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Spin-$\frac{1}{2}$ system coupled to a single mode: a resolvent expansion of the time-dependent solution

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Abstract. In order to describe the dynamics of a spin-oscillator Hamiltonian analytically, a second-order differential equation for the transition probability amplitude is established by means of a transcription into the Bargmann space of entire functions. The solution of the differential equation is given by a resolvent expansion whose zeroth-order member is in general exact up to fourth order in time; for various degenerate parameter values, however, it is exact for all times. The Laplace transform of any higher-order member is given explicitly.

1. Introduction

For a particle with spin $\frac{1}{2}$ coupled to a boson field mode (Schweber 1967, Reik *et al* 1982, 1985), exact solutions are of great interest because this simple looking but nevertheless non-trivial system serves as an archetypal model for a large variety of physical situations ranging from atomic physics and quantum optics to solid state physics. Let us give just a few examples from among these topics: a single atom coupled to an electromagnetic field (Dicke 1954), quantum diffusion (mode-assisted tunnelling) (Leggett *et al* 1987, Wagner and Vázquez-Márquez 1987, Weiss *et al* 1987), quantum chaos (Graham and Höhnerbach 1984) and laser action in vibronic systems (Schwendimann *et al* 1988).

Stationary isolated exact solutions were first found in the case of a Jahn-Teller system which is closely related to our model (Judd 1979). Attempts to construct exact solutions in the complete parameter space were advanced systematically by Reik *et al* (1982, 1985) by means of function theoretical methods in the spirit of Schweber (1967). In contrast to these treatments Schwendimann and Sigmund (1986) looked for time-dependent solutions.

Apart from the ubiquity of the model, there is still another motivation for investigating the coupled spin-oscillator system. Until now rather elaborate methods have been developed in order to determine the eigenvalues and eigenfunctions with high precision. However, these methods involve a considerable amount of mathematics. Therefore, one still feels the need to find novel, effective and even simpler schemes.

In the present paper (in contrast to most others in this field) we are interested in solutions which evolve in time in order to describe the dynamics of the system. Within the framework of an iteration procedure, we solve the time-dependent Schrödinger equation in a projected form, thus obtaining solutions for the transition probability

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amplitudes. Initial and final states of the system are allowed to be arbitrary. Our description is quite valuable for a large number of problems in physics (see above), at least as long the (generally non-stationary) initial state can be prepared, say, as a single eigenstate of some zeroth-order Hamiltonian. Since we do not deal with stationary states of the system, our results look formally quite different to previously published results. In summary, it seems to us that we have found a new and promising pathway towards the goal of constructing exact solutions.

Concerning a more explicit characterisation of the model, we deal in this paper with a spin-oscillator Hamiltonian which is a somewhat extended variant of that usually seen in the literature. This variant has been derived in RWA from a model Hamiltonian for an active centre of a vibronic laser (Schwendimann and Sigmund 1986):

$$H = 2\Delta\sigma_z + \Omega b^\dagger b + \lambda\sigma_z(b^\dagger + b) + \gamma\sigma_+ + \gamma^*\sigma_- \tag{1.1}$$

where $[b, b^\dagger] = 1$ and $[\sigma_+, \sigma_-] = 2\sigma_z$, $[\sigma_z, \sigma_\pm] = \pm\sigma_\pm$, $\sigma_z^2 = I$, λ denotes the particle-mode coupling and Ω is the mode frequency. $|\gamma|$ characterises the strength of tunnelling if the Hamiltonian is seen as describing a two-site system where tunnelling assisted by a single mode occurs. Δ takes account of an asymmetry in the potentials of the two sites. Equation (1.1) reduces to a form more frequently investigated if γ is real and Δ vanishes.

A transformed version of (1.1) turns out to be more convenient for our purposes. With

$$\tilde{H} = U^{-1}HU \qquad U = \exp[(\lambda/\Omega)\sigma_z(b - b^\dagger)] \tag{1.2}$$

the new Hamiltonian becomes (the prime indicating neglect of a parameter-dependent energy shift $E_s = -\Omega\delta^2/4$)

$$\begin{aligned} &\tilde{H}' = 2\Delta\sigma_z + \Omega b^\dagger b + \gamma V(\delta)\sigma_+ + \gamma^* V(-\delta)\sigma_- \\ &V(\pm\delta) = \exp[\pm\delta(b - b^\dagger)] \qquad \delta = -\lambda/\Omega. \end{aligned} \tag{1.3}$$

This paper is organised as follows. In § 2 equations for the transition probability amplitude are derived from (1.3), they suggest a change from a description in occupation number space to a formulation in Bargmann space where one deals with coherent states of Bargmann or Glauber type (Bargmann 1961, 1962, Glauber 1963). The function theoretical consequences of this transcription are drawn; they apply to the problem of solving a second-order differential equation obtained for the Laplace transform (with regard to the time) of the transition probability amplitude. In § 3 a resolvent expansion is developed in order to solve the differential equation. Only a particular initial condition as the simplest case is treated (cf §§ 3.1 and 3.3). The solution in zeroth order is analysed by means of combinatorics (cf § 3.2). In § 4.1 a rather explicit form for any member of the resolvent expansions with arbitrary initial conditions is deduced (§§ 3.1 and 3.3 may be read as an introduction to this comprehensive section). In § 4.2 the correct symmetry behaviour under time reversal is subsequently imposed. In § 4.3 the inverse Laplace transformation is explicitly performed. Section 4.4 is left to a listing of exact limiting cases in the parameter space and to the estimation of the time region where our solutions for arbitrary system parameters are reasonable. In § 4.5 the question of convergence of the present resolvent expansion is examined.

Finally, a remark on the notation: since in our calculations the parameters of the Hamiltonian (1.3), i.e. Δ, Ω, γ, γ^* and δ, will separate into the sets $\{\Delta, \Omega, \gamma, \gamma^*\}$ and

$\{\delta\}$ throughout the paper, we shall denote the former set by α for the purpose of a compact notation.

2. Second-order differential equations for the transition probability amplitudes

We want to solve the Schrödinger equation for the Hamiltonian (1.3) ($\alpha = \{\lambda, \Omega, \gamma, \gamma^*\}$)

$$\frac{\partial}{\partial t}|\Psi(\alpha, \delta; t)\rangle = -\mathrm{i}H(\alpha, \delta)|\Psi(\alpha, \delta; t)\rangle \tag{2.1}$$

where without loss of generality a product state

$$|\Psi(\alpha, \delta; 0)\rangle = |n\uparrow\rangle \tag{2.2}$$

is chosen as the initial state. Here n indicates the occupation number of a harmonic oscillator and $\uparrow$ and $\downarrow$ represent spin-$\frac{1}{2}$ states. Our problem is equivalent to that of calculating the transition probability amplitudes which arise as coefficients if the time-dependent solution vector is decomposed along the complete set of product states $|m\uparrow\downarrow\rangle$:

$$|\Psi(\alpha, \delta; t)\rangle = \sum_m |m\uparrow\rangle\langle\uparrow m|\Psi(\alpha, \delta; t)\rangle + \sum_m |m\downarrow\rangle\langle\downarrow m|\Psi(\alpha, \delta; t)\rangle. \tag{2.3}$$

Multiplying (2.1) from the left by an arbitrary state $\langle\uparrow m|$ we obtain

$$(\partial/\partial t)\langle\uparrow m|\Psi(\alpha, \delta; t)\rangle = -\mathrm{i}(\Delta + m\Omega)\langle\uparrow m|\Psi(\alpha, \delta; t)\rangle - \mathrm{i}\gamma\langle\downarrow m|V(\delta)|\Psi(\alpha, \delta; t)\rangle. \tag{2.4a}$$

Note that the last term is a superposition of transition probability amplitudes

$$\langle\downarrow m|V(\delta)|\Psi(\alpha, \delta; t) = \sum_k \langle m|V(\delta)|k\rangle\langle\downarrow k|\Psi(\alpha, \delta; t)\rangle. \tag{2.5}$$

We complete (2.4a) by the equation of motion for the sum (2.5)

$$\begin{aligned}(\partial/\partial t)&\langle\downarrow m|V(\delta)|\Psi(\alpha, \delta; t)\rangle \\ &= \mathrm{i}\Delta\langle\downarrow m|V(\delta)|\Psi(\alpha, \delta; t)\rangle - \mathrm{i}\Omega\langle\downarrow m|V(\delta)b^\dagger b|\Psi(\alpha, \delta; t)\rangle \\ &\quad - \mathrm{i}\gamma^*\langle\uparrow m|\Psi(\alpha, \delta; t)\rangle\end{aligned} \tag{2.4b}$$

where clearly (2.4a) and (2.4b) have to be complemented by their initial conditions

$$\langle\uparrow m|\Psi(\alpha, \delta; 0)\rangle = \delta_{m,n} \qquad \langle\downarrow m|V(\delta)|\Psi(\alpha, \delta; 0)\rangle = 0. \tag{2.6}$$

Unfortunately, the system (2.4) is not closed on account of the second term on the right-hand side of (2.4b). Therefore let us switch over from oscillator state vectors $\langle n|$ to Bargmann vectors $\langle\xi^*|$ (Bargmann 1961, 1962, Schweber 1967)

$$\langle\xi^*| = \sum_{k=0}^{\infty} \frac{\xi^k}{\sqrt{k!}}\langle k| \qquad \xi \in \mathbb{C}. \tag{2.7}$$

These new vectors are indicated by small Greek characters to avoid confusion. By virtue of this replacement the operators $b^\dagger$ and b are realised by $b^\dagger \to \xi$ and $b \to \partial/\partial\xi$, if acting to the left. More explicitly, we multiply (2.1) from the left by $\langle\uparrow\xi^*|V(-\delta)$, use the identities

$$\begin{aligned}\langle\xi^*|V(-\delta) &= \exp(-\tfrac{1}{2}\delta^2)\exp(\delta\xi)\langle\xi^* - \delta| \\ \langle\xi^*|V(-\delta)b^\dagger b &= (\xi - \delta)(\partial/\partial\xi - \delta)\langle\xi^*|V(-\delta)\end{aligned} \tag{2.8}$$

and arrive at

$$[\partial/\partial t + i\Delta + i\Omega(\xi-\delta)\,\partial/\partial\xi]\langle\uparrow\xi^*-\delta|\Psi(\alpha,\delta;t)\rangle$$
$$= -i\gamma\langle\downarrow\xi^*|\Psi(\alpha,\delta;t)\rangle\exp(\tfrac{1}{2}\delta^2-\delta\xi) \tag{2.9a}$$
$$[\partial/\partial t - i\Delta + i\Omega\xi\,\partial/\partial\xi]\langle\downarrow\xi^*|\Psi(\alpha,\delta;t)\rangle$$
$$= -i\gamma^*\langle\uparrow\xi^*-\delta|\Psi(\alpha,\delta;t)\rangle\exp(-\tfrac{1}{2}\delta^2+\delta\xi) \tag{2.9b}$$

with initial conditions corresponding to (2.6).

With regard to the formal solution of (2.1) and (2.2), i.e.

$$|\Psi(\alpha,\delta;t)\rangle = \exp(-iH(\alpha,\delta)t)|n\uparrow\rangle \tag{2.10}$$

the following notation is self-explanatory:

$$\begin{aligned}\langle\uparrow\downarrow\xi^*|\Psi(\alpha,\delta;t)\rangle &= G_{\uparrow\downarrow,n\uparrow}(\xi;\alpha,\delta;t)\\ \langle\uparrow\downarrow m|\Psi(\alpha,\delta;t)\rangle &= G_{\uparrow\downarrow m,n\uparrow}(\alpha,\delta;t).\end{aligned} \tag{2.11}$$

The Laplace transforms (with respect to the variable t) of $G_{\uparrow\downarrow,n\uparrow}$ and $G_{\uparrow\downarrow m,n\uparrow}$ are denoted by $g_{\uparrow\downarrow,n\uparrow}(\xi;\alpha,\delta;s)$ and $g_{\uparrow\downarrow m,n\uparrow}(\alpha,\delta;s)$, respectively. The initial value problem (2.9) is now cast into the form

$$[s+i\Delta+i\Omega(\xi-\delta)\partial/\partial\xi]g_{\uparrow,n\uparrow}(\xi-\delta;\alpha,\delta;s)$$
$$= -i\gamma g_{\downarrow,n\uparrow}(\xi;\alpha,\delta;s)\exp(\tfrac{1}{2}\delta^2-\delta\xi)+\langle\xi^*-\delta|n\rangle \tag{2.12a}$$
$$(s-i\Delta+i\Omega\xi\,\partial/\partial\xi)g_{\downarrow,n\uparrow}(\xi;\alpha,\delta;s) = -i\gamma^* g_{\uparrow,n\uparrow}(\xi-\delta;\alpha,\delta;s)\exp(-\tfrac{1}{2}\delta^2+\delta\xi). \tag{2.12b}$$

What about the integration constants in the variable ξ? To answer this question, one uses the fact that

$$g_{\uparrow\downarrow,n\uparrow}(\xi;\alpha,\delta;s) = \sum_{k=0}^{\infty}\frac{\xi^k}{\sqrt{k!}}\,g_{\uparrow\downarrow k,n\uparrow}(\alpha,\delta;s) \tag{2.13}$$

is an entire function in ξ. As is well known (Schweber 1967), this is a feature which holds quite generally: let, in $\langle\xi^*|f\rangle$, f be an arbitrary normalisable vector, then it is easily proved by means of standard convergence criteria that

$$|\langle\xi^*|f\rangle| \leqslant \|f\|\sum_{k=0}^{\infty}\frac{|\xi|^k}{\sqrt{k}} \qquad \|f\| = \langle f|f\rangle^{1/2} \tag{2.14}$$

has an infinite radius of convergence. The extension to vectors such as (2.10) is obvious. Therefore the solution of (2.12) has to lie in the space of entire functions; this fixes the integration constants because the solution vector (2.10) is unique. The inverse formulae to (2.13) are

$$g_{\uparrow m,n\uparrow}(\alpha,\delta;s) = \frac{1}{\sqrt{m!}}\frac{\partial^m}{\partial\xi^m}\,g_{\uparrow,n\uparrow}(\xi-\delta;\alpha,\delta;s)|_{\xi=\delta} \tag{2.15a}$$

$$g_{\downarrow m,n\uparrow}(\alpha,\delta;s) = \frac{1}{\sqrt{m!}}\frac{\partial^m}{\partial\xi^m}\,g_{\downarrow,n\uparrow}(\xi;\alpha,\delta;s)|_{\xi=0}. \tag{2.15b}$$

Similar equations hold also for the t-dependent expressions. These inverse formulae allow us to return to the $G_{\uparrow\downarrow m,n\uparrow}(\alpha,\delta;t)$ we were originally interested in.

To deal with the system (2.12), we eliminate (2.12a) and get

$$D(\xi,\partial/\partial\xi;\alpha,\delta;s)g_{\downarrow,n\uparrow}(\xi;\alpha,\delta;s) = -i\gamma^*\langle\xi^*|V(-\delta)|n\rangle \tag{2.16}$$

with the differential operator

$$D(\xi, \partial/\partial\xi; \alpha, \delta; s) = [s + i\Delta + i\Omega(\xi - \delta)(\partial/\partial\xi - \delta)][s - i\Delta + i\Omega\xi\,\partial/\partial\xi] + |\gamma|^2 \tag{2.17}$$

and the inhomogeneity

$$\langle\xi^*|V(-\delta)|n\rangle = \exp(-\tfrac{1}{2}\delta^2)\exp(\delta\xi)\langle\xi^* - \delta|n\rangle = \exp(-\tfrac{1}{2}\delta^2)(1/\sqrt{n!})(\xi - \delta)^n \exp(\delta\xi). \tag{2.18}$$

The 'spin-up' counterpart to (2.16), written as similarly to (2.16) as possible, is

$$\hat{D}(\xi, \partial/\partial\xi; \alpha, \delta; s) g_{\uparrow,n\uparrow}(\xi - \delta; \alpha, \delta; s)\exp(-\tfrac{1}{2}\delta^2 + \delta\xi)$$
$$= (s - i\Delta + i\Omega\xi\,\partial/\partial\xi)\langle\xi^*|V(-\delta)|n\rangle \tag{2.19}$$

where in $\hat{D}$ the two expressions in the square brackets of D are just interchanged. Of more practical interest is the form resulting from (2.4*b*):

$$-i\gamma^* G_{\uparrow m,n\uparrow}(\alpha, \delta; t) = \sum_k (\partial/\partial t - i\Delta + ik\Omega)\langle m|V(\delta)|k\rangle G_{\downarrow k,n\uparrow}(\alpha, \delta; t) \tag{2.20}$$

which connects both types of solutions and may be used once $G_{\downarrow k,n\uparrow}(\alpha, \delta; t)$ is known.

As we do not know of any analytical solution of (2.16) or (2.19) in general, we shall develop a step by step expansion in §§ 3 and 4. This expansion is a resolvent expansion (cf § 3.3); the tricky point is to find a zeroth-order solution as starting point which is optimal in some definite sense (cf §§ 3.1 and 4.1). After solving (2.16) and (2.19) by means of the expansion to some degree of accuracy, we have to transform back to the approximate $g_{\uparrow\downarrow m,n\uparrow}(\alpha, \delta; s)$ in a way corresponding to (2.15). Thus we conclude that we must also require approximate ('perturbative') solutions of (2.16) and (2.19) to lie in the space of entire functions.

3. Low-order approximations with restriction to the oscillator ground state as initial state

A most crucial point is to iterate (2.12) or its equivalents (2.16) and (2.19) in a satisfactory way. Of course, it is not sufficient to proceed from exactly solvable Hamiltonians belonging to decoupled spin-oscillator systems, i.e. from (1.3) with either $\delta = 0$ or $\gamma = 0$; each of the two possibilities simply proves too poor to be taken as a basis for a pertubation theoretical treatment. Rather we have to look for more sophisticated methods such as starting from an appropriate differential operator $D^{(0)}$, where we reject an interpretation of $D^{(0)}$ as stemming from an underlying Hamiltonian via a transcription of the Schrödinger equation into the Bargmann space of entire functions. As such an ansatz $D^{(0)}$ *may depend on the initial state*, we confine ourselves to the initial state $|0\uparrow\rangle$ in this section.

3.1. Solution in the zeroth-order approximation

The reasoning that led us to an optimal starting point $D^{(0)}$ consists of two parts.

(i) If the transformed system (1.3) decouples ($\delta = 0$ and/or $\gamma = 0$), the occupation number of the oscillator state cannot change in time. According to (2.15*a*), $g_{\uparrow,0\uparrow}(\xi; \alpha, \delta; s)$ cannot depend on ξ at all, because all $g_{\uparrow m,0\uparrow}(\alpha, \delta; s)$ with $m \neq 0$ have to vanish. Therefore the term containing $\partial/\partial\xi$ in (2.12*a*) can be dropped in the limiting cases of decoupling.

(ii) There is an indication that one may neglect the term containing $\partial/\partial\xi$ also in the case $\chi \neq 0$, $\delta \neq 0$. Let the initial state be arbitrary for the moment. One observes that (2.4*a*) and (2.4*b*), restricted to $m = 0$, are identical with (2.9*a*) and (2.9*b*), if one subsequently equates $\xi = \delta$ in both equations. These identities hold because

$$\langle\uparrow\xi^* - \delta|\Psi(\alpha, \delta; t)\rangle|_{\xi=\delta} = \langle\uparrow m|\Psi(\alpha, \delta; t)\rangle|_{m=0} \tag{3.1a}$$

$$\langle\downarrow\xi^*|\Psi(\alpha, \delta; t)\rangle|_{\xi=\delta} = \exp(\tfrac{1}{2}\delta^2)\langle\downarrow m|V(\delta)|\Psi(\alpha, \delta; t)\rangle|_{m=0} \tag{3.1b}$$

(the last equation is easily deduced from writing the first equality of (2.8) to the left of $V(\delta)|\Psi(\alpha, \delta; t)\rangle$). Hence it is tempting to set $\xi = \delta$ in (2.12*a*) or, equivalently, in the first bracket of (2.17) from the very beginning so that (2.16) could be easily solved. Of course this procedure is not quite correct because the order of the differential equation (2.16) is reduced and an integration constant gets lost. We hope, however, to deal with a case which is very robust with respect to approximations—at least for small times t—if the initial amplitude $G_{\uparrow 0,n\uparrow}(\alpha, \delta; 0)$ is maximal; this fixes n at $n = m = 0$ as in the preceding paragraph.

In this approximation (2.16)-(2.18) become

$$D_0^{(0)}(\xi, \partial/\partial\xi; \alpha; s)g_{\downarrow,0\uparrow}^{(0)}(\xi; \alpha, \delta; s) = -i\gamma^* \exp(-\tfrac{1}{2}\delta^2)\exp(\delta\xi) \tag{3.2}$$

with

$$D_0^{(0)}(\xi, \partial/\partial\xi; \alpha; s) = s^2 + \Delta^2 + |\gamma|^2 + (s + i\Delta)i\Omega\xi\,\partial/\partial\xi. \tag{3.3}$$

$D_0^{(0)}$ no longer depends on δ, its lower index characterises the initial state. Equation (3.2) with (3.3) is easily solved (the homogeneous solution is found by a temporary substitution $\xi \to \exp(\eta)$, $\xi\partial/\partial\xi \to \partial/\partial\eta$, whereas a particular solution is built by expanding both the solution and the inhomogeneity in powers of ξ). One gets

$$g_{\downarrow,0\uparrow}^{(0)}(\xi; \alpha, \delta; s) = C(\alpha, \delta; s)\xi^{-[(s^2+\Delta^2+|\gamma|^2)/i\Omega(s+i\Delta)]}$$

$$-i\gamma^* \exp(-\tfrac{1}{2}\delta^2)\sum_k \frac{\delta^k\xi^k}{k!}\frac{1}{d_{k,0}(\alpha; s)} \tag{3.4}$$

with

$$d_{k,0}(\alpha; s) = s^2 + \Delta^2 + |\gamma|^2 + (s + i\Delta)ik\Omega. \tag{3.5}$$

The homogeneous solution has in general a winding point in $\xi = 0$, hence contradicting our requirement of § 2 that the solution be an entire function. To ensure that the exponent of ξ be zero or a positive integer, the integration constant C has to behave like a δ function in the variable s. As this solution does not make sense as a Laplace transform, the homogeneous part has to be dropped.

Performing both limiting procedures, $\xi \to \delta$ according to (3.1*b*) as well as $\xi \to 0$ after differentiation according to (2.15*b*), and using

$$\langle 0|V(\delta)|k\rangle = \langle k|V(-\delta)|0\rangle = \exp(-\tfrac{1}{2}\delta^2)\delta^k/\sqrt{k!} \tag{3.6}$$

we are led to

$$\left[\sum_k \langle 0|V(\delta)|k\rangle g_{\downarrow k,0\uparrow}(\alpha, \delta; s)\right]^{(0)} = -i\gamma^* \sum_k \langle 0|V(\delta)|k\rangle\langle k|V(-\delta)|0\rangle \frac{1}{d_{k,0}(\alpha; s)} \tag{3.7}$$

and

$$g_{\downarrow k,0\uparrow}^{(0)}(\alpha, \delta; s) = -i\gamma^* \frac{\langle k|V(-\delta)|0\rangle}{d_{k,0}(\alpha; s)} \tag{3.8}$$

respectively. Hence by means of our function theoretical requirement we have introduced the correct linear dependence of the solution on the inhomogeneity, and (3.7)

has the correct linear dependence on the terms given by (3.8), i.e. the matrix elements of $V(\delta)$ in front of (3.7) are not affected by the approximation.

The zeros of $d_{k,0}(\alpha; s)$

$$\begin{aligned} s_{k,0,\pm}(\alpha) &= -ik(\Omega/2) \pm i q_{k,0}(\alpha) \\ q_{k,0}(\alpha) &= [(\Delta - k\Omega/2)^2 + |\gamma|^2]^{1/2} \end{aligned} \tag{3.9}$$

appear in the complex inversion formula of the Laplace transformation which applies as long as $g^{(\nu)}_{\uparrow\downarrow m,n\uparrow}(\alpha, \delta; s)$ is a rational function in s

$$G^{(\nu)}_{\uparrow\downarrow m,n\uparrow}(\alpha, \delta; t) = \sum \operatorname{res} \exp(st) g^{(\nu)}_{\uparrow\downarrow m,n\uparrow}(\alpha, \delta; s). \tag{3.10}$$

Equation (3.10) leads in zeroth-order approximation to

$$G^{(0)}_{\downarrow k,0\uparrow}(\alpha, \delta; t) = -i\gamma^* \langle k| V(-\delta)|0\rangle \exp[-ik(\Omega/2)t] \frac{\sin(q_{k,0}(\alpha)t)}{q_{k,0}(\alpha)}. \tag{3.11}$$

3.2. Interpretation of the zeroth-order solution (in the case $\Delta = 0$)

How good is solution (3.11)? In order to answer this question, we first note that (3.11) and its corresponding 'spin-up' solution fulfil both initial conditions (2.6) automatically (because (2.6) is treated exactly by the intermediary Laplace transformation, i.e. independently from the choice of $D_0^{(0)}$). It is easily shown in a second step that (2.20), taken for $n = 0$, also holds after replacing the terms G by $G^{(0)}$. Since this modification of equation (2.20) connects zeroth-order solutions with both kinds of initial conditions (2.6) by differentiating with respect to t, solution (3.11) must be exact in zeroth- *and first*-order in t. Actually, (3.11) is much better as is shown by a somewhat tedious expansion of both the exact solution (in powers of H) and (3.11) (in powers of t):

$$\begin{aligned} &\langle\downarrow k| \exp(-iH(\alpha, \delta)t)|0\uparrow\rangle - \langle\downarrow k| \exp(-iH(\alpha, \delta)t)|0\uparrow\rangle^{(0)} \\ &\quad = i(t^5/5!)|\gamma|^2\gamma^*\Omega^2\langle k| V(-\delta)|0\rangle(\delta^2 - k) + O(t^6). \end{aligned} \tag{3.12}$$

Thus (3.11) represents an excellent approximation, better than by means of an exactly solvable Hamiltonian (note that this characterisation only counts the order in t up to which the approximation is exact; determining the (maximal) time beyond which the infinite-series solution in t becomes questionable is a somewhat different problem requiring explicit knowledge of the parameters α, δ and will be dealt with in § 4.4).

Let us elucidate (3.12) in detail. It is appropriate to introduce the abbreviations

$$H = \underbrace{2\Delta\sigma_z}_{A} + \underbrace{\Omega b^+ b}_{B} + \underbrace{\gamma\sigma_+ V(\delta)}_{C_+} + \underbrace{\gamma^*\sigma_- V(-\delta)}_{C_-}. \tag{3.13}$$

For the following it is important that B commutes with C_+C_- and C_-C_+. Furthermore, because of the algebra of the operators σ_+ and σ_-, in non-vanishing matrix elements $\langle\downarrow| \ldots |\uparrow\rangle$, the total number of operators C has to be odd, their sequence being alternating

$$\ldots C_- \ldots C_+ \ldots C_- \ldots C_+ \ldots C_- \ldots \tag{3.14}$$

with C_- on the outsides. Now we write down in 'alphabetical order' all permutations of operators stemming from H^5 and going with $\gamma^*|\gamma|^2\Omega^2$, under the restriction (3.14)

$$\begin{aligned} &\underline{BBC_-C_+C_-} + \underline{BC_-BC_+C_-} + \underline{BC_-C_+BC_-} + \underline{BC_-C_+C_-B} \\ &\quad + \underline{C_-BBC_+C_-} + C_-BC_+BC_- + \underline{C_-BC_+C_-B} \\ &\quad + \underline{C_-C_+BBC_-} + \underline{C_-C_+BC_-B} + \underline{C_-C_+C_-BB}. \end{aligned} \tag{3.15}$$

The terms with broken underlines vanish (the B act either directly or through the operator pair C_+C_- on the ground state on the right); the fully underlined terms (the B act either directly or through the pair C_-C_+ to the left) prove as reproduced by expanding (3.11) to fifth order in t; the only term not reproduced by expanding (3.11) is that where the commutators $[B, C_+]$ and $[B, C_-]$ (which introduce the parameter δ) would be needed for the evaluation.

It is worth noting that the expression $\langle\downarrow 0|V(\delta)\exp(-\mathrm{i}Ht)|0\uparrow\rangle^{(0)}$, whose exact form $\langle\downarrow 0|V(\delta)|\exp(-\mathrm{i}Ht)|0\uparrow\rangle$ was one of our starting points in this section (cf (3.1*b*)), is even exact up to the *fifth* order in t. This is easily explained by applying $\langle 0|C_+$ to (3.15) or $\Sigma\langle 0|V(\delta)|k\rangle$ to (3.12) (in the latter case use (3.6) and collect terms in powers of δ).

One may wonder whether an interpretation of (3.11) as a partial sum of the kind described above for the fifth order in t holds for all powers of t up to infinite order. For the special case $\Delta = 0$ (i.e. the operator Δ does not occur) such a guess reduces to a rather simple but enlightening combinatorial problem.

Theorem. At each order in t solution (3.11) (in the case $\Delta = 0$) results from the corresponding exact expression by keeping, from the complete expansion of the latter in operator sequences, only such sequences where the B act through (repetitions of) pairs C_-C_+ to the left.

Sketch of the proof. From the series expansion of (3.11)

$$\exp(-\tfrac{1}{2}\mathrm{i}k\Omega t)\frac{\sin(qt)}{t} = \sum_{l=0}^{\infty}\frac{1}{l!}(-\tfrac{1}{2}\mathrm{i}k\Omega)^l t^l \times\left(t-\frac{1}{3!}q^2t^3+\frac{1}{5!}q^4t^5\mp\ldots\right) \qquad q = q_{k,0}(\alpha) \tag{3.16}$$

we pick out the terms of Nth order in t and (assuming the theorem to be true) equate their sum with the value which results from that subclass of operator sequences in the exact solution where an operator C_- appears on the right of H^N and a permutation with repetition of the operators B and C_-C_+ on its left. By equating in any power of, say, C_-C_+ (the power of B is then given) we are left with the following relation which has to be checked:

$$\sum_{\nu=0}^{[M/2]}\binom{M+1}{2\nu+1}\binom{\nu}{\mu} = 2^{M-2\mu}\binom{M-\mu}{\mu} \qquad \mu = 0,\ldots,[M/2]. \tag{3.17}$$

$M+1$ is the (even or odd) order in t, μ the order in C_-C_+, $[M/2]$ represents the nearest integer less than or equal to $M/2$. As (3.17) proves to be true, the theorem is proven, too.

We have the feeling that this combinatorial analysis could as well be extended to the case $\Delta \neq 0$; a still more extended procedure might be a promising method to deal even with the complicated operator algebra occurring in higher-order members of the resolvent expansion.

In any case, our present examination shows very nicely how in (3.11) the higher-order terms in t still try to 'simulate' the exact values. Let us now look for a first improvement (which affects all higher-order terms in t simultaneously).

3.3. First-order correction

We define the difference between the exact differential operator D (2.17) and the approximate operator $D^{(0)}$ (3.3) as a 'perturbation' $D_0^{(s)}$

$$D_0^{(s)}(\xi, \partial/\partial\xi; \alpha, \delta; s) = i\Omega(\xi - \delta)(\partial/\partial\xi - \delta)(s - i\Delta + i\Omega\xi\partial/\partial\xi). \tag{3.18}$$

Our iterative procedure for constructing the exact solution $g = g^{(0)} + g^{(1)} + \ldots$ is formally described by casting (2.16) into the form

$$[D^{(0)} + D^{(s)}][g^{(0)} + g^{(1)} + \ldots] = \text{inhomogeneous} \tag{3.19}$$

and solving it by the scheme

$$D^{(0)} g^{(0)} = \text{inhomogeneous} \tag{3.20a}$$

$$D^{(0)} g^{(\nu)} = -D^{(s)} g^{(0)} \qquad \nu = 1, 2, \ldots \tag{3.20b}$$

where the only solutions admitted are those which are entire functions in ξ. This approach is equivalent to a resolvent expansion of the operator D

$$\frac{1}{D^{(0)} + D^{(s)}} = \frac{1}{D^{(0)}} - \frac{1}{D^{(0)}} D^{(s)} \frac{1}{D^{(0)}} \pm \ldots. \tag{3.21}$$

With the aid of

$$D_0^{(s)}(\xi, \partial/\partial\xi; \alpha, \delta; s)\xi^k = i\Omega(s - i\Delta + i\Omega k)[(\delta^2 + k)\xi^k - \delta\xi^{k+1} - \delta k\xi^{k-1}] \tag{3.22}$$

we derive the first-order correction from (3.20b) with $\nu = 1$:

$$g^{(1)}_{\downarrow,0\uparrow}(\xi; \alpha, \delta; s) = -\gamma^* \Omega \exp(-\tfrac{1}{2}\delta^2) \sum_k \frac{\delta^k}{k!} \left((\delta^2 + k) \frac{\xi^k}{d_{k,0}(\alpha; s)} - \delta \frac{\xi^{k+1}}{d_{k+1,0}(\alpha; s)} - \delta k \frac{\xi^{k-1}}{d_{k-1,0}(\alpha; s)} \right) \frac{s - i\Delta + i\Omega k}{d_{k,0}(\alpha; s)} \tag{3.23}$$

based on $g^{(0)}$ (equation (3.4) with $C = 0$). Now we use the identity following from (3.5)

$$\frac{s - i\Delta + i\Omega k}{d_{k,0}(\alpha; s)} = \frac{1}{s + i\Delta} \left(1 - \frac{|\gamma|^2}{d_{k,0}(\alpha; s)} \right) \tag{3.24}$$

where the term 1 can be dropped because it does not contribute to the sum in (3.23) as is easily seen after collecting the terms under the sum in common powers of ξ (by renaming the summation indices). After (2.15b) is performed, the final result is

$$g^{(1)}_{\downarrow k,0\uparrow}(\alpha, \delta; t) = |\gamma|^2 \gamma^* \Omega \langle k | V(-\delta) | 0 \rangle \times \sum \text{res} \frac{\exp(ts)}{(s + i\Delta) d_{k,0}(\alpha; s)} \times \left(\frac{\delta^2 + k}{d_{k,0}(\alpha; s)} - \frac{\delta^2}{d_{k+1,0}(\alpha; s)} - \frac{k}{d_{k-1,0}(\alpha; s)} \right). \tag{3.25}$$

We leave the explicit evaluation to § 4.3 (cf equation (4.24) for $n = 0$) in a more general context. In appendix 1 we list a collection of powerful sum rules on residues of rational functions we have derived by mathematical induction. Those rules prove to be an adequate tool for examining expressions such as (3.25) in powers of t. By expanding $\exp(ts)$ in a Taylor series in t, (A1.2a) states that (3.25) vanishes up to third order in t (one has to identify the s_i with $-i\Delta$ and the zeros given by (3.9)).

Using (A1.2*b*) one sees that the numerators in the brackets of (3.25) cancel exactly; the first non-vanishing expression is that given by (3.12) which is exactly reproduced by (A1.2*c*). As we shall see in § 4.1, the terms up to the fifth order in t are not affected within a higher-order resolvent expansion ($\nu > 1$) so that our results of § 3.2 are completely confirmed.

Finally, the reader is warned of taking (3.25) too literally since later on we shall apply a slight modification which acts on terms in t of sixth order and above (cf § 4.2). We are now sufficiently prepared to attack the general case of arbitrary initial states.

4. Series expansion for arbitrary initial states

This section comprises a generalisation of the results of the previous section in that ansatz (3.3) is extended to arbitrary initial states. In § 4.1 our main results in each order of correction are presented. They are slightly modified in § 4.2 in order to impose the correct symmetry behaviour under time reversal. In § 4.3 the inverse Laplace transformation is explicitly performed with regard to the first and second order of the resolvent expansion; brief instructions are given on how to deal with higher orders, combining symbolic and numerical procedures in a computer-aided calculation. In § 4.4 exactly solvable limiting cases in the parameter space are listed; a method for estimating the range of validity in time for arbitrary parameters is given. Section 4.5 is reserved for the difficult problem of convergence of the present resolvent expansion.

4.1. Resolvent expansion to arbitrary order

Partly using arguments about the decoupled spin-oscillator system as in § 3.1 and partly using symmetry arguments with regard to time reversal, we are led to the ansatz

$$D_n^{(0)}(\xi, \partial/\partial\xi; \alpha; s) = (s - \mathrm{i}\Delta + \mathrm{i}\Omega\xi\partial/\partial\xi)(s + \mathrm{i}\Delta + \mathrm{i}\Omega n) + |\gamma|^2 \tag{4.1}$$

where n characterises the initial state. The zeroth-order equation corresponding to (3.2) is

$$D_n^{(0)}(\xi, \partial/\partial\xi; \alpha; s) g_{\downarrow,n\uparrow}^{(0)}(\xi; \alpha, \delta; s) = -\mathrm{i}\gamma^* \sum_k \frac{\xi^k}{\sqrt{k!}} f_{k,n}(\delta). \tag{4.2}$$

Here we have introduced a new notation for the matrix elements of the operator $V(\delta)$ as explained in appendix 2. From

$$D_n^{(0)}(\xi, \partial/\partial\xi; \alpha; s)\xi^k = d_{k,n}(\alpha; s)\xi^k \tag{4.3}$$

with

$$d_{k,n}(\alpha; s) = (s - \mathrm{i}\Delta + \mathrm{i}\Omega k)(s + \mathrm{i}\Delta + \mathrm{i}\Omega n) + |\gamma|^2 \tag{4.4}$$

we obtain

$$g_{\downarrow,n\uparrow}^{(0)}(\xi; \alpha, \delta; s) = -\mathrm{i}\gamma^* \sum_k \frac{\xi^k}{\sqrt{k!}} \frac{f_{k,n}(\delta)}{d_{k,n}(\alpha; s)} \tag{4.5}$$

and

$$G_{\downarrow k,n\uparrow}^{(0)}(\alpha, \delta; t) = -\mathrm{i}\gamma^* f_{k,n}(\delta) \exp[-\tfrac{1}{2}\mathrm{i}(k+n)\Omega t] \frac{\sin(q_{k,n}(\alpha)t)}{q_{k,n}(\alpha)} \tag{4.6}$$

with the definitions

$$q_{k,n}(\alpha)=(p_{k,n}^2(\alpha)+|\gamma|^2)^{1/2} \qquad p_{k,n}(\alpha)=\Delta-\tfrac{1}{2}(k-n)\Omega. \tag{4.7}$$

Equations (4.4), (4.5) and (4.6) are generalisations of (3.5), (3.4) and (3.11), respectively. We stress an important characteristic of $d_{k,n}(\alpha; s)$ in (4.5) which ensures that (4.6) has the correct symmetry with regard to time reversal: $d_{k,n}(\alpha; s)$ is of a form which leaves the solution (4.6) unchanged under the simultaneous replacements $k\leftrightarrow n$, $\Delta\leftrightarrow-\Delta$, $\delta\leftrightarrow-\delta$. Such an invariance is a general property of the *exact* solution evolving under the Hermitian Hamiltonian $H(\alpha, \delta)$.

We comment that we failed in generalising the theorem of § 3.2 into an expansion in t of (4.6). In detail, we tried to keep (in the corresponding exact expressions) only those sequences of operators (cf § 3.2) where the B act either through the pairs C_-C_+ to the left, or through the pairs C_+C_- to the right. However, we got incorrect weight factors in front of general powers of k and n so that (4.6), taken to some order in t, was not reproduced.

Now we turn to the first-order correction. The difference between the exact differential operator (2.17) and $D_n^{(0)}$ (4.1), i.e. $D_n^{(s)}=D-D_n^{(0)}$, acts on ξ^k as follows:

$$D_n^{(s)}(\xi, \partial/\partial\xi; \alpha, \delta; s)\xi^k=\mathrm{i}\Omega(s-\mathrm{i}\Delta+\mathrm{i}\Omega k)[(\delta^2+k-n)\xi^k-\delta\xi^{k+1}-\delta k\xi^{k-1}]. \tag{4.8}$$

The solution of (3.20*b*) ($\nu=1$) based on (4.5) is

$$g_{\downarrow,n\uparrow}^{(1)}(\xi; \alpha, \delta; s)=-\gamma^*\Omega\sum_k\frac{f_{k,n}(\delta)}{\sqrt{k!}} \times\left((\delta^2+k-n)\frac{\xi^k}{d_{k,n}(\alpha; s)}-\delta\frac{\xi^{k+1}}{d_{k+1,n}(\alpha; s)}-\delta k\frac{\xi^{k-1}}{d_{k-1,n}(\alpha; s)}\right)\frac{s-\mathrm{i}\Delta+\mathrm{i}\Omega k}{d_{k,n}(\alpha; s)}. \tag{4.9}$$

We now relabel the summation indices in such a way that the same power ξ^k appears in each of the three numerators in the brackets, and use

$$\frac{s-\mathrm{i}\Delta+\mathrm{i}\Omega k}{d_{k,n}(\alpha; s)}=\frac{1}{s+\mathrm{i}\Delta+\mathrm{i}\Omega n}\left(1-\frac{|\gamma|^2}{d_{k,n}(\alpha; s)}\right). \tag{4.10}$$

Again as in (3.24) the term 1 can be dropped, but now on account of (A2.4), thus revealing an intimate interplay between our n-dependent ansatz (4.1) and a set of recurrence relations involving Laguerre polynomials with a common lower index n. The result is

$$G_{\downarrow k,n\uparrow}^{(1)}(\alpha, \delta; t)=|\gamma|^2\gamma^*\Omega\sum\operatorname{res}\frac{\exp(ts)}{(s+\mathrm{i}\Delta+\mathrm{i}\Omega n)d_{k,n}(\alpha; s)} \times\left((\delta^2+k-n)\frac{f_{k,n}(\delta)}{d_{k,n}(\alpha; s)}-\delta\sqrt{k}\,\frac{f_{k-1,n}(\delta)}{d_{k-1,n}(\alpha; s)}-\delta\sqrt{k+1}\,\frac{f_{k+1,n}(\delta)}{d_{k+1,n}(\alpha; s)}\right). \tag{4.11}$$

The same procedure is repeated in all higher-order corrections, the only difference being that the intermediate step of employing (4.10) and dropping the term 1 no longer applies. Since the other intermediate step, i.e. relabelling the summation indices, is sufficiently easy to handle, the calculus can be done rather explicitly. After defining the coefficients

$$C_{k,n}^{[0]}=\delta^2+k-n, \qquad C_{k,n}^{[-1]}=-\sqrt{k}\delta \qquad C_{k,A}^{[1]}=-\sqrt{k+1}\delta \tag{4.12}$$

(4.11) is transcribed into

$$G^{(1)}_{\downarrow k,n\uparrow}(\alpha,\delta;t)=|\gamma|^2\gamma^*\Omega\sum \operatorname{res}\frac{\exp(ts)}{(s+i\Delta+i\Omega n)d_{k,n}(\alpha;s)}\sum_{l=-1}^{1}C^{[l]}_{k,n}\frac{f_{k+l,n}(\delta)}{d_{k+l,n}(\alpha;s)} \tag{4.13}$$

which serves as the basis for the higher members of the series

$$\begin{aligned}G^{(\nu)}_{\downarrow k,n\uparrow}(\alpha,\delta;t)=i|\gamma|^2\gamma^*(-i\Omega)^{\nu}\sum \operatorname{res}&\frac{\exp(ts)}{(s+i\Delta+i\Omega n)d_{k,n}(\alpha;s)}\\ &\times\sum_{l_1=-1}^{1}C^{[l_1]}_{k,n}\frac{s-i\Delta+i\Omega(k+l_1)}{d_{k+l_1,n}(\alpha;s)}\times\ldots\\ &\times\sum_{l_{\nu-1}=-1}^{1}C^{[l_{\nu-1}]}_{k+l_1+\ldots+l_{\nu-2},n}\frac{s-i\Delta+i\Omega(k+l_1+\ldots+l_{\nu-1})}{d_{k+l_1+\ldots+l_{\nu-1},n}(\alpha;s)}\\ &\times\sum_{l_\nu=-1}^{1}C^{[l_\nu]}_{k+l_1+\ldots+l_{\nu-1},n}\frac{f_{k+l_1+\ldots+l_\nu,n}(\delta)}{d_{k+l_1+\ldots+l_\nu,n}(\alpha;s)}\\ &\nu=2,3,\ldots.\end{aligned} \tag{4.14}$$

Note that at each step of increasing the accuracy (i.e. $\nu\to\nu+1$) the number of terms is tripled on account of (4.8).

As for the iteration of the 'spin-up' solution (with the zeroth-order operator $s+i\Delta+i\Omega n$ on the left of (2.12a) and (2.12b) left unchanged), we proved an equation resembling (2.20)

$$G^{(\nu)}_{\uparrow m,n\uparrow}(\alpha,\delta;t)=-\frac{1}{i\gamma^*}\sum_k(\partial/\partial t-i\Delta+ik\Omega)f_{m,k}(-\delta)G^{(\nu)}_{\downarrow k,n\uparrow}(\alpha,\delta;t). \tag{4.15}$$

Formulae (4.14) and (4.15) jointly with (4.4) and (A2.2) represent quite general results for the time behaviour of the transition probability amplitudes, calculated in any order of correction; hence the evolution of the system is completely described. Because of (A1.2a), (A1.2b) and (A2.4), the corrections $G^{(\nu)}_{\downarrow k,n\uparrow}(\alpha,\delta;t)$ ($\nu\geqslant 1$) vanish up to the $(3+\nu)$th power in t, i.e. they are exact up to the $(4+\nu)$th power. The 'spin-up' terms in comparison with the former 'spin-down' terms are exact to one less order due to differentiating once with respect to t in (4.15).

Partly in anticipation of the intention of the next section, we now give some particular results. Starting from the generalisation of (3.12)

$$\begin{aligned}\langle\downarrow k|\exp(-iH(\alpha,\delta)t)|n\uparrow\rangle^{(1)}=&-i(t^5/5!)|\gamma|^2\gamma^*\Omega^2\delta[\sqrt{k}f_{k-1,n}(\delta)\\ &-\sqrt{k+1}f_{k+1,n}(\delta)]+O(t^6)\end{aligned} \tag{4.16}$$

(found by applying (A1.2c) on (4.11)), one proves for the form *symmetrised* in the initial and final oscillator states

$$\langle\downarrow m|V(\delta)\exp(-iH(\alpha,\delta)t)|n\uparrow\rangle^{(1)}+m\leftrightarrow n=O(t^6). \tag{4.17}$$

For the proof that (4.17) cancels in fifth order one has simply to insert a complete set of intermediate states on the right of $V(\delta)$. It is easily deduced from (4.17) that

$$\langle\downarrow\Phi|V(\delta)\exp(-iH(\alpha,\delta)t)|\Phi\uparrow\rangle^{(1)}=O(t^6) \tag{4.18}$$

holds for any *real* linear combination $|\Phi\rangle$ in terms of states $|n\rangle$. Equation (4.18), being in agreement with a statement on $\langle\downarrow 0|V(\delta)\exp(-iHt)|0\uparrow\rangle^{(0)}$ in § 3.2, demonstrates that the quality of our approach is even improved for particular state vectors.

4.2. Symmetrisation in initial and final states: time evolution of the original (untransformed) system

By inspection of the 'spin-up' counterpart to (4.6) which follows from (4.15)

$$G^{(0)}_{\uparrow m,n\uparrow}(\alpha,\delta;t)=\sum_k f_{m,k}(-\delta)f_{k,n}(\delta)\exp[-\tfrac{1}{2}\mathrm{i}(k+n)\Omega t]$$
$$\times\left(\cos(q_{k,n}(\alpha)t)-\mathrm{i}p_{k,n}(\alpha)\frac{\sin(q_{k,n}(\alpha)t)}{q_{k,n}(\alpha)}\right) \tag{4.19}$$

(cf definitions (4.7) for $q_{k,n}$ and $p_{k,n}$) one concludes that in general the expressions $G^{(\nu)}$ may lack the correct symmetry behaviour under time reversal (or, in the example under consideration, with respect to simply interchanging initial and final states). This happens because we have treated the evolution of the system from the very beginning in an unsymmetrical fashion by shifting operations (e.g. those in (2.8)) only to the left. Of course, the total sum of contributions to a given power of t behaves *a priori* correctly under time reversal. Consider a 'spin-down' example: as (4.6) has the correct invariance described below (4.7) in all powers of t, the only correction in the fifth power of t, i.e. (4.16), must also reveal this invariance, which is indeed the case on account of (A2.5). Hoping to get better results quite generally at any level of approximation, we shall now impose the correct symmetry behaviour on the corrections $G^{(\nu)}$.

The problem of installing the correct symmetry properties on the matrix elements $G^{(\nu)}_{\uparrow\downarrow m,n\uparrow}$ evolving under the (Hermitian) Hamiltonian $H(\alpha,\delta)$ is easily overcome by choosing suitable linear combinations $G^{[\nu]}_{\uparrow\downarrow m,n\uparrow}$ consisting of two matrix elements $G^{(\nu)}_{\uparrow\downarrow m,n\uparrow}$ of the same order ν where m and n are interchanged and some signs of the system parameters may be changed. Subsequently, at any order ν of the expansion (3.20), the terms $G^{(\nu)}$ have to be replaced by the new combinations $G^{[\nu]}$. That is, we replace at any order ν of the expansion (3.20) those terms which are denoted by an upper index $^{(\nu)}$ by terms with an upper index $^{[\nu]}$. Our final results are

$$G^{[\nu]}_{\downarrow m,n\uparrow}(\alpha,\delta;t)=\tfrac{1}{2}[G^{(\nu)}_{\downarrow m,n\uparrow}(\alpha,\delta;t)+G^{(\nu)}_{\downarrow n,m\uparrow}(\bar\alpha,-\delta;t)] \qquad \bar\alpha=\{-\Delta,\Omega,\gamma,\gamma^*\} \tag{4.20}$$

$$\langle\downarrow m|\exp(-\mathrm{i}H_{\mathrm{orig}}t)|n\uparrow\rangle^{[\nu]}\exp(\mathrm{i}E_{\mathrm{s}}t)$$
$$=\sum_{m'}\sum_{n'}f_{m,m'}(-\tfrac{1}{2}\delta)G^{[\nu]}_{\downarrow m',n'\uparrow}(\alpha,\delta;t)f_{n',n}(-\tfrac{1}{2}\delta) \tag{4.20'}$$

$$G^{[\nu]}_{\uparrow m,n\uparrow}(\alpha,\delta;t)=\tfrac{1}{2}[G^{(\nu)}_{\uparrow m,n\uparrow}(\alpha,\delta;t)+G^{(\nu)}_{\uparrow n,m\uparrow}(\alpha,\delta;t)] \tag{4.21}$$

$$\langle\uparrow m|\exp(-\mathrm{i}H_{\mathrm{orig}}t)|n\uparrow\rangle^{[\nu]}\exp(\mathrm{i}E_{\mathrm{s}}t)$$
$$=\sum_{m'}\sum_{n'}f_{m,m'}(\tfrac{1}{2}\delta)G^{[\nu]}_{\uparrow m',n'\uparrow}(\alpha,\delta;t)f_{n',n}(-\tfrac{1}{2}\delta)$$
$$=-\frac{1}{2\mathrm{i}\gamma^*}\sum_k\left(\frac{\partial}{\partial t}-\mathrm{i}\Delta+\mathrm{i}k\Omega\right)$$
$$\times\sum_l[f_{m,k}(-\tfrac{1}{2}\delta)G^{(\nu)}_{\downarrow k,l\uparrow}(\alpha,\delta;t)f_{l,n}(-\tfrac{1}{2}\delta)+m\leftrightarrow n]. \tag{4.21'}$$

In (4.20') and (4.21') we have reintroduced the original Hamiltonian (1.1) by inverting the unitary transformation (1.2) thus connecting with our original problem (E_{s} is the energy shift defined jointly with (1.3)). The transition probability amplitudes of the transformed system are given by (4.14) and (4.15). For practical purposes, examination of these two latter equations may suffice in most cases.

We note that by means of (4.17) $G^{[1]}_{\uparrow m,n\uparrow}(\alpha, \delta; t)$ is better than $G^{(1)}_{\uparrow m,n\uparrow}(\alpha, \delta; t)$ by one order in t so that $G^{[0]}_{\uparrow m,n\uparrow}(\alpha, \delta; t)$ is correct up to the fourth power of t (just like the corresponding 'spin-down' term). This fact strongly assures that *symmetrisation indeed improves our expansion.* Equation (4.18) holds as well under replacing H by H_{orig}.

4.3. *Evaluation of the residues*

In our general formula (4.14), we have still to evaluate the residues stemming from inverting the Laplace transformation originally introduced in (2.12). Clearly, if in (4.14) the k indices in multiple products of the $d_{k,n}$ become identical, multiple poles arise whose residues can be evaluated by a standard formula of function theory which serves for calculating the residuum of an analytical function $F(s)$ in a pole s_0 of mth order:

$$\operatorname{res} F(s)|_{s=s_0} = \frac{1}{(m-1)!} \frac{\mathrm{d}^{m-1}}{\mathrm{d}s^{m-1}} [F(s)(s-s_0)^m]|_{s=s_0}. \tag{4.22}$$

In using (4.22), one has to be sure that there are no other (overlooked) degeneracies which would lead to divergences (which could be balanced only by additional limiting procedures). Now an explicit investigation of the positions of the poles yields the most pleasing result that there are no other degeneracies (besides those originating from identical k indices) except in cases which comprise pathological values of the oscillator state numbers and system parameters, i.e. $\Omega \to 0$, $|k-n| \to \infty$, $\gamma \to 0$ and $|\gamma| \to \infty$. An accidental degeneracy in the sense of crossing poles induced by smoothly turning the parameters can never occur.

Now we are able to make use of (4.22) for the explicit evaluation of the two lowest-order corrections of (4.6). As can be easily shown, the total sum of residues stemming from the pole $(s+\mathrm{i}\Delta+\mathrm{i}\Omega n)^{-1}$ vanishes in (4.14) for arbitrary ν as a consequence of (A2.4) so that the evaluation is simplified. For the purpose of a convenient representation we define

$$\begin{aligned} u_{k,n,\pm}(\alpha) &= v_{k,n,\pm}(\alpha) - (\Delta + n\Omega) \\ v_{k,n,\pm}(\alpha) &= p_{k,n}(\alpha) \pm q_{k,n}(\alpha) \end{aligned} \tag{4.23}$$

where the u are the imaginary parts of the zeros of (4.4) and abbreviations (4.7) are used. Then the first-order correction is

$$\begin{aligned} G^{(1)}_{\downarrow k,n\uparrow}(\alpha, \delta; t) = |\gamma|^2 \gamma^* \Omega \Bigg[& -\frac{(\delta^2 + k - n) f_{k,n}(\delta)}{4|\gamma|^2 q^2_{k,n}(\alpha)} \sum_{\pm} \exp(\mathrm{i} u_{k,n,\pm}(\alpha) t) \\ & \times \left(\mathrm{i}t + \frac{v_{k,n,\pm}(\alpha)}{|\gamma|^2} \mp \frac{1}{q_{k,n}(\alpha)} \right) v_{k,n,\mp}(\alpha) \\ & + \frac{\delta \sqrt{k} f_{k-1,n}(\delta)}{2|\gamma|^4 \Omega} \sum_{l=0,1} (-1)^l \sum_{\pm} \exp(\mathrm{i} u_{k-l,n,\pm}(\alpha) t) \frac{\pm v^2_{k-l,n,\mp}(\alpha)}{q_{k-l,n}(\alpha)} \\ & - \frac{\delta \sqrt{k+1} f_{k+1,n}(\delta)}{2|\gamma|^4 \Omega} \sum_{l=0,1} (-1)^l \sum_{\pm} \exp(\mathrm{i} u_{k+l,n,\pm}(\alpha) t) \frac{\pm v^2_{k+l,n,\mp}(\alpha)}{q_{k+l,n}(\alpha)} \Bigg]. \end{aligned} \tag{4.24}$$

The next higher correction is given in appendix 3. From definitions (4.23) we read off

that each term in (4.24) and (A3.2) has its counterpart where the roots q (4.7) are replaced by their negative values so that in all non-vanishing higher-order terms in t (starting from the fifth order as discussed in § 4.1) only *integral* powers of the system parameters result.

We point out that (4.24) and (A3.1) are of great practical use as they enable the time evolution of the transition probabilities to be plotted as a function of the five system parameters, in this connection not only making (4.6) exact up to the sixth order in t, but also correcting (4.6) up to infinite order in t to an extent which depends on the actual parameter values α and δ (as will be elucidated in the next section).

A point of interest is the *numerical stability* of equations (4.24) and (A3.1) (for instance, if one wishes to plot them with the aid of a computer). One easily recognises that the numerical stability in the sum over all residues is weakened if two or more poles approach each other. Thus from the foregoing discussion in this section concerning the degeneracies we conclude that the numerical accuracy is not reduced as long as one keeps oneself far enough from the pathological cases mentioned above.

In this context, the following should be remarked with regard to the algebraic form of (4.24) and (A3.1). In order to increase the numerical accuracy in these equations for small γ, we have replaced $(v_{k,n,-})^{-1}$ (cf equation (4.23)) by its algebraic equivalent $(-v_{k,n,+})/|\gamma|^2$ in all contributions proportional to positive powers of $(v_{k,n,-})^{-1}$. The reason for this replacement is that for small γ values $v_{k,n,-}$ is the difference of two almost equal terms which apparently leads to a loss of accuracy in precisely those terms which contribute considerably to the total result.

Because of the rather lengthy form of (A3.2) it seems impossible to treat higher corrections in an analytical way. There is, however, the possibility of a computer-aided calculation. It would be desirable that a program written for this purpose would deal with higher derivatives with respect to s in a *symbolic* way; fortunately, only elementary functions in s (whose derivatives stay in the frame of the same functions) are involved in (4.14). In detail, such a program had for fixed $l_1, \ldots, l_\nu$ to identify the multiplicity of the appearing poles, to evaluate their residues by (4.22), and to add them up; subsequently the summation on the $l_1, \ldots, l_\nu$ had to be executed.

4.4. Limiting cases in the parameter space: estimation of the range of validity in time

Let us discuss the transformed system (1.3) for simplicity. Without loss of generality we may set $\Omega = 1$ (i.e. we measure the time t with Ω as unit).

According to our detailed discussion at the beginning of § 3.1, the approaches (3.3) and (4.1) contain the fact that the cases $\delta \to 0$ and/or $\gamma \to 0$ are exactly solved already in the zeroth-order approximation, i.e. by (4.6) and (4.19) (symmetrisation according to § 4.2 is superfluous). In detail, for $\delta \to 0$ the well known Rabi solution (Rabi 1937) for a two-level system is obtained with $f_{k,n}(0) = \delta_{k,n}$, $q_{k,n}(\alpha) = q_{\mathrm{Rabi}}(\alpha) = (\Delta^2 + |\gamma|^2)^{1/2}$. In the case $\gamma \to 0$, the system remains in its initial state apart from a time dependent phase factor which clearly solves (2.4*a*).

However, there are still other limits which are also solved in zeroth-order approximation, namely $|\gamma| \to \infty$, Δ/γ zero or finite ($q_{k,n}(\alpha)$ is replaced by $q_{\mathrm{Rabi}}(\alpha)$ which gives rise to rapid oscillations) and $\delta \to \infty$ and/or $\Delta \to \infty$ (the system remains in its initial state).

For arbitrary parameters, one has to estimate an upper bound T of the time interval $0 < t < T$ in which a (symmetrised) approximation of order ν, $\tilde{G}^{[\nu]}$ $(= G^{[0]} + \ldots + G^{[\nu]})$, does not deviate too much from the exact transition probability amplitude. For this aim, we propose to check simply how well the conservation of the norm for the total

transition probability, say, in the approximate form

$$\sum_{k=0}^{\infty} |\tilde{G}^{[\nu]}_{\downarrow k,n\uparrow}(\alpha, \delta; t)|^2 + \sum_{k=0}^{\infty} |\tilde{G}^{[\nu]}_{\uparrow k,n\uparrow}(\alpha, \delta; t)|^2 \approx 1 \tag{4.25}$$

is fulfilled within the interval; the two terms on the left are the conditional probabilities of finding the spin in the lower and upper state if the system was in the state $|n\uparrow\rangle$ at $t=0$. The difference of these two terms is of particular physical interest because it approximates the expectation value of $-2\sigma_z(t)$ in νth order.

In all limiting cases listed above, the sign of equality holds in (4.25), and T goes to infinity. We note that in these cases quite simple tests of consistency are available: one can check whether the higher-order corrections tend to zero. In doing so, we obtain that not only the first correction (4.11) itself vanishes but also the sum over k of the squared moduli of (4.11) (whether symmetrised or not). For instance, in the case $\delta \to \infty$, only the infinite tail from some large k_0 can contribute to the latter sum because of the k dependence of $f_{k,n}(\delta)$; but then, because of the smoothness of the denominator $d_{k,n}(\alpha; s)$ in (4.11) as a function of k, equation (A2.4) applies so that no contribution to the sum remains at all. These considerations can be extended to higher corrections whether of the first or second term in (4.25).

4.5. The question of convergence

Finally, let us turn to the question of whether the solution $G_{\downarrow k,n\uparrow}(\alpha, \delta; t)$ written as an infinite series $G = G^{(0)} + G^{(1)} + \ldots$ in terms of (4.14) has to be interpreted as an asymptotic solution rather than the equality still being strictly exact. Our feeling is that as long as the Taylor series in t for the exact transition probability amplitude G exists for all t, the exact equality holds. That is, we quote that the convergence of the resolvent expansion is only limited by the analytical properties of the expanded function $G(t)$. In other words, from § 4.1 we know that the members of the Taylor series for G and for its νth approximation $G^{(0)} + \ldots + G^{(\nu)}$ are the same up to the $(4+\nu)$th power in t; we hope that the difference between the νth approximation of G and its truncated Taylor series (with members up to the $(4+\nu)$th power in t only) tends to zero in the limit $\nu \to \infty$. We leave this question open to discussion.

Of course, for physical applications the question of convergence is of minor importance if one is only interested in lower approximations. On the other hand, supposing convergence is secured, we have constructed an *analytic* solution for our problem with a rather intricate Hamiltonian, a kind of solution which many other people have previously sought by dealing with the stationary states of the system.

5. Conclusions

In order to avoid conventional paths in exactly treating the coupled spin-oscillator model, we have developed an iteration scheme (mathematically to be characterised as a resolvent expansion) for constructing time-dependent solutions. These solutions are given in the form of transient probability amplitudes for arbitrary initial and final states. Our approach is quite natural to describe the dynamics of the system. For instance, elimination of the final states of the bosonic subsystem leads to a description of the averaged motion of the spin (or of the tunnelling particle in the two-site system, depending on the interpretation of the model).

Independently of the values of the five system parameters, already the zeroth-order solution is exact up to the fourth order in time. We explicitly give the Laplace transforms (with regard to the time) of any higher-order member of the resolvent expansion. We have performed the inverse Laplace transformation for the first and second member. Furthermore, brief instructions are given on how to deal with the inverse Laplace transformation quite generally by means of a computer program.

A most striking feature of our approach is that several limiting cases with regard to the parameter values are treated exactly. In particular, those cases are contained where the coupling parameter and the tunnel parameter vanish or become infinite. For intermediate values of these parameters, the time region of validity is restricted. It can be expected, however, that even the first-order term of the resolvent expansion leads to fairly exact results within a large time region of physical interest. Examination of the complete parameter space was beyond the scope of our work, but concrete problems should surely be attacked in the future. A general method for estimating the time region of validity is given.

The difficult (and purely mathematical) question of whether or not the resolvent expansion converges in a strict sense is left open to a further discussion.

In addition to our thorough investigation of the coupled spin-oscillator system, we have made a first step in handling the intricate problem of operator algebra in the time-dependent solutions of the system equations by means of combinatorics.

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Appendix 1

By starting from

$$\sum \operatorname{res} \frac{1}{(s-s_1)\ldots(s-s_n)} = \delta_{n,1} \tag{A1.1}$$

the following relations may be derived by mathematical induction:

$$\sum \operatorname{res} \frac{s^m}{(s-s_1)\ldots(s-s_n)} = 0 \qquad \text{for } 0 \leqslant m < n-1 \tag{A1.2a}$$

$$\sum \operatorname{res} \frac{s^{n-1}}{(s-s_1)\ldots(s-s_n)} = 1 \tag{A1.2b}$$

$$\sum \operatorname{res} \frac{s^n}{(s-s_1)\ldots(s-s_n)} = s_1 + s_2 + \ldots \tag{A1.2c}$$

$$\sum \operatorname{res} \frac{s^{n+1}}{(s-s_1)\ldots(s-s_n)} = s_1^2 + s_2^2 + \ldots + s_1 s_2 + s_1 s_3 + \ldots \tag{A1.2d}$$

$$\sum \operatorname{res} \frac{s^{n+2}}{(s-s_1)\ldots(s-s_n)} = s_1^3 + \ldots + s_1^2 s_2 + \ldots + s_1 s_2 s_3 + \ldots . \tag{A1.2e}$$

The s_i are the (not necessarily distinct) zeros of polynomials in the variable s occurring in the denominators. By combinatorics it is ensured that odd powers in the roots q (cf equation (3.9)) cancel as should be the case in a series expansion of (2.10), where only entire powers of the system parameters occur.

Appendix 2

We write the matrix elements of the operator $V(\delta)$, known as the Frank-Condon overlap integral, in a frequently used notation

$$f_{m,n}(\delta) = \langle m|V(-\delta)|n\rangle = \langle n|V(\delta)|m\rangle \qquad \delta \in \mathbb{R}. \tag{A2.1}$$

Its explicit form which is immediately deduced from (2.18)

$$\begin{aligned} f_{m,n}(\delta) &= \exp(-\tfrac{1}{2}\delta^2)\frac{1}{\sqrt{m!}}\frac{1}{\sqrt{n!}}\sum_{\nu=0}^{\infty}\nu!\binom{m}{\nu}\binom{n}{\nu}\delta^{m-\nu}(-\delta)^{n-\nu} \\ f_{m,n}(\delta) &= f_{n,m}(-\delta) \end{aligned} \tag{A2.2}$$

is usually written in an unsymmetrical form (Wagner 1959, Koide 1960)

$$f_{m,n}(\delta) = \exp(-\tfrac{1}{2}\delta^2)\delta^{m-n}\sqrt{\frac{n!}{m!}}\,L_n^{m-n}(\delta^2) \tag{A2.3}$$

where L_m^{n-m} is a (generalised) Laguerre polynomial.

The following recurrence relations, holding for integer k and n, are easily proved by collecting terms in common powers of δ and converting the resulting coefficients by means of well known properties of the binomial coefficients with integral arguments:

$$(\delta^2+k-n)f_{k,n}(\delta) - \delta\sqrt{k}f_{k-1,n}(\delta) - \delta\sqrt{k+1}f_{k+1,n}(\delta) = 0 \tag{A2.4}$$

$$\sqrt{k}f_{k-1,n}(\delta) - \sqrt{k+1}f_{k+1,n}(\delta) = -\sqrt{n}f_{k,n-1}(\delta) + \sqrt{n+1}f_{k,n+1}(\delta). \tag{A2.5}$$

Appendix 3

The second-order correction of (4.6) is

$$G^{(2)}_{\downarrow k,n\uparrow}(\alpha, \delta; t) = \mathrm{I} + \mathrm{II} + \mathrm{III} \tag{A3.1}$$

where

$$\begin{aligned} \mathrm{I} = |\gamma|^2\gamma^*\Omega^2(\delta^2+k-n)^2 f_{k,n}(\delta)\tfrac{1}{8}\sum_{\pm}\exp(\mathrm{i}u_{k,n,\pm}(\alpha)t)\frac{\pm v^2_{k,n,\mp}(\alpha)}{|\gamma|^2 q^3_{k,n}(\alpha)} \\ \times\left[\tfrac{1}{2}t^2 - \mathrm{i}t\left(\frac{2p_{k,n}(\alpha)}{|\gamma|^2} \mp \frac{3}{2q_{k,n}(\alpha)}\right)\right. \\ \left. - \frac{v^2_{k,n,\mp}(\alpha)}{|\gamma|^4} - \frac{3}{2q^2_{k,n}(\alpha)} + \frac{1}{|\gamma|^2}\left(1 \pm \frac{3p_{k,n}(\alpha)}{q_{k,n}(\alpha)}\right)\right] \end{aligned} \tag{A3.2a}$$

$$\begin{aligned} \mathrm{II} = |\gamma|^2\gamma^*\Omega^2\{&(\delta^2+k-n)[-\delta\sqrt{k}f_{k-1,n}(\delta)A_{k,k-1,k}(\alpha; t) - \delta\sqrt{k+1}f_{k+1,n}(\delta)A_{k,k+1,k}(\alpha; t)] \\ &- \delta\sqrt{k}[(\delta^2+k-1-n)f_{k-1,n}(\delta)A_{k-1,k,k-1}(\alpha; t) \\ &- \delta\sqrt{k}f_{k,n}(\delta)A_{k,k-1,k-1}(\alpha; t)] \\ &- \delta\sqrt{k+1}[(\delta^2+k+1-n)f_{k+1,n}(\delta)A_{k+1,k,k+1}(\alpha; t) \\ &- \delta\sqrt{k+1}f_{k,n}(\delta)A_{k,k+1,k+1}(\alpha; t)]\} \end{aligned} \tag{A3.2b}$$

where

$$A_{k,k',k''}(\alpha;t)=\sum{}' \operatorname{res}\exp(ts)(s-i\Delta+i\Omega k'')\frac{1}{s+i\Delta+i\Omega n}\frac{1}{d_{k,n}^2(\alpha)}\frac{1}{d_{k',n}(\alpha)}$$

$$=\frac{1}{4\Omega(k'-k)}\sum_{\pm}\exp(iu_{k,n,\pm}(\alpha)t)\frac{v_{k,n,\mp}^2(\alpha)}{|\gamma|^4 q_{k,n}^2(\alpha)}$$

$$\times\left[\left(it+\frac{2v_{k,n,\mp}(\alpha)}{|\gamma|^2}\mp\frac{1}{q_{k,n}(\alpha)}\right)[v_{k,n,\mp}(\alpha)-\Omega(k''-k)]-1\right]$$

$$+B_{k,k''}(\alpha;t)-B_{k',k''}(\alpha,t)$$

and

$$B_{k,k''}(\alpha;t)=\frac{1}{2|\gamma|^6\Omega^2}\sum_{\pm}\exp(iu_{k,n,l}(\alpha)t)\frac{\pm v_{k,n,\mp}^3(\alpha)}{q_{k,n}(\alpha)}[v_{k,n,\mp}(\alpha)-\Omega(k''-k)]$$

$$\mathrm{III}=|\gamma|^2\gamma^*\Omega^2[\delta^2\sqrt{k}\sqrt{k-1}f_{k-2,n}(\delta)C_{k-1,n}(\alpha;t)$$

$$+\delta^2\sqrt{k+1}\sqrt{k+2}f_{k+2,n}(\delta)C_{k+1,n}(\alpha;t)] \qquad \text{(A3.2}c\text{)}$$

where

$$C_{k,n}(\alpha;t)=\frac{1}{2|\gamma|^6\Omega^2}\left(\sum_{\pm}\exp(iu_{k,n,\pm}(\alpha)t)\frac{\pm v_{k,n,\mp}^4(\alpha)}{q_{k,n}(\alpha)}\right.$$

$$\left.-\tfrac{1}{2}\sum_{l=-1,1}\sum_{\pm}\exp(iu_{k+l,n,\pm}(\alpha)t\frac{\pm v_{k+l,n,\mp}^3(\alpha)}{q_{k+l,n}(\alpha)}[v_{k+l,n,\mp}(\alpha)+l\Omega]\right).$$

The terms I, II, III in (A2.2) correspond respectively to the cases where three or two pairs of poles coincide, or no degeneracy occurs at all (in each term the residues of $(s+i\Delta+i\Omega n)^{-1}$ are omitted because they cancel altogether).

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