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S-matrix for generalized Landau–Zener problem

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Abstract. The Schrödinger equation $i\dot{\Psi} = (A + Bt)\Psi$ with constant Hermitian matrices A and B is studied. In the form where B is diagonalized, this equation is a generalization of the *Landau–Zener* problem to an arbitrary number of crossing energy levels. An approach—the *independent crossing approximation*—leading to a partial understanding of the general case in terms of the two-level problem is introduced. It is found that certain S-matrix elements (and thus the corresponding transition probabilities) for the general problem are *exactly* given by formulae of unexpected simplicity, suggesting that some kind of general analytic solution might exist. The full S-matrix is calculated for a solvable special case of the problem. The solution of another special case, previously discovered for systems with three states, is generalized to any number of states. The asymptotic behaviour of the system is discussed in general and given explicitly to lowest order in $1/t$.

1. Introduction

Generally it is very difficult to obtain analytic results for Schrödinger equations with time-dependent Hamiltonians. The most simple kind of time dependence one can imagine—at least in a formal sense—is a linear one, corresponding to a Schrödinger equation of the form $i\dot{\Psi}(t) = (A + Bt)\Psi(t)$ with Hermitian (say $n \times n$) matrices A and B. In the form where B is diagonalized, this equation is generally referred to as the *level crossing* or (for $n = 2$) *Landau–Zener* problem. Applications include nuclear [3] and atomic [4] collisions, quantum optics [5] and atoms in time-dependent electric [6, 7] or magnetic [8] fields. Our motivation for working on this problem is that it describes (in some approximation) a uniformly accelerated particle coupled to a bath of harmonic excitations [9]. Even though the case of two levels (degrees of freedom) was studied and solved already in 1932 by Zener [10], Landau [11], Stückelberg [12] and Majorana [13], the general (n-level) problem still is an area of active research. Analytic results have been obtained for some special cases involving more than two degrees of freedom [1, 14], but no general solution for $n \geqslant 3$ has so far been found.

The central result of this paper is that some of the transition probabilities for the fully general n-level problem are *exactly* given by a simple formula. This formula is—via an approximation scheme introduced below—naturally obtained as an *approximate* result in the limit where the crossings of pairs of levels are well separated. Furthermore, we extend the analytic work done so far and discuss the asymptotic behaviour of the equation under consideration. The formula mentioned above, together with the analytic results found previously and in this paper, leads us

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to believe that a general analytic solution to the level-crossing problem might exist. This paper may be seen as an invitation to the reader to try and find it. To that end we also attempted to briefly summarize some of the previous work in a coherent form and include all the information known to us which might be useful for further investigations.

The detailed organization of this paper is as follows. In section 2 we state the problem under consideration in a more precise form, and introduce important notation and general concepts. After a brief discussion of the two-level case (section 3) we show how in the limit of *independent crossings* some transition probabilities for the general problem can be obtained approximately from the known two-level probabilities (section 4). In section 5 we make the important discovery that some of these approximate formulae actually hold *exactly* in the fully general case. The most important special cases for which analytic results have been found so far are discussed in section 6. We give a simple analytic solution and calculate the full S-matrix for the *equal-slope* case, and we generalize the solution to the *bowtie* case (found by Carroll and Hioe [1] for three states) to any number of states. Two important cases for which no analytic solution is yet known, the $1+n$ case and the three-level problem, are studied in section 7, followed by a short summary (section 8). In the appendix we discuss the asymptotic behaviour of the solutions and give an accurate definition of the S-matrix for our problem.

2. General discussion, notation

We are considering the differential equation

$$\mathrm{i}\dot{\Psi}(t) = (A + Bt)\Psi(t) \tag{1}$$

where A and B are Hermitian matrices and Ψ is a vector with complex components ψ_k. This is a system of first-order complex linear differential equations. It conserves probability (i.e. $|\Psi|^2 = \sum_k |\psi_k|^2$ remains constant) and phase space volume†. Our goal is to find some kind of analytic expression for its solutions or for the S-matrix defined by it (see below).

Equation (1) possesses several symmetries (i.e. operations on the matrices A and B corresponding to redefinitions of Ψ or the time t that leave the above form of the equation unchanged):

$$\begin{aligned}
&\text{(I)} && \mathrm{A} \to \mathrm{A} + \mu\mathbf{1} && (\Psi = \mathrm{e}^{\mathrm{i}\mu t}\Psi') \\
&\text{(II)} && \mathrm{B} \to \mathrm{B} + \mu\mathbf{1} && (\Psi = \mathrm{e}^{\mathrm{i}\mu t^2/2}\Psi') \\
&\text{(III)} && \mathrm{A} \to -\mathrm{A}^*,\ \mathrm{B} \to -\mathrm{B}^* && (\Psi = \Psi'^*) \\
&\text{(IV)} && \mathrm{A} \to \mathrm{A} + \mu\mathrm{B} && (\mathrm{t} = \mathrm{t}' + \mu) \\
&\text{(V)} && \mathrm{A} \to \mu\mathrm{A},\ \mathrm{B} \to \mu^2\mathrm{B} && (\mathrm{t} = \mu\mathrm{t}',\ \mu > 0) \\
&\text{(VI)} && \mathrm{A} \to -\mathrm{A}, && (\mathrm{t} = -\mathrm{t}') \\
&\text{(VII)} && \mathrm{A} \to \mathrm{UAU}^\dagger,\ \mathrm{B} \to \mathrm{UBU}^\dagger && (\Psi = U\Psi',\ U \text{ unitary}).
\end{aligned} \tag{2}$$

† Here the volume is defined by the integration measure $\mathrm{d}V = \prod_k \mathrm{d}(\mathrm{Re}\,\psi_k)\,\mathrm{d}(\mathrm{Im}\,\psi_k)$.

Because we can diagonalize B in (1) by an appropriate unitary transformation (operation (VII) above), in the following we can assume that B is real and diagonal; denote its diagonal elements (or eigenvalues) by b_k ($k = 1, \ldots, n$). If B has multiple eigenvalues, then we can diagonalize A in the corresponding subspaces, such that $a_{kl} = 0$ if $k \neq l$ and $b_k = b_l$ (this will also be assumed in the following). Note that we still have the freedom to modify our equation using the symmetries (I) to (VI) and a subgroup of (VII) (U diagonal) without affecting the above assumptions.

Denoting the elements of A by $a_{kk} = \epsilon_k$ and $a_{kl} = v_{kl}$ (for $k \neq l$) in order to make our notation more intuitive, we can now write (1) in the more concrete form

$$\mathrm{i}\begin{pmatrix} \dot{\psi}_1 \\ \vdots \\ \vdots \\ \dot{\psi}_n \end{pmatrix} = \begin{pmatrix} \epsilon_1 + b_1 t & v_{12} & \cdots & v_{1n} \\ v_{21} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & v_{n-1,n} \\ v_{n1} & \cdots & v_{n,n-1} & \epsilon_n + b_n t \end{pmatrix} \begin{pmatrix} \psi_1 \\ \vdots \\ \vdots \\ \psi_n \end{pmatrix} \tag{3}$$

with $\epsilon_k, b_k \in \mathbb{R}$, $v_{lk} = v_{kl}^* \in \mathbb{C}$, and $v_{kl} = 0$ whenever $b_k = b_l$.

In physical terms we can interpret our equation as describing a quantum mechanical system with some number n of *states* or *levels* whose *unperturbed energies* $E_k(t) = \epsilon_k + b_k t$ are linear functions of time, and which are coupled by the constant off-diagonal matrix elements v_{kl}; ψ_k is the *amplitude* for the system to be in state k. Unless we have the trivial case where all the eigenvalues of B are equal, there will be pairs (k, l) of levels, whose unperturbed energies $E_k(t)$ and $E_l(t)$ cross at some point in time—thus the name 'level-crossing problem'.

What kind of behaviour do we expect from the solutions of (3)? If all the couplings v_{kl} are equal to zero, the time evolution of the system is trivial—the different degrees of freedom are decoupled and the general solution is $\psi_k(t) = c_k \mathrm{e}^{-\mathrm{i}\phi_k(t)}$, with arbitrary constants c_k and the phases $\phi_k(t)$ being defined by $\phi_k(t) = \int_0^t (\epsilon_k + b_k t')\,\mathrm{d}t' = \epsilon_k t + \frac{1}{2} b_k t^2$. If on the other hand there are non-zero couplings, transitions between different states become possible, and things are more complicated. However, for large times t the terms $b_k t$ on the diagonal will cause more and more rapid relative oscillations between the different amplitudes, and thus suppress the mixing due to the coupling terms. This becomes clearer if we write down our equation in the interaction picture, i.e. transform to new variables Ψ^{I} defined by $\psi_k(t) = \mathrm{e}^{-\mathrm{i}\phi_k(t)} \psi_k^{\mathrm{I}}(t)$. In terms of Ψ^{I}, (3) becomes

$$\mathrm{i}\dot{\Psi}^{\mathrm{I}}(t) = C(t)\Psi^{\mathrm{I}}(t) \qquad \text{with} \begin{cases} c_{kk}(t) = 0 \\ c_{kl}(t) = v_{kl}\mathrm{e}^{\mathrm{i}(\phi_k(t) - \phi_l(t))} \qquad (k \neq l). \end{cases} \tag{4}$$

We see that the non-zero elements of $C(t)$ oscillate increasingly faster as the time gets larger (recall that $v_{kl} = 0$ if $b_k = b_l$).

In fact, numerical integrations show (and in appendix A we will prove) that the absolute values $|\psi_k(t)|$ of our amplitudes approach limits for $t \to \pm\infty$, or, in other words, that for all k and l the limit

$$S_{kl} = \lim_{\substack{t' \to \infty \\ t \to -\infty}} |U_{kl}(t', t)| \tag{5}$$

exists† (where $U(t', t)$ is the time evolution operator for our equation). In physical terms this means that there are well defined transition probabilities S_{kl}^2 for the system

† Unless $k \neq l$, $b_k = b_l$ and $\epsilon_k = \epsilon_l$; see the footnote in appendix A for a remark on that case.

to go from state l at time $t \to -\infty$ to state k at $t \to +\infty$. The matrix defined by (5) will in the following be referred to as the S-matrix for our problem (note that in appendix A we will give a more precise definition of the S-matrix which—in contrast to (5)—also retains phase information).

Since the transition probabilities are the quantities of physical interest, our task is to calculate the S-matrix defined by (5), i.e. to determine its dependence on the parameters v_{kl}, b_k and ϵ_k. From the above definition of the S-matrix it follows that it is invariant under the symmetry operations (2) (I)–(V) and (VII) (for diagonal U). This restricts the possible forms an explicit formula for elements of S can have. In particular, for a pair of levels k and l with a crossing (i.e. for which $b_k \neq b_l$), the *Landau–Zener* (LZ) parameter

$$z_{kl} = \frac{|v_{kl}|^2}{|b_k - b_l|} \tag{6}$$

is essentially the only combination of the parameters pertaining to this crossing (b_k, b_l, ϵ_k, ϵ_l, v_{kl}, v_{lk}) which is invariant under the above symmetry operations (i.e. any invariant function depending only on these six parameters can be written as a function of z_{kl}). The LZ parameters will play a very important role in the following—all transition probabilities for which explicit formulae have been found so far (in this paper or previously) are simple functions of the z_{kl}. For use in the following, let us also define

$$p_{kl} = \mathrm{e}^{-\pi z_{kl}} \qquad \text{and} \qquad q_{kl} = \sqrt{1 - p_{kl}^2}. \tag{7}$$

3. Two degrees of freedom

The simplest non-trivial case of the general level-crossing problem is the one with two degrees of freedom and $b_1 \neq b_2$:

$$\mathrm{i}\begin{pmatrix} \dot{\psi}_1 \\ \dot{\psi}_2 \end{pmatrix} = \begin{pmatrix} \epsilon_1 + b_1 t & v \\ v^* & \epsilon_2 + b_2 t \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}. \tag{8}$$

It was first solved in 1932 by Zener [10], Landau [11], Stückelberg [12] and Majorana [13] (see also Wannier [15] for a particularly concise approach). The two-level case is a special instance of the equal-slope case discussed in section 6.1, so that our calculation of the S-matrix for that case also applies here. It is given by

$$S = \begin{pmatrix} p & q \\ q & p \end{pmatrix} \tag{9}$$

where $p = \mathrm{e}^{-\pi z}$, $q = \sqrt{1 - p^2}$ and $z = |v|^2/|b_2 - b_1|$ is the LZ parameter defined above. According to the discussion in the previous section it follows from symmetry considerations alone that the S-matrix for the two-level case must be a function of z only, but it seems remarkable that the functional dependence is of such a simple form†.

† Note that (9) is an instance of the *adiabatic theorem*: the probability for leaving the instantaneous ground state of the system (state 1 for $t \to -\infty$ and state 2 for $t \to +\infty$, if $b_1 > b_2$) is exponentially small in the limit of slow passage ($|b_2 - b_1| \to 0$).

In words we can summarize this result as follows. If the system is originally in one of its two states, then the crossing of the two levels results in a reduction in the amplitude in the original state by a factor which is essentially the exponential of the squared coupling divided by the rate of relative energy change. The other state picks up the amount of amplitude dictated by probability conservation. To gain some intuition of how the amplitudes evolve in time, see figure 1.

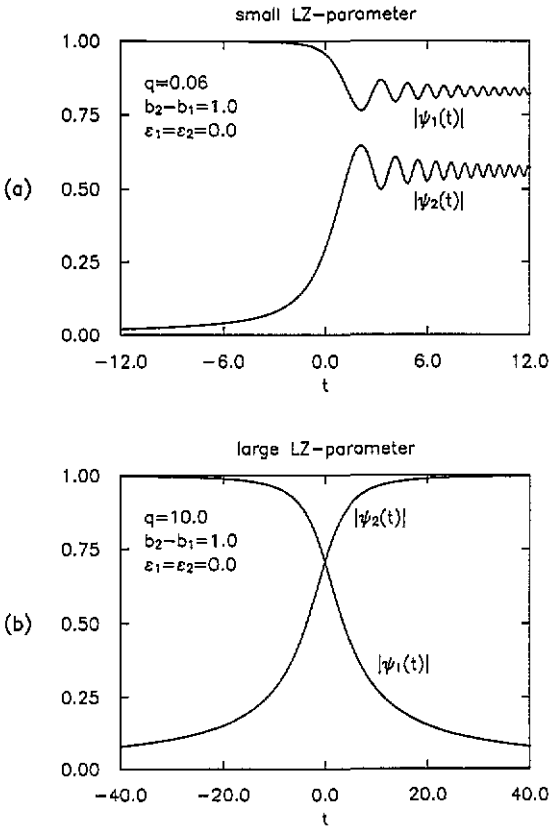

Figure 1. Time evolution of the complex amplitudes (i.e. their magnitudes) for the two-level problem, with the system initially in state 1. In (a) the LZ parameter is relatively small ($q = 0.06$), while in (b) it is fairly large ($q = 10$). Even though the detailed time evolution is very different, in both cases large amounts of amplitude are exchanged only at times close to $t = 0$ (when the levels cross).

4. Independent crossing approximation (ICA)

Since the S-matrix for the case of two levels can be calculated, but no general solution for three or more levels exists, one may ask to what extent or under which circumstances the general case can be understood in terms of crossings of pairs of the levels involved. From the plots in the previous section, or by looking at the problem in the interaction picture (equation (4)), one sees that significant amounts

of amplitude are exchanged between two states k and l only near the time when the two levels cross (i.e. when $E_k(t) = E_l(t)$). Thus we expect that if all crossings are well separated (and there are no multiple crossings, i.e. crossings of more than two levels at one point), they can be considered as independent of each other and each of them is described by the S-matrix (9). This approach will in the following be referred to as the *independent crossing approximation* (ICA).

What kind of information the ICA yields is best explained by use of an example. Consider the 'level-crossing diagram' in figure 2(a). Say initially the system is in state 1, i.e. $|\psi_1| = 1$, $|\psi_2| = |\psi_3| = 0$. Then at the crossing of levels 1 and 3, the amplitude splits up according to (9); the amount p_{13} remaining in state 1 splits up again at the crossing (1–2). Note that in this case we obtain values for all the final amplitudes (and thus the corresponding S-matrix elements); the crossing (2–3) never comes into play, because all the amplitude is in state 1 when it takes place.

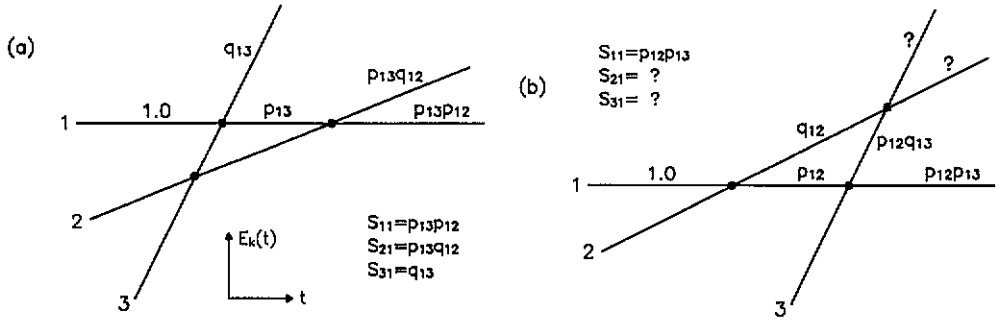

Figure 2. Schematic illustration of the ICA rule for three levels. (a) and (b) show the two possible orderings of the crossings. Note that in (a) all three final amplitudes can be predicted, but in (b) only one of them.

In contrast to the previous example, now consider figure 2(b) (which differs from 2(a) only in the ordering of the crossings). If the system initially is in state 1, the amplitude first splits at the crossing (1–2), and then the amount remaining in state 1 splits again at (1–3). But now *both* the levels 2 and 3 have non-zero amplitude *before* they cross, and (since our method is not taking into account any phase information) we cannot predict the final amplitudes for those two levels.

So our knowledge of the S-matrix for the two-level problem enables us to predict—in the limit of well separated crossings—some, but by no means all, transition probabilities for the general case. Whether a particular transition probability can be predicted or not may depend on the ordering of the crossings (as seen above), or on the existence of couplings (for example, if $v_{12} = 0$ in figure 2(b), then $q_{12} = 0$ and approximations for all final amplitudes can be obtained).

However, there are some 'special' matrix elements which can *always* be predicted by the ICA: the diagonal elements S_{kk} corresponding to states k with maximum or minimum slope ($b_k = \max_{l=1,\dots,n}\{b_l\}$, or $b_k = \min_{l=1,\dots,n}\{b_l\}$). The values obtained are

$$S_{kk} \approx \prod_{\substack{l=1,\dots,n \\ b_l \neq b_k}} p_{kl} \tag{10}$$

(every level l with $b_l \neq b_k$ crosses the level k and thus reduces $|\psi_k|$ by the factor p_{kl}; because the level k has maximum or minimum slope, no amplitude that has branched off from it at some point can ever return).

By improving the above method and taking into account phase information, we could also obtain approximations for all other S-matrix elements. However, due to interference effects, the elements so obtained would depend on the separations of the crossings (i.e. the ϵ_k) very sensitively and thus do not approach limits as the crossings are separated more and more. In contrast to that, the matrix elements obtainable without the use of phase information do not depend on the ϵ_k at all (for a given ordering of the crossings).

In the following we will see that the ICA not only offers some intuition by allowing a simple (though only partial) understanding of the general n-level problem in terms of single crossings (in the limit of these being well separated), but that some 'approximate' results predicted by it actually are *exact*.

5. General formula for 'special' S-matrix elements

From the derivation of formula (10) one would not expect it to be useful unless the crossings of level k with the other levels are well separated from each other and from all the other crossings. However, to our surprise we found in numerical simulations that (10) is an *exact* result which holds always except in the very special case where there is another level l with identical unperturbed energy as level k. Let us write down this statement in accurate form.

Consider the differential equation (3). If the level k has minimum or maximum slope ($b_k = \min_{l=1,\ldots,n}\{b_l\}$, or $b_k = \max_{l=1,\ldots,n}\{b_l\}$), and there is no other level with the same unperturbed energy (i.e. there is no $l \neq k$ with $b_l = b_k$ *and* $\epsilon_l = \epsilon_k$), then the diagonal S-matrix element S_{kk} (defined by (5)) corresponding to that level is *exactly* given by

$$S_{kk} = \prod_{\substack{l=1,\ldots,n \\ b_l \neq b_k}} p_{kl} = \exp\left(-\pi \sum_{\substack{l=1,\ldots,n \\ b_l \neq b_k}} z_{kl}\right) = \exp\left(-\pi \sum_{\substack{l=1,\ldots,n \\ b_l \neq b_k}} \frac{|v_{kl}|^2}{|b_k - b_l|}\right). \tag{11}$$

Formula (11) agrees with all analytic results found so far (see section 6) and we also verified it by numerous highly accurate numerical integrations, so that we have no doubts about the correctness of the above statement. Note that the one and only restriction (that there may be no other level with identical unperturbed energy) to the validity of (11) is easy to understand (see the footnote in appendix A).

The structure and simplicity of formula (11) reflects the way it was obtained in the previous section; every level l crossing the level k contributes a factor of $\exp(-\pi z_{kl})$. S_{kk} only depends on the LZ parameters pertaining to the level k, and not on the ϵ_l and the couplings between the other levels. Note that in contrast to this, the other S-matrix elements *do* depend on the ϵ_k (see section 7.2) and thus cannot be given by formulae as simple as (11).

The fact that some (at least two) transition probabilities for the fully general problem are given by such simple expressions, suggests that a general analytic solution might exist or a more complete understanding of the problem in terms of two-level crossings might be possible. Unfortunately we have not yet been able to find a general proof of (11). In the next section we will discuss special cases of (3), for which analytic solutions—of course in agreement with (11)—exist.

6. Analytical solutions to special cases

In spite of the simplicity and generality of the formula (11) discovered in the previous section, analytic solutions to equation (3) (and thus proofs for (11)) have so far only been found for some special cases of fairly limited scope. In the following subsections we will discuss the two most general of these†. They both have in common that they apply to any number of levels, they contain the two-level problem as a special case, and there is a special level which is coupled to all the others, but no two of these are coupled to each other.

6.1. The equal-slope case

Assume that all but one of the eigenvalues b_k of B in (1) are equal. Then we can use the symmetry transformations (2) to write (3) in the form

$$\mathrm{i}\begin{pmatrix}\dot{\psi}_0\\ \dot{\psi}_1\\ \vdots\\ \dot{\psi}_n\end{pmatrix}=\begin{pmatrix}bt & v_1 & \dots & v_n\\ v_1^* & \epsilon_1 & \dots & 0\\ \vdots & \vdots & \ddots & \vdots\\ v_n^* & 0 & \dots & \epsilon_n\end{pmatrix}\begin{pmatrix}\psi_0\\ \psi_1\\ \vdots\\ \psi_n\end{pmatrix} \tag{12}$$

with $b \neq 0$ and the ϵ_k ordered according to $\epsilon_1 < \epsilon_2 < \ldots < \epsilon_n$ (assume that no two of the ϵ are equal; also assume for definiteness that $b > 0$). We have a 'special' degree of freedom ψ_0, and n others which are not coupled to each other and for which the unperturbed energies as functions of time have equal slopes (see figure 3). This special case of the level-crossing problem was first considered by Demkov [14] in 1966; in the same year the S-matrix element S_{00} (i.e. the reduction of amplitude in the special state due to its interaction with the others) was determined by Osherov [17] (see also [18]). We will in the following calculate the full S-matrix.

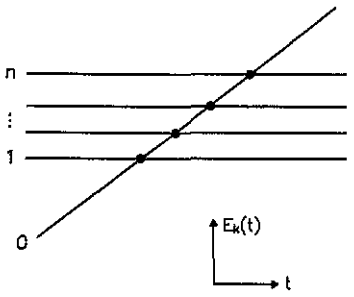

Figure 3. Unperturbed energy levels as functions of time for the equal-slope case. One level crosses a number of other ones which all have equal slope and thus do not cross each other.

Equation (12) is straightforward to solve via Fourier transformation. Writing it down component by component and Fourier transforming according to $\Psi(t) = \int_C \mathrm{d}\omega\, \mathrm{e}^{-\mathrm{i}\omega t}\hat{\Psi}(\omega)$ (where the contour C will be specified later) gives

$$\begin{cases}\omega\hat{\psi}_0 = -\mathrm{i}b\dfrac{\mathrm{d}\hat{\psi}_0}{\mathrm{d}\omega} + \displaystyle\sum_{k=1}^{n} v_k\hat{\psi}_k\\ \omega\hat{\psi}_k = \epsilon_k\hat{\psi}_k + v_k^*\hat{\psi}_0 \qquad (k = 1,\ldots,n).\end{cases} \tag{13}$$

† In fact, to our knowledge the only other case solved so far is the 'SU(2)' case $\mathrm{i}\dot{\Psi} = (J_x + btJ_z)\Psi$ (with the matrices J_x and J_z being n-dimensional representations of the corresponding angular momentum operators; see [16]). But since there is essentially only one free parameter, this case is very special and not important to our work here.

Solving the n lower equations for $\hat{\psi}_k$ gives $\hat{\psi}_k = (v_k^*/(\omega - \epsilon_k))\hat{\psi}_0$; inserting this into the first equation results in a first-order linear differential equation in $\hat{\psi}_0$, which is solved by $\hat{\psi}_0(\omega) = \exp[(\mathrm{i}/2b)\omega^2] \prod_k (\omega - \epsilon_k)^{-\mathrm{i}z_k}$, where the $z_k = |v_k|^2/b$ are the by now familiar LZ parameters. So we obtain

$$\psi_k(t) = \int_C \mathrm{d}\omega \exp(-\mathrm{i}\omega t + (\mathrm{i}/2b)\omega^2)\psi_k(\omega)$$

$$\begin{cases} \psi_0(\omega) = \prod_k (\omega - \epsilon_k)^{-\mathrm{i}z_k} \\ \psi_k(\omega) = \dfrac{v_k^*}{\omega - \epsilon_k}\psi_0(\omega) \qquad (k = 1, \ldots, n) \end{cases} \tag{14}$$

By inserting (14) into the components of (12) we can easily check that we actually have a solution (because of the factor $\exp(\mathrm{i}/2b)\omega^2$ in our integrals, any choice of the contour C originating and ending at $\pm\mathrm{e}^{\mathrm{i}\pi/4}\infty$ will ensure that all integrals converge and any boundary terms from partial integrations vanish).

In appendix B we will describe how the above integral representation yields a complete set of solutions, from which the S-matrix can be obtained. It is given by

$$\begin{pmatrix} p_1 \cdots p_n & q_1 p_2 \cdots p_n & q_2 p_3 \cdots p_n & q_3 p_4 \cdots p_n & \cdots & q_n \\ q_1 & p_1 & 0 & 0 & \cdots & 0 \\ p_1 q_2 & q_1 q_2 & p_2 & 0 & \cdots & 0 \\ p_1 p_2 q_3 & q_1 p_2 q_3 & q_2 q_3 & p_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ p_1 \cdots p_{n-1} q_n & q_1 p_2 \cdots p_{n-1} q_n & q_2 p_3 \cdots p_{n-1} q_n & q_3 p_4 \cdots p_{n-1} q_n & \cdots & p_n \end{pmatrix} \tag{15}$$

with $p_k = \mathrm{e}^{-\pi z_k}$ and $q_k = \sqrt{1 - p_k^2}$.

Note that the S-matrix elements do not depend on the ϵ_k (for a given ordering of those). The same is true for predictions of the ICA, and in fact it is quite easy to see that here the ICA predicts values for all S-matrix elements, and they all agree with (15)—in other words, the ICA is exact for the equal-slope case. Formula (15) (together with the assumed ordering of the ϵ_k) implies that some S-matrix elements perform discontinuous jumps if for a pair l, m of indices the sign of $\epsilon_m - \epsilon_l$ changes. At first glance this 'infinitely sensitive' dependence of the S-matrix on the ϵ_k seems counter-intuitive, but it can be accounted for by the fact that the time it takes the levels l and m to equilibrate, diverges for $|\epsilon_m - \epsilon_l| \to 0$. We also want to remark that the S-matrix (15) depends very sensitively on the equality of the slopes of levels $1, \ldots, n$—small differences between these slopes may lead to large deviations of the S_{kl} from (15).

6.2. The bowtie case

Another case for which an explicit solution exists is the one where all levels are crossing at the same point (see figure 4), and there is one special degree of freedom, say ψ_0, coupled to all the others, but with those not being coupled to each other.

Using (2) this case can be written in the form

$$\mathrm{i}\begin{pmatrix}\dot{\psi}_0\\ \dot{\psi}_1\\ \vdots\\ \dot{\psi}_n\end{pmatrix}=\begin{pmatrix}0 & v_1 & \dots & v_n\\ v_1^* & b_1 t & \dots & 0\\ \vdots & \vdots & \ddots & \vdots\\ v_n^* & 0 & \dots & b_n t\end{pmatrix}\begin{pmatrix}\psi_0\\ \psi_1\\ \vdots\\ \psi_n\end{pmatrix}. \tag{16}$$

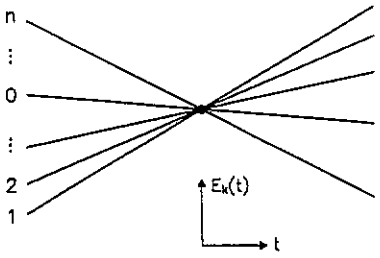

Figure 4. Unperturbed energy levels as functions of time for the bowtie case. All levels cross at one point in time. Levels 1 to n are not coupled to each other, but all of them may be coupled to level 0.

Note that we have a time-reversal symmetry here: if $(\psi_0(t);\psi_1(t),\dots,\psi_n(t))$ is a solution, then $(\psi_0(-t);-\psi_1(-t),\dots,-\psi_n(-t))$ also is. This implies that there is a complete basis of solutions for which ψ_0 is even and the ψ_k $(k=1,\dots,n)$ are odd or *vice versa*. This special case was first considered and solved by Carroll and Hioe [1, 2] for $n=2$ (i.e. for three levels; note that the time-reversal symmetry is crucial for their solution). They also calculate the matrix of transition probabilities [1]; it is interesting to note that not only the 'special' transition probabilities agree with (11), but that also all the other ones are very simple functions (polynomials of degree $\leqslant 4$) of the familiar parameters $p_k=\exp(-\pi z_k)$ (with $z_k=|v_k|^2/|b_k|$, $k=1,2$).

Rewriting their solution in our notation and generalizing it to any number of levels we obtain

$$\begin{aligned}\psi_0(t)&=t\int_C \mathrm{d}u\,\mathrm{e}^{(-\mathrm{i}/2)ut^2}\psi_0(u) \qquad & \psi_0(u)&=u^{-1/2-\mathrm{i}/2\sum_k \tilde{z}_k}\prod_k (u-b_k)^{\mathrm{i}\tilde{z}_k/2}\\ \psi_k(t)&=\int_C \mathrm{d}u\,\mathrm{e}^{-(\mathrm{i}/2)ut^2}\psi_k(u) \qquad & \psi_k(u)&=\frac{v_k^*}{u-b_k}\psi_0(u)\end{aligned} \tag{17}$$

with $\tilde{z}_k=|v_k|^2/b_k$. It is straightforward to verify that (17) solves (16) for $t\neq 0$ (as long as the contour C begins and ends at $\mathrm{Im}\,(u)=-\infty$). In order to calculate the S-matrix, special attention has to be given to the point $t=0$, where the integral for $\psi_0(t)$ does not converge [2]. It might be interesting to calculate the S-matrix for more than three degrees of freedom from (17); we have not attempted this yet.

7. Discussion of two unsolved cases

After having discussed the most general solutions found so far, let us now turn to two (in some sense) rather simple cases which have not been solved yet. We will see that the $1+n$ case (which contains both the cases considered in section 6) can be rewritten as an integral equation, and we will attempt to gain some insight by studying the case of three levels.

7.1. The 1+n case

Consider the situation where the *only* restriction is that there is a special state ψ_0, such that all the other states may be coupled to ψ_0, but not to each other†. Using symmetries (I) and (II) in (2), we can obtain $\epsilon_0 = b_0 = 0$, so that (3) takes the form

$$\mathrm{i}\begin{pmatrix} \dot{\psi}_0 \\ \dot{\psi}_1 \\ \vdots \\ \dot{\psi}_n \end{pmatrix} = \begin{pmatrix} 0 & v_1 & \dots & v_n \\ v_1^* & \epsilon_1 + b_1 t & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ v_n^* & 0 & \dots & \epsilon_n + b_n t \end{pmatrix} \begin{pmatrix} \psi_0 \\ \psi_1 \\ \vdots \\ \psi_n \end{pmatrix}. \tag{18}$$

This case is the most simple generalization of *both* the solvable special cases discussed in the previous section.

Because the levels $1, \dots, n$ are not coupled to each other, (18) can be written as an integral equation in terms of ψ_0. To do this, first write down (18) component by component in the interaction picture (see section 2):

$$\begin{aligned} \mathrm{i}\dot{\psi}_0 &= \sum_{k=1}^{n} v_k \mathrm{e}^{-\mathrm{i}\phi_k(t)} \psi_k^{\mathrm{I}} \\ \mathrm{i}\dot{\psi}_k^{\mathrm{I}} &= v_k^* \mathrm{e}^{\mathrm{i}\phi_k(t)} \psi_0 \qquad (k = 1, \dots, n). \end{aligned} \tag{19}$$

This can be transformed to a Volterra integro-differential equation (with degenerate kernel) by integrating the second set of equations and inserting into the first one. For the initial condition $\psi_0(t_0) = 1$, $\psi_k(t_0) = 0$ $(k = 1, \dots, n)$ we get

$$\dot{\psi}_0(t) = \int_{t_0}^{t} \mathrm{d}s\, L(t,s)\psi_0(s) \qquad \text{with} \qquad L(t,s) = -\sum_k |v_k|^2 \mathrm{e}^{\mathrm{i}\phi_k(s) - \mathrm{i}\phi_k(t)}. \tag{20}$$

Integrating both sides yields the Volterra integral equation

$$\psi_0(t) = 1 + \int_{t_0}^{t} \mathrm{d}s\, K(t,s)\psi_0(s)$$

with

$$K(t,s) = -\sum_k |v_k|^2 \mathrm{e}^{\mathrm{i}\phi_k(s)} \int_s^t \mathrm{d}y\, \mathrm{e}^{-\mathrm{i}\phi_k(y)}. \tag{21}$$

Equation (21) is more general than all special cases solved so far, but nevertheless it may be easier to solve than the fully general problem (which cannot be converted to an integral equation in any obvious way). In the limit $t_0 \to -\infty$ the above initial condition implies $|\psi_0(t \to \infty)| = S_{00}$; if the b_k $(k = 1, \dots, n)$ are either all positive or all negative, then S_{00} is a 'special' matrix element (see section 5) to which formula (11) applies, and the final amplitude in state 0 should have the simple form $|\psi_0(\infty)| = \exp(-\pi \sum_{k=1}^{n} z_k)$ with $z_k = |v_k|^2/|b_k|$. Unfortunately we have not (yet) been able to solve (21) or even calculate $|\psi_0(\infty)|$.

† This case corresponds (in some approximation) to the problem of a uniformly accelerated particle coupled to the elementary excitations of a solid or liquid, which was our original motivation to study the level-crossing problem.

7.2. *Three degrees of freedom*

The smallest system for which no explicit solution is known is the case of three degrees of freedom with no two of the b_k being equal. So, to gain some intuition about the general problem, it should be instructive to study the behaviour of the S-matrix in this case. Because of $b_1 \neq b_2$, we can obtain $\epsilon_1 = \epsilon_2 = 0$ by use of the symmetries (I) and (IV) in (2), and write (3) as

$$\mathrm{i}\begin{pmatrix}\dot{\psi}_1\\ \dot{\psi}_2\\ \dot{\psi}_3\end{pmatrix} = \begin{pmatrix} b_1 t & v_{12} & v_{13}\\ v_{12}^* & b_2 t & v_{23}\\ v_{13}^* & v_{23}^* & \epsilon_3 + b_3 t\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\end{pmatrix}. \tag{22}$$

We will also assume that the b_k are ordered according to $b_1 < b_2 < b_3$, so that formula (11) applies to S_{11} and S_{33}, but not to S_{22}. In the following we study the dependence of the S-matrix on ϵ_3 and compare the results to (11) and the ICA predictions.

First let us consider the case where all three levels are coupled to each other and look at the S-matrix elements corresponding to the initial condition of all amplitude in state 1 (figure 5(a)). We see that—in agreement with our general statement (11)—S_{11} is independent of ϵ_3 and exactly given by the prediction of the independent crossing approximation. S_{21} and S_{31} approach limits for $\epsilon_3 \to +\infty$, but not for $\epsilon_3 \to -\infty$; instead they continue to oscillate, with the amplitudes of the oscillations approaching constant values and the frequency increasing proportionally to ϵ_3. This is exactly what we expect from the discussion in the context of the ICA in section 4 (note that the limits $\epsilon_3 \to +\infty$ and $\epsilon_3 \to -\infty$ correspond to figures 2(a) and (b) respectively).

From all that has been said up to now, it seems as if all predictions of the ICA which do not depend on the ordering of the crossings (i.e. on the ϵ_k), might be exact. But this is not the case—consider figure 5(b), where the S-matrix elements S_{k2}, $k = 1, 2, 3$, are plotted for the case where levels 1 and 3 are not coupled to each other. Now the ICA predicts $S_{22} = p_{12}p_{23}$ independently of the ordering of the crossings, and—in contrast to the case of S_{21} and S_{31} above—it gives no *a priori* reason why S_{22} would have to depend on ϵ_3. But it is clear from the graph that, even though S_{22} approaches the limit $p_{12}p_{23}$ for $\epsilon_3 \to \pm\infty$, $S_{22} = p_{12}p_{23}$ does *not* hold exactly†. Thus it seems that formula (11) exclusively applies to the S-matrix elements specified in section 5.

8. Summary, outlook

All transition probabilities for special cases of the level-crossing problem which have been determined analytically so far (see section 6.1 and the work by Carroll and Hioe [1, 16], have the common feature that they are polynomials in the parameters p_{kl} defined at the end of section 2. Furthermore, we have found that certain 'special' transition probabilities for the fully general problem are given *exactly* by the very simple formula (11), which—in the limit of independent crossings—arises naturally from the well known solution of the two-level case. The simple form and generality

† Note that the symmetry $S_{22}(-\epsilon_3) = S_{22}(\epsilon_3)$ evident in the plot is no mystery—it follows from the behaviour of the S-matrix under the symmetry operations in (2).

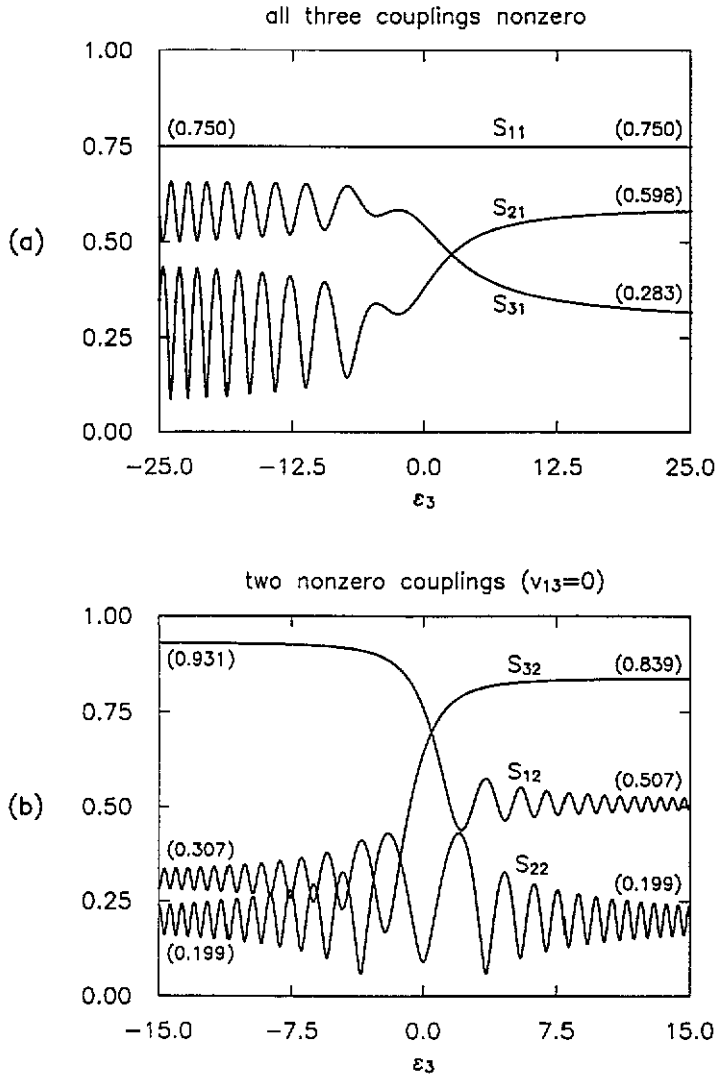

Figure 5. S-matrix elements for the three-level problem as functions of ϵ_3 (with $\epsilon_1 = \epsilon_2 = 0$). Graph (a) shows the S-matrix elements S_{k1} for $k = 1, 2, 3$ (in other words, the final amplitudes $|\psi_k(\infty)|$ for the initial condition of the system being in state 1) for the case where all three levels are coupled to each other. In (b) one of the couplings (v_{13}) is equal to zero and the system initially is in state 2. The parameter values used are $v_{12} = 0.28$, $v_{13} = 0.2$, $v_{23} = 0.75$, $b_1 = 0.0$, $b_2 = 1.0$, $b_3 = 3.0$ for (a), and $v_{12} = 0.8$, $v_{13} = 0$, $v_{23} = 0.44$, $b_1 = 0.0$, $b_2 = 2.0$, $b_3 = 3.0$ for (b); the numbers in brackets are the predictions given by the ICA.

of (11) suggest that one should be able to find an analytic proof for it, that a more complete understanding of the general problem in terms of two-level crossings might be possible, or that there might even be a general analytic solution to equation (3).

In contrast to that, as of yet explicit solutions (and thus proofs of (11)) have only been found for fairly limited special cases of the problem, and even in these cases considerable amounts of tedious work [2] were sometimes necessary to calculate

transition probabilities. In fact, even though there are many ways to write the solution for the two-level problem, it seems that even for this most simple case, no one has yet given a nice expression which is symmetric in the parameters corresponding to the two levels.

Thus our conclusion is that perhaps the right approach for tackling (3) has not been found yet and there is a nice solution to be discovered. We hope that this paper will inspire one of its readers to find it.

Acknowledgments

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Appendix A. Asymptotic behaviour

In this appendix we will study the asymptotic behaviour of the solutions to (3) in some detail. This will enable us to prove the existence of the S-matrix for our problem and give an improved definition of it that also contains phase information (in contrast to the definition in section 2).

The discussion in section 2 (and our numerical work) suggest that there are solutions $\Psi^{-(l)}$ and $\Psi^{+(l)}$ of (3) corresponding to the system being in the state l for $t \to -\infty$ and $t \to +\infty$ respectively. Or, in other words, solutions whose components $\psi_k^{\pm(l)}$ satisfy

$$\lim_{t\to-\infty} |\psi_k^{-(l)}(t)| = \delta_{kl} \qquad \lim_{t\to+\infty} |\psi_k^{+(l)}(t)| = \delta_{kl}. \tag{23}$$

Our explicit solution for the equal-slope case (see appendix B) suggests that to lowest order in $1/t$ the asymptotic solutions might have the form

$$\psi_l^{\pm(l)}(t) \sim |t|^{iA_l} e^{-i\phi_l(t)} \qquad \psi_k^{\pm(l)}(t) \sim \frac{B_{kl}}{t}\psi_l^{\pm(l)}(t) \qquad (k \neq l) \tag{24}$$

with constants A_l and B_{kl}. This motivates the ansatz

$$\begin{aligned} \psi_l^{\pm(l)}(t) &= |t|^{iA_l} e^{-i\phi_l(t)}(1 + \alpha_{l1}t^{-1} + \alpha_{l2}t^{-2} + \cdots) \\ \psi_k^{\pm(l)}(t) &= |t|^{iA_l} e^{-i\phi_l(t)}(\beta_{kl1}t^{-1} + \beta_{kl2}t^{-2} + \cdots) \qquad (k \neq l). \end{aligned} \tag{25}$$

Inserting (25) into (3) and collecting terms of equal order in $1/t$ yields equations for the coefficients A_l, α_{lj} and β_{klj}. Some tedious work shows that, if there is no level $k \neq l$ for which $b_k = b_l$ *and* $\epsilon_k = \epsilon_l$, all the equations can be satisfied and all the coefficients are uniquely determined†. In particular, we obtain

$$A_l = \sum_{\substack{k=1,\ldots,n \\ b_k \neq b_l}} \frac{|v_{kl}|^2}{b_k - b_l} \qquad \text{and} \qquad B_{kl} = \beta_{kl1} = \begin{cases} -\dfrac{v_{kl}}{b_k - b_l} & \text{for } b_k \neq b_l \\ 0 & \text{otherwise.} \end{cases} \tag{26}$$

† If there is a number of levels, say $k_1, \ldots, k_r$, with identical values of b_k and ϵ_k, then asymptotic states $\psi^{\pm(l)}$ satisfying (23) can, in general, only be defined after a suitable unitary transformation is performed in the subspace of the amplitudes $\psi_{k_1}, \ldots, \psi_{k_r}$ (and all other such subspaces with identical values of b_k and ϵ_k). We will not discuss this complication any further.

Thus the $\psi_k^{\pm(l)}(t)$ have asymptotic expansions as in (25), and to lowest order in $1/t$ they are given by (24) with A_l and B_{kl} as in (26). Note that the above formulae are identical for $t \to +\infty$ and $t \to -\infty$.

Clearly both the $\Psi^{-(l)}$ and the $\Psi^{+(l)}$ $(l = 1, \ldots, n)$ are complete sets of solutions, so that there are uniquely defined coefficients $\tilde{S}_{kl}$ satisfying

$$\Psi^{-(l)} = \sum_{k=1}^{n} \tilde{S}_{kl} \Psi^{+(k)}. \tag{27}$$

If we expand a solution $\Psi(t)$ in terms of the asymptotic states as $\Psi = \sum_l c_l^- \Psi^{-(l)} = \sum_l c_l^+ \Psi^{+(l)}$, then (27) implies $c_k^+ = \sum_l \tilde{S}_{kl} c_l^-$. In that sense the matrix $\tilde{S}$ completely describes the evolution of our system from $t = -\infty$ to $t = \infty$. Or, in other words, equation (3) can be viewed as a scattering problem with asymptotic states $\Psi^{\pm(l)}$ and the S-matrix being given by $\tilde{S}$. The magnitudes of its elements agree with the S-matrix defined in section 2 (i.e. $|\tilde{S}_{kl}| = S_{kl}$), but in contrast to S the improved S-matrix $\tilde{S}$ also contains phase information. Note that (24) together with (26) can be used to obtain accurate numerical results for $\tilde{S}$.

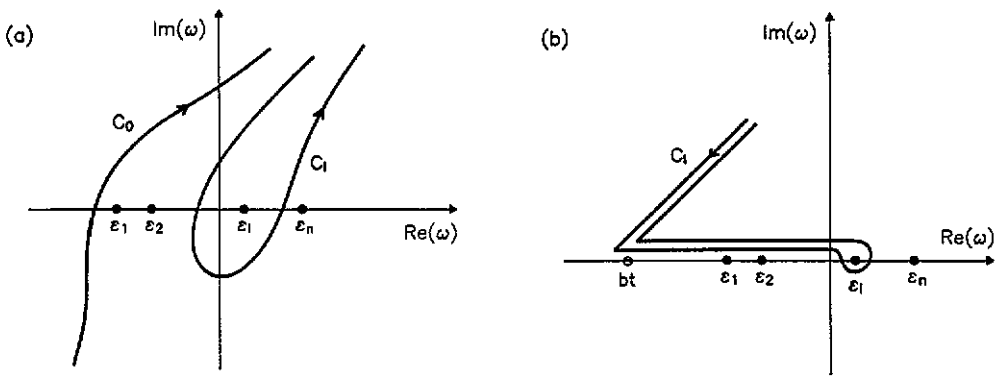

Figure A1. (a) shows the topology of the contours used to calculate the S-matrix for the equal slope case. C_0 goes from $-e^{i\pi/4}\infty$ to $+e^{i\pi/4}\infty$ and has all the singularities on its right. C_l $(l = 1, \ldots, n)$ starts and ends at $+e^{i\pi/4}\infty$, and encloses the singularity $\omega = \epsilon_l$ only. In (b) an example of a deformed contour $(l = 1, \ldots, n$; for the limit $t \to -\infty)$ is given.

Appendix B. *S*-matrix for equal-slope case

Here we will describe how the S-matrix (15) can be obtained from the integral representation (15). To be able to calculate the S-matrix, we need a complete set of solutions to (12). Consider the $n + 1$ different contours $C_0, \ldots, C_n$ shown in figure A1(a), and denote the solution obtained from C_l by $\Psi^{(l)}$ $(l = 0, \ldots, n)$. We need to evaluate the asymptotic behaviour of the components $\psi_k^{(l)}$ $(k = 0, \ldots, n)$ of the $\Psi^{(l)}$ for $t \to \pm\infty$. To do this, let us deform the contours such that their endpieces go from $\omega = bt$ to $\pm e^{i\pi/4}\infty$, and all other parts remain close to the real

axis (see figure A1(b) for an example). Then we can argue that (in the limit $t \to \pm\infty$) contributions of O(1) to $\psi_k^{(l)}(t)$ only can come from the saddle point $\omega = bt$ for $k = 0$, and from the neighbourhood of the singularity at $\omega = \epsilon_k$ for $k = 1, \ldots, n$. Omitting further details, we get for $t \to -\infty$:

$$\begin{aligned}
&\psi_0^{(0)}(t) \sim F_0(t)\mathrm{e}^{\pi(z_1+\cdots+z_n)} \\
&\psi_l^{(l)}(t) \sim F_l(t)\mathrm{e}^{3\pi z_l/2}\mathrm{e}^{\pi(z_{l+1}+\cdots+z_n)} \qquad (l = 1, \ldots, n) \\
&\psi_k^{(l)}(t) = \mathrm{O}(1/t) \qquad (k \neq l)
\end{aligned} \tag{28}$$

and, for $t \to +\infty$,

$$\begin{aligned}
&\psi_0^{(0)}(t) \sim F_0(t) \\
&\psi_k^{(0)}(t) \sim -F_k(t)\mathrm{e}^{(\pi/2)z_k}\mathrm{e}^{\pi(z_{k+1}+\cdots+z_n)} \qquad (k = 1, \ldots, n) \\
&\psi_0^{(l)}(t) \sim F_0(t)(\mathrm{e}^{2\pi z_l} - 1) \\
&\psi_k^{(l)}(t) = \mathrm{O}(1/t) \qquad (1 \leqslant k < l) \\
&\psi_l^{(l)}(t) \sim F_l(t)\mathrm{e}^{\pi z_l/2}\mathrm{e}^{\pi(z_{l+1}+\cdots+z_n)} \\
&\psi_k^{(l)}(t) \sim F_k(t)(1 - \mathrm{e}^{2\pi z_l})\mathrm{e}^{\pi z_k/2}\mathrm{e}^{\pi(z_{k+1}+\cdots+z_n)} \qquad (k > l)
\end{aligned} \tag{29}$$

(where $l = 1, \ldots, n$ in the last four equations), with

$$F_0(t) = \mathrm{e}^{\mathrm{i}\pi/4}\mathrm{e}^{-\mathrm{i}bt^2/2}|bt|^{-\mathrm{i}(z_1+\cdots+z_n)}(2\pi b)^{1/2}$$

and, for $k = 1, \ldots, n$,

$$F_k(t) = v_k^*\mathrm{e}^{\mathrm{i}\epsilon_k^2/(2b)}\mathrm{e}^{-\mathrm{i}\epsilon_k t}|t|^{\mathrm{i}z_k}\exp\left(-\mathrm{i}\sum_{m\neq k} z_m \ln|\epsilon_m - \epsilon_k|\right)2\sinh(\pi z_k)\Gamma(-\mathrm{i}z_k). \tag{30}$$

Note that, because of $\lim_{t\to-\infty}\psi_k^{(l)}(t) = 0$ for $k \neq l$, the $\Psi^{(l)}$ are (up to constant factors) identical with the asymptotic solutions $\Psi^{-(l)}$ defined in appendix A, and so the S-matrix (without phase information) is given by $S_{kl} = |\psi_k^{(l)}(\infty)|/|\psi_l^{(l)}(-\infty)|$. Using the identity $|\Gamma(\mathrm{i}z)| = (\pi/z\sinh(\pi z))^{1/2}$ (z real), we get from the above

$$\begin{aligned}
&S_{00} = \mathrm{e}^{-\pi(z_1+\cdots+z_n)} \\
&S_{k0} = \mathrm{e}^{-\pi(z_1+\cdots+z_{k-1})}(1 - \mathrm{e}^{-2\pi z_k})^{1/2} \qquad (k = 1, \cdots, n) \\
&S_{0l} = (1 - \mathrm{e}^{-2\pi z_l})^{1/2}\mathrm{e}^{-\pi(z_{l+1}+\cdots+z_n)} \\
&S_{kl} = 0 \qquad (1 \leqslant k < l) \\
&S_{ll} = \mathrm{e}^{-\pi z_l} \\
&S_{kl} = (1 - \mathrm{e}^{-2\pi z_l})^{1/2}\mathrm{e}^{-\pi(z_{l+1}+\cdots+z_{k-1})}(1 - \mathrm{e}^{-2\pi z_k})^{1/2} \qquad (k > l)
\end{aligned} \tag{31}$$

(where the index l always runs from 1 to n). This, rewritten in terms of the p_k and q_k, yields the S-matrix (15) in section 6.1.

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