity well, $v = 0$ and $v \neq 0$, is important:
for $v \neq 0$:

$$\alpha = c^{-2}k^2 - \left(\frac{t^*t}{vc^4} - d\right) + i\frac{2t^*t}{vc^4}k^5 + O(k^6)$$

for $v = 0$:

$$\alpha = c^{-2}k^2 + i\frac{t^*t}{2c^4}k^3 + O(k^4). \tag{17}$$

In all the cases $\alpha(k)$ is an analytic function of k in some neighbourhood of $k = 0$, which is a zero point of second order, so the function can be inverted to give k as an analytic function of the square root of α [9, 10]. Its expansion is:
for $v \neq 0$:

$$\begin{aligned} k &= c\alpha^{1/2} + \frac{1}{2}\left(t^*t\frac{c}{v} - c^5 d\right)\alpha^{3/2} - it^*t\frac{c^2}{v^2}\alpha^2 + O(\alpha^{5/2}) \\ E &= c^2\alpha + \left(t^*t\frac{c^2}{v} - c^6 d - \frac{c^4}{12}\right)\alpha^2 - it^*t\frac{2c^3}{v^2}\alpha^{5/2} + O(\alpha^3) \end{aligned} \tag{18}$$

for $v = 0$:

$$\begin{aligned} k &= c\alpha^{1/2} - i\frac{t^*t}{4}\alpha + O(\alpha^{3/2}) \\ E &= c^2\alpha - it^*t\frac{c}{2}\alpha^{3/2} + O(\alpha^2). \end{aligned} \tag{19}$$

3 Discussion

The model has been chosen to investigate the basic mathematical structure, with best possible ease in computation. The impurity's potential and the perturbation are therefore assumed to act locally at one point only. ¿From there on everything is as general as possible. For the closed channel the inner–channel part of the perturbing potential has been set equal to one in equation (6). The reason is the following: If it were zero, the bound state would under perturbation not turn into a resonance, but would remain a bound state. (This can be checked with the ansatz of a wave function $\Phi_n = \begin{pmatrix} e^{-\gamma n} \\ a \cdot e^{-\kappa n} \end{pmatrix}$, and proceeding in a similar way as for the resonance.) So we are only interested in the case where this inner channel perturbation is strictly positive, and we may use the freedom of shifting the normalization between the coupling constant and the potential V, to set this matrix element equal to one.

The threshold behaviour of the open channel, connected with the absence or presence of an impurity well, determines the leading term for the imaginary part: If $v \neq 0$, there is a nonvanishing effective range of the impurity, the continuum wave functions at low energy tend to stay away from it. The transition probability from the bound state to the continuum increases with the coupling constant α more slowly than in other cases. If $v = 0$, there is no effective range, the transitions are not hindered, and the high spectral density of the continuum effects an increase of Im $(E(\alpha))$ faster than α^2. These effects will be discussed in closer detail for the continuum models.

4 The simplified lattice model

To pave the way for simple continuum models, we simplify this two–band model by ignoring any inner–channel effects in the closed channel, except for the change in energy. So we replace H_α by $PH_\alpha P$, with the projection operator

$$P = \begin{pmatrix} |\varphi\rangle\langle\varphi| & 0 \\ 0 & 1 \end{pmatrix} \tag{20}$$

where $|\varphi\rangle$ is the unperturbed bound state (2).

So we work in the restricted Hilbert space $P[\ell^2(\mathbf{N}) \oplus \ell^2(\mathbf{N})] \cong \mathbf{C} \oplus \ell^2(\mathbf{N})$, where the closed channel is represented by only one state. Moreover, we feel free to replace the inner–channel part u of the perturbation V by t^*t, because the leading terms in the expansion of 16b are identical to those of 16a.

The Hilbert space is $\mathcal{H} = \mathbf{C} \oplus \ell^2(\mathbf{N})$, the Hamiltonian $H_\alpha = H_0 + \alpha V$,

$$H_0 = \begin{pmatrix} 0 & 0 \\ 0 & K - v\delta_{n0} \end{pmatrix}, \qquad V = \begin{pmatrix} c^2 & ct^*\delta_{n0} \\ ct\delta_{n0} & t^*t\delta_{n0} \end{pmatrix}. \tag{21}$$

With the ansatz for the unnormalized resonance wave function

$$\Psi = \begin{pmatrix} 1 \\ a \cdot e^{ikn} \end{pmatrix} \tag{22}$$

inserted into $(H_\alpha - E)\Psi = 0$, we get

$$\begin{aligned} E &= 2(1-\cos k) \\ a &= (E/\alpha c - c)/t^* \\ \alpha &= \frac{c^{-2}(1-\cos k)(v+2i\sin k)}{v/2 + i\sin k + t^* t c^{-2}(1-\cos k)}. \end{aligned} \tag{23}$$

This α is an analytic function of k, with the power series in a neighbourhood of the origin

$$\alpha = \begin{cases} c^{-2}k^2 + \left(\frac{t^*t}{vc^4} - \frac{1}{12c^2}\right)k^4 - ik^5 + O(k^6) & \text{for } v \neq 0 \\ c^{-2}k^2 + i\frac{t^*t}{2c^4}k^3 + O(k^4) & \text{for } v = 0. \end{cases} \tag{24}$$

These functions can be inverted to a function of $\sqrt{\alpha}$, analytic in a neighbourhood of the origin:
For $v \neq 0$:

$$\begin{aligned} k &= c\alpha^{1/2} + \left(\frac{t^*t}{2vc^2} - \frac{1}{24}\right)c^3\alpha^{3/2} - i\frac{t^*tc^2}{v^2}\alpha^2 + O(\alpha^{5/2}) \\ E &= c^2\alpha + \frac{t^*tc^2}{v}\alpha^2 - i\frac{2t^*tc^3}{v^2}\alpha^{5/2} + O(\alpha^3). \end{aligned} \tag{25}$$

For $v = 0$:

$$\begin{aligned} k &= c\alpha^{1/2} - i\left(\frac{t^*t}{4}\right)\alpha + O(\alpha^{3/2}) \\ E &= c^2\alpha - i\frac{t^*tc}{2}\alpha^{3/2} + O(\alpha^2). \end{aligned} \tag{26}$$

The leading contributions both to the real part and to the imaginary part of the energy in (25) and (26) are identical to those in the formulas (18) and (19).

5 A simple continuum model

The studies of the lattice model encourages us to use two simple building blocks: To keep only a single bound state, representing the closed channel, and to consider a rank one operator as the perturbation V, coupling the bound state to the open channel. In the open channel we consider the particle to be free. Everything is reflection or rotation invariant in one or three dimensions.

The Hilbert space is now

$$\mathcal{H} = \mathbf{C} \oplus \mathcal{L}^2(\mathbf{R}_+) = \left\{ \begin{pmatrix} p \\ |\psi\rangle \end{pmatrix}, p \in \mathbf{C}, |\psi\rangle = \psi(x) \in \mathcal{L}^2(\mathbf{R}_+) \right\}.$$

As Hamiltonian we consider

$$H_\alpha = H_0 + \alpha V, \qquad H_0 = \begin{pmatrix} 0 & 0 \\ 0 & K_\nu \end{pmatrix}, \qquad V = \begin{pmatrix} c^2 & c\langle v| \\ c|v\rangle & |v\rangle\langle v| \end{pmatrix} \tag{27}$$

with $c > 0$, $v(x) = O(e^{-\kappa x})$ for some $\kappa > 0$, as $x \to \infty$. The kinetic energy, plus the angular momentum barrier, is either

$$K_\nu = -\frac{d^2}{dx^2} + \frac{\ell(\ell+1)}{x^2}, \qquad \ell = \nu - \frac{1}{2} \in \mathbf{N} \tag{28}$$

with Dirichlet–boundary conditions at $x = 0$, or $K_\nu = -d^2/dx^2$ with Neumann boundary conditions at $x = 0$ and $\nu = -1/2$. The models in one dimension are either of parity -1 or $+1$, concerning the reflection at $x = 0$ in $\mathcal{L}^2(\mathbf{R})$. They can thus be reduced to models on the half line $\mathbf{R}_+$, with $\nu = \pm 1/2$, the sign of ν corresponding to the sign of the parity.

The index ν is chosen in such a way that it coincides with the standard indication of the Bessel functions, which, multiplied by $\sqrt{\pi k x/2}$, give the eigenfunctions of K_ν.

The **formal** ansatz for the resonance wave function at positive α is

$$\Psi_\alpha = \begin{pmatrix} 1 \\ \psi_\alpha(x) \end{pmatrix}, \tag{29}$$

supposed to be a solution of the differential equation

$$(H_\alpha - E(\alpha))\Psi_\alpha = 0, \tag{30}$$

with the asymptotic behaviour

$$\psi_\alpha(x) \sim e^{ikx} \quad \text{at } x \to \infty, \text{ with Im } (k) < 0, \text{ Re } (k) > 0. \tag{31}$$

A discussion of this asymptotic behaviour would involve mathematical subtleties, especially if $v(x)$ is not of compact support. So we will instead analyze these formulas first for negative coupling constants α. There we get unnormalized bound states Ψ_α with negative energies $E(\alpha)$, the asymptotic behaviour as in (31), but with $k = k(\alpha) = i\sqrt{-E(\alpha)}$. Then we may consider the analytic continuation of $E(\alpha)$ and $\psi_\alpha(x)$ to positive α. This is again achieved by inverting the function $\alpha(k)$.

Inserting (27) and (29) into (30) gives the pair of equations

$$\begin{aligned} \alpha c^2 + \alpha c \langle v|\psi_\alpha\rangle - E &= 0 \\ (K_\nu - E)|\psi_\alpha\rangle + \alpha(c + \langle v|\psi_\alpha\rangle)|v\rangle &= 0. \end{aligned} \tag{32}$$

The second equation is transformed to

$$|\psi_\alpha\rangle = -\alpha(c + \langle v|\psi_\alpha\rangle)(K_\nu - E)^{-1}|v\rangle = -\frac{E}{c}(K_\nu - E)^{-1}|v\rangle. \tag{33}$$

Multiplying (33) by $\langle v|$, and eliminating $\langle v|\psi_\alpha\rangle$ from the pair of equations, we get

$$\alpha = \frac{E}{c^2 - E\,\langle v|(K_\nu - E)^{-1}|v\rangle}. \tag{34}$$

For negative real energies E, (34) gives negative real α. In the uniformizing variable k, this function $\alpha(k)$ can be analytically continued into the region Im $(k) > -\kappa$ (Appendix

A). In the appendix B we prove that the energies $E = k^2$ in the unphysical sheet, giving positive real $\alpha(k)$, are actually poles of the resolvent of H_α. In appendix A it is shown that

$$\langle v|(K_\nu - k^2)^{-1}|v\rangle = F(k) - ik^{2\nu}G(k), \tag{35}$$

with $F(k)$ and $G(k)$ analytic functions of k, real and even for $k \in \mathbf{R}$. $G(0)$ is the absolute square of a scaled transition matrix element from $|v\rangle$ into the continuum of K_ν at energy zero: $|t|^2 = G(0)$. The analytic function $\alpha(k)$ can be split into a real and an imaginary part, for $k \in \mathbf{R}$, and expanded in powers of k:

$$\alpha(k) = \frac{k^2}{c^2 - k^2F(k) - ik^{2\nu+2}G(k)} = \frac{k^2}{c^2} + O(k^4) + i\left[\frac{|t|^2}{c^4}k^{2\nu+4} + O(k^{2\nu+6})\right]. \tag{36}$$

To invert it, we have to form the square root:

$$\alpha^{1/2}(k) = \frac{k}{c} + O(k^3) + i\left[\frac{|t|^2}{2c^3}k^{2\nu+3} + O(k^{2\nu+5})\right]. \tag{37}$$

In both equations the remaining contributions, which we indicate by the order of their leading terms, have real–valued expansion coefficients. The inversion of this function near $k = 0$ gives the searched for expansions of k and of E in the square root of the coupling constant:

$$k(\alpha^{1/2}) = c\alpha^{1/2} + O(\alpha^{3/2}) - i\left[\frac{c^{2\nu+1}}{2}|t|^2\alpha^{\nu+3/2} + O(\alpha^{\nu+5/2})\right] \tag{38}$$

$$E(\alpha^{1/2}) = c^2\alpha + O(\alpha^2) - i\left[c^{2\nu+2}|t|^2\alpha^{\nu+2} + O(\alpha^{\nu+3})\right]. \tag{39}$$

6 Discussion

The leading term in the expansion of the real part of the resonance energy is precisely as in ordinary first order perturbation theory. The leading term in the expansion of the negative imaginary part increases as $\alpha^{3/2}$ for $\nu = -1/2$, where standard FGR would give infinity times α^2. In the other cases, for $\nu \geq 1/2$, the increase is slower than α^2. Now it turns out that the leading term in the expansion can be calculated with a

modified FGR:

As a *first step* one has to take into account the shift in energy of the bound state to $E_\alpha = c^2\alpha$.
Then as a *second step* one has to proceed with standard FGR, applied to the bound state with the shifted energy.

In the present case this procedure gives the transition matrix element to the wave function $b_\nu(kx)$ in the open channel (see appendix A)

$$t_k := \sqrt{\frac{2}{\pi}}\, c \int_0^\infty v^*(x) b_\nu(kx)dx \overset{k\to 0}{\sim} ck^{\nu+1/2}\sqrt{\frac{2}{\pi}}\, t. \tag{40}$$

The spectral density is $1/2k$. Evaluating all the contributions at $k = \sqrt{E_\alpha}$, one gets

$$\frac{\Gamma}{2} = |\mathrm{Im}\ E(\alpha)| = \frac{\pi}{2k}|t_k|^2\alpha^2 = c^{2\nu+2}|t|^2\alpha^{\nu+2}, \tag{41}$$

precisely the leading term in (39).

Concerning the relevance of the model for physics, one has to observe, that the wave functions in the continuum of an open channel with a short range potential behave as in the open channel without a potential and with Dirichlet b.c., *unless there is a zero energy bound state or innerchannel–resonance*. In an open channel with $\ell = 0$ and a zero–energy resonance, the wave functions behave as in the open channel with Neumann b.c. and the transition matrix element into the continuum stays finite at $E = 0$.

The exponential fall off of the perturbing potential in the model corresponds to the exponential decrease of the bound state wave function to be incorporated in the model: Consider the case of two particles with the bound state Φ in the closed channel,

$$\Phi(\vec{x}, \vec{y}) = \varphi_1(\vec{x})\varphi_2(\vec{y})$$

perturbed by an interaction $\alpha W(\vec{x}-\vec{y})$. It enables transitions into an open channel, where the second particle with y–coordinate is still bounded with the wave function $\varphi_3(\vec{y})$, but the first particle is free. In this open channel the general wave function is

$$\Psi(x, y) = \psi(\vec{x})\varphi_3(\vec{y}),$$

the transition matrix element is

$$\langle\Psi|\alpha W|\Phi\rangle = \langle\psi|\alpha v\rangle$$

with

$$v(\vec{x}) = \varphi_1(\vec{x}) \int d^3y\, W(\vec{x}-\vec{y})\varphi_3^*(\vec{y})\varphi_2(\vec{y}).$$

The decay of $v(\vec{x})$ is thus determined by the decay of the bound state wave function $\varphi_1(\vec{x})$.

There remains the problem of the behaviour of continuum wave function in the open channel in the presence of a long range potential.

Appendix A: Analytic continuation

The solutions to the differential equation

$$((K_\nu - k^2)f)(x) = 0$$

are given by the transformed Bessel and Hankel functions b_ν and e_ν:

$$\begin{aligned} b_\nu(kx) &:= (\pi kx/2)^{1/2} J_\nu(kx) \\ e_\nu(kx) &:= (\pi kx/2)^{1/2} H_\nu^{(1)}(kx). \end{aligned} \tag{A.1}$$

The asymptotic behaviour is [11]

$$b_\nu(kx) \overset{kx\to 0}{\sim} \frac{\sqrt{\pi}}{\Gamma(\nu+1)} \left(\frac{kx}{2}\right)^{\nu+1/2} \tag{A.2}$$

$$e_\nu(kx) \overset{kx\to\infty}{\sim} e^{i(kx-\pi(\nu+1/2)/2)}. \tag{A.3}$$

The Wronskian

$$b_\nu \frac{d}{dx} e_\nu - e_\nu \frac{d}{dx} b_\nu = ik. \tag{A.4}$$

The Green's function $G_{\nu,k}(x,y)$, the kernel of the resolvent $(K_\nu - k^2)^{-1}$ for Im $k > 0$, is thus

$$G_{\nu,k}(x,y) = \frac{i}{k}\left[\Theta(y-x) b_\nu(kx) e_\nu(ky) + \Theta(x-y) b_\nu(ky) e_\nu(kx)\right]. \tag{A.5}$$

For half–integer valued ν, it is an entire function of k.

Since in the limit $x \to \infty$ $v(x) = O(e^{-\kappa x})$, the integration

$$\int_0^\infty dx \int_0^\infty dy\ v^*(x) G_{\nu,k}(x,y) v(y)$$

converges for Im $k > -\kappa$. So does the integration with $G_{\nu,k}$ replaced by the kernel $\frac{d}{dk}(kG_{\nu,k})$, and the existence of a continuation of the analytic function

$$kQ(x) := k\langle v|(K_\nu - k^2)^{-1}|v\rangle$$

is established for Im $k > -\kappa$. In order to distinguish between real and imaginary coefficients of the expansions, we use the transformed Neumann functions

$$n_\nu(kx) := (\pi kx/2)^{1/2} N_\nu(kx)$$

and split

$$e_\nu = b_\nu + i n_\nu. \tag{A.6}$$

The Green's function is now written as

$$G_{\nu,k}(x) = \frac{i}{k} b_\nu(ky) b_\nu(kx) + \frac{1}{k}\left[\Theta(y-x) n_\nu(ky) b_\nu(kx) + \Theta(x-y) b_\nu(ky) n_\nu(kx)\right]. \tag{A.7}$$

The Bessel and Neumann functions take real values at positive real arguments. So, *for positive real* k, we may split $Q(k)$ into real and imaginary parts:

$$Q(k) = F(k) + ik^{2\nu} G(k) \tag{A.8}$$

$$F(k) = -\frac{1}{k}\int_0^\infty dx \int_0^\infty dy\ \Theta(y-x) n_\nu(ky) b_\nu(kx)\left[v^*(y)v(x) + v(y)v^*(x)\right]. \tag{A.9}$$

The product $n_\nu(ky)b_\nu(kx)$ lifts the singularity of $1/k$. For half–integer–valued ν, $F(k)$ has an analytic expansion in powers of k^2.

$$G(k) = k^{-(2\nu+1)}\left|\int_0^\infty dx\ v^*(x) b_\nu(kx)\right|^2 \xrightarrow{k\to 0} |t|^2, \tag{A.10}$$

with the "scaled transition matrix element"

$$t := \lim_{k\to 0} k^{-(\nu+1/2)}\int_0^\infty dx\ v^*(x) b_\nu(kx) = \frac{\sqrt{\pi}}{2^{\nu+1/2}\Gamma(\nu+1)}\int_0^\infty dx\ v^*(x) x^{\nu+1/2}. \tag{A.11}$$

At $k \sim 0$, $G(k)$ has an analytic expansion in powers of k^2.

Appendix B: Poles of the resolvent

We split the Hamiltonian H_α as

$$H_\alpha = L + W, \qquad L := \begin{pmatrix} \alpha c^2 & 0 \\ 0 & K + \alpha|v\rangle\langle v| \end{pmatrix}, \qquad W := \begin{pmatrix} 0 & \alpha c\langle v| \\ \alpha c|v\rangle & 0 \end{pmatrix} \tag{B.1}$$

(we simply write K instead of K_ν) and use the iterated resolvent equation in the Hilbert space $\mathbf{C}\oplus\mathcal{L}^2(\mathbf{R})$

$$\begin{aligned} (H_\alpha - E)^{-1} &= (L - E + W)^{-1} = \frac{1}{L-E} - \frac{1}{L-E}W\frac{1}{L-E+W} = \\ &= \frac{1}{L-E} - \frac{1}{L-E}W\frac{1}{L-E} + \frac{1}{L-E}W\frac{1}{L-E}W\frac{1}{L-E+W} \end{aligned} \tag{B.2}$$

to calculate the matrix element with $\begin{pmatrix} 1 \\ |0\rangle \end{pmatrix}$:

$$r := (1, \langle 0|)\frac{1}{L+W-E}\begin{pmatrix} 1 \\ |0\rangle \end{pmatrix}. \tag{B.3}$$

We get

$$r = \frac{1}{\alpha c^2 - E} + \frac{\alpha^2 c^2}{\alpha c^2 - E}\left\langle v\left|\frac{1}{K + \alpha|v\rangle\langle v| - E}\right|v\right\rangle r. \tag{B.4}$$

Again we use the resolvent equation, now in the smaller Hilbert space $\mathcal{L}^2(\mathbf{R}_+)$:

$$\frac{1}{K - E + \alpha|v\rangle\langle v|} = \frac{1}{K-E} - \frac{\alpha}{K-E}|v\rangle\langle v|\frac{1}{K - E + \alpha|v\rangle\langle v|}. \tag{B.5}$$

Taking the expectation value of (B.5) with $|v\rangle$, we get an equation, to be transformed to

$$\left\langle v\left|\frac{1}{K - E + \alpha|v\rangle\langle v|}\right|v\right\rangle = \frac{\langle v|\frac{1}{K-E}|v\rangle}{1 + \alpha\langle v|\frac{1}{K-E}|v\rangle}. \tag{B.6}$$

Inserting (B.6) in (B.4) and solving for r results in

$$r = \frac{1 + \alpha\langle v|(K-E)|v\rangle}{\alpha c^2 - E - \alpha E\langle v|(K-E)^{-1}|v\rangle}. \tag{B.7}$$

Due to the asymptotic bound at large x

$$v(x) = O(e^{-\kappa x}), \tag{B.8}$$

the matrix element $\langle v|(K-k^2)^{-1}|v\rangle$ can be continued to an analytic function of k, for $\mathrm{Im}\, k > -\kappa$. The poles of the matrix element $r = r(k)$ in this region are the zeroes of the denominator of (B.7). Finding these zeroes amounts to solving equ. (34).

Other matrix elements of the resolvent involve the same denominator.

References

[1] R.G. Newton: Scattering Theory of Waves and Particles. Springer, New York, Heidelberg, Berlin 1982

[2] J.J. Sakurai: Modern Quantum Mechanics. Benjamin, Menlo Park 1985

[3] C. Cohen–Tannoudji, B. Diu, F. Laloë: Quantum Mechanics Vol. II. Hermann, Paris 1977

[4] W. Thirring: Lehrbuch der Mathematischen Physik Band 3: Quantenmechanik von Atomen und Molekülen. Zweite Auflage, Springer, Wien, New York 1994

[5] J. Aguilar, J.M. Combes: A Class of Analytic Perturbations for One–Body Schrödinger Hamiltonians. Commun. Math. Phys. **22**, 269–79 (1971);
E. Balslev, J.M. Combes: Spectral Properties of Many–Body Schrödinger Operators with Dilation–Analytic Interactions. Commun. Math. Phys. **22**, 280–94 (1971)

[6] B. Baumgartner: Peculiar effects from number theory for doubly excited Rydberg states of two–electron ions. J. Phys. **B 27**, L1–L6 (1994)

[7] B.K. Ridley: Quantum Processes in Semiconductors. Clarendon Press, Oxford 1993

[8] G. Gamow: Zur Quantentheorie des Atomkernes. Z. Phys. **51**, 204–212 (1928)

[9] W.F. Osgood: Lehrbuch der Funktionentheorie I. R.G. Teubner, Leipzig, Berlin 1928

[10] W.I. Smirnov: Lehrgang der höheren Mathematik III/2. VEB Deutscher Verlag der Wissenschaften, Berlin 1971

[11] M. Abramowitz, I.A. Stegun: Handbook of Mathematical Functions. Dover Publications, New York 1965