

General solution of quantum mechanical equations of motion with time-dependent Hamiltonians: a Lie algebraic approach.

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Abstract

The unitary operators $U(t)$, describing the quantum time evolution of systems with a time-dependent Hamiltonian, can be constructed in an explicit manner using the method of time-dependent invariants. We clarify the role of Lie-algebraic techniques in this context and elaborate the theory for $SU(2)$ and $SU(1,1)$. In these cases we give explicit formulas for obtaining general solutions from special ones. We show that the constructions known as Magnus expansion and Wei-Norman expansion correspond with different representations of the rotation group. A simpler construction is obtained when representing rotations in terms of Euler angles.

Progress can be made if one succeeds in finding a non-trivial special solution of the equations of motion. Then the general solution can be derived by means of the Lie theory. The problem of evaluating the evolution of the system is translated from a noncommutative integration in the sense of Dyson into an ordinary commutative integration.

The two main applications of our method are reviewed, namely the Bloch equations and the harmonic oscillator with time-dependent frequency. Even in these well known examples some new results are obtained.

1 Introduction

Assume that a time-dependent Hamiltonian $H(t)$ is given. The axioms of quantum mechanics require that it is a selfadjoint operator in Hilbert space. The solution of the time dependent Schrödinger equation

$$i\frac{d\psi}{dt} = H(t)\psi(t) \quad (1)$$

is formally given by $\psi(t) = U(t)\psi(0)$ with unitary operators $U(t)$ satisfying $U(0) = \mathbb{I}$ and

$$i\left(\frac{d}{dt}U(t)\right)U^*(t) = H(t). \quad (2)$$

The time evolution can be extended to density operators (positive trace-class operators with trace 1) by the relation

$$\rho(t) = U(t)\rho(0)U^*(t). \quad (3)$$

They satisfy von Neumann's equations of motion

$$\frac{d}{dt}\rho(t) = i[\rho(t), H(t)]. \quad (4)$$

Explicit expressions for $U(t)$ in function of the given $H(t)$ are usually difficult to obtain. The mathematical origin of the difficulties is that Hamiltonians $H(t)$ and $H(t')$ at unequal times $t \neq t'$ do not necessarily commute with each other. Much progress has been made in the case that the time-dependent Hamiltonian can be written as a linear combination of constant operators S_1, S_2, \dots, S_n , generating a finite dimensional Lie algebra

$$H(t) = \sum_{j=1}^n h_j(t)S_j. \quad (5)$$

The generators satisfy the commutation relations

$$[S_j, S_m] = i \sum_l \omega_{jml} S_l, \quad (6)$$

with structure constants ω_{jml} . Then the time evolution of the generators can be written as

$$U(t)S_jU^*(t) = \sum_m u_{mj}(t)S_m, \quad (7)$$

with coefficients $u_{mj}(t)$ solution of

$$\frac{d}{dt}u_{mj}(t) = \sum_{ls} \omega_{lsm} h_l(t) u_{sj}(t). \quad (8)$$

Note that (7) is not the time evolution in the Heisenberg picture. The latter is given by $U^*(t)S_jU(t)$ instead of $U(t)S_jU^*(t)$.

Using (7) one can obtain the general solution of the von Neumann equation (4), with arbitrary initial conditions of the form

$$\rho(t=0) = C + \sum_j a_j(0)S_j. \quad (9)$$

The operator C is an arbitrary operator commuting with all generators S_j . The solution is

$$\rho(t) = C + \sum_j a_j(t)S_j, \quad (10)$$

with

$$a_j(t) = \sum_m u_{jm}(t)a_m(0). \quad (11)$$

The problem remains to obtain an explicit expression for the unitary operators $U(t)$. See for instance [1, 2] and the references quoted there. These authors show that one can write $U(t)$ as an ordered product

$$U(t) = e^{g_1(t)S_1} e^{g_2(t)S_2} \dots e^{g_n(t)S_n}, \quad (12)$$

where the complex functions $g_1(t), \dots, g_n(t)$ are solutions of some set of non-linear differential equations. In this way the problem is reduced to a well-known but rather difficult classical (this is, non-quantum) problem of solving sets of equations. This method has been elaborated by many authors, including [3, 4, 6, 8, 19, 20, 22]. A related topic is that of the superposition principle for nonlinear equations, see for instance [29, 39].

Alternatively, one assumes that a particular solution $\rho_s(t)$ of von Neumann's equation (4) is known. This special solution was called a time-dependent invariant in [3]. We use the existence of such special solutions as a starting point for constructing unitary operators $U(t)$, based on an idea of [35].

The next Section describes in general terms the method of constructing $U(t)$. Section 3 explains how the assumption, that the Hamiltonian $H(t)$ can be expanded in terms of generators of a Lie algebra, helps to apply the method. Subsequent Sections specialise the method for $SU(2)$ and $SU(1,1)$. Applications start in Section 6. The discussion of the obtained results follows in Section 10.

2 Method

Assume that there is given a time-dependent Hamiltonian $H(t)$ and a special solution $\rho_s(t)$ of the von Neumann equation (4) and $\frac{d\rho_s(t)}{dt} \neq 0$ for almost all t . Can one construct unitary operators $U(t)$ solving (2)? The method described below requires two steps to do so.

First step Determine unitary operators $V(t)$ such that

$$\rho_s(t) = V(t)\rho_s(0)V^*(t). \quad (13)$$

If $\rho_s(t)$ has a discrete spectrum, as is the case for a density operator, then this can be obtained in principle by diagonalising $\rho_s(t)$. The unitary $V(t)$ transforms the basis in which $\rho_s(0)$ is diagonal to the basis where $\rho_s(t)$ is diagonal. In practical applications we use special solutions obtained by some concrete technique (expansions in generators of a Lie algebra, Darboux transformations, etc.), and the very form of a given method typically suggests the shape of $V(t)$.

With this $V(t)$ one can construct a Hamiltonian $K(t)$ by

$$K(t) = i \frac{dV}{dt} V^*(t). \quad (14)$$

In general, this Hamiltonian differs from the given $H(t)$, in which case $V(t)$ is not a solution of (2), which is the defining equation of $U(t)$.

Second step Assume now that $\rho_s(0)$ is self-adjoint, as is the case for a density operator. Then generically operators commuting with $\rho_s(0)$ are functions of $\rho_s(0)$ in the sense of spectral theory. Comparing (13) with (3) shows that $U(t)V^*(t)$ commutes with $\rho_s(t)$ and

$V^*(t)U(t)$ commutes with $\rho_s(0)$. Hence, if $\rho_s(0)$ is multiplicity free, there exists a real function $f_t(x)$ such that

$$U(t) = e^{if_t(\rho_s(t))} V(t) = V(t) e^{if_t(\rho_s(0))}. \quad (15)$$

It remains to determine this function $f_t(x)$. Combine (15) with (2) to obtain

$$\frac{d}{dt} f_t(\rho_s(0) - C) = U^*(t) \{K(t) - H(t)\} U(t) = V^*(t) \{K(t) - H(t)\} V(t). \quad (16)$$

The r.h.s. of this equation is known from the first step of the method. Hence the function $df_t(x)/dt$ can be determined. To this purpose, the r.h.s. of (16) has to be written as a function of $\rho_s(0)$. Next, $f_t(x)$ is obtained by integration.

Summing up, if for a given time-dependent Hamiltonian $H(t)$ we know $V(t)$ corresponding to some explicit solution $\rho_s(t)$, such $\rho_s(0)$ is multiplicity free, then the problem of defining the evolution of the system is translated from noncommutative integrations in the sense of Dyson to an ordinary commutative integration.

3 Lie algebras

Assume now that $H(t)$ is a linear combination of generators S_1, \dots, S_n of a Lie algebra, with commutation relations as given by (6), and that the special solution $\rho_s(t)$ is of the form (10). We first study the time evolution of the coefficients $a_j(t)$ as elements of a Lie algebra, represented in \mathbb{R}^n .

Introduce the Killing form

$$\langle a|b \rangle = \langle b|a \rangle = - \sum_{mn} \left(\sum_j \omega_{jmn} a_j \right) \left(\sum_l \omega_{lnm} b_l \right). \quad (17)$$

The minus sign is needed because of the imaginary factor i in the definition (6) of the structure constants. Introduce the Lie bracket $a \times b = -b \times a$ by

$$(a \times b)_l = \sum_{jm} a_j b_m \omega_{jml}. \quad (18)$$

A well-known property of the Killing form, consequence of the Jacobi identity, is that

$$\langle a \times b|c \rangle = \langle a|b \times c \rangle. \quad (19)$$

This will be used often.

The Hamiltonian $K(t)$ can be written as

$$K(t) = \sum_j k_j(t) S_j. \quad (20)$$

One has

$$\begin{aligned} i \sum_j \frac{da_j}{dt} S_j &= i \frac{d}{dt} \rho_s(t) = [K(t), \rho_s(t)] \\ &= i \sum_{jm} k_j(t) a_m(t) \omega_{jml} S_l. \end{aligned} \quad (21)$$

This implies

$$\frac{da_j}{dt} = \sum_{ml} k_m(t) a_l(t) \omega_{mlj}. \quad (22)$$

Introduce the notation \dot{a} for the vector with components da_j/dt . From (22) then follows that $\dot{a} = k \times a$.

Let us assume that the Killing form is non-degenerate. This is known to be the case if and only if the Lie algebra is semi-simple.

Lemma 1 *Assume that the Killing form is non-degenerate. Fix $a \in \mathbb{R}^n$ such that $\langle a|a \rangle \neq 0$. Assume that the Killing form of the Lie algebra is such that $\langle b|a \rangle = 0$ implies that there exists $c \in \mathbb{R}^n$ such that $b = a \times c$. Then $a \times u = 0$ and $\langle u|a \rangle = 0$ together imply $u = 0$.*

Proof

Let d be arbitrary in \mathbb{R}^n . Write

$$d = \frac{\langle d|a \rangle}{\langle a|a \rangle} a + b, \quad (23)$$

with $\langle b|a \rangle = 0$. By assumption one can write $b = a \times c$ so that

$$d = \frac{\langle d|a \rangle}{\langle a|a \rangle} a + a \times c. \quad (24)$$

Now calculate, using $a \times u = 0$ and $\langle u|a \rangle = 0$,

$$\langle d|u \rangle = \langle a \times c|u \rangle = \langle c|u \times a \rangle = 0. \quad (25)$$

Since d is arbitrary and the Killing form is non-degenerate there follows that $u = 0$. □

Proposition 1 *Let be given a special solution $\rho_s(t)$ of the form*

$$\rho_s(t) = C + \sum_j a_j(t) S_j, \quad (26)$$

where C commutes with all S_j . Assume that $\langle a(0)|a(0) \rangle \neq 0$ and that $\langle b|a(0) \rangle = 0$ implies that there exists $c \in \mathbb{R}^n$ such that $b = a(0) \times c$. Assume also that the Killing form is non-degenerate. Then one has

$$H(t) = K(t) + \alpha(t) \{ \rho_s(t) - C \}. \quad (27)$$

with

$$\alpha(t) = \frac{\langle a|h - k \rangle}{\langle a|a \rangle}. \quad (28)$$

Proof

Note that

$$\dot{a} = h \times a = k \times a. \quad (29)$$

Let $r = h - k$. Then one has $0 = r \times a$. Let $u = r - \alpha(t)a$ with $\alpha(t)$ given by (28). Then a short calculation yields $\langle u|a \rangle = 0$ and $a \times u = 0$. By the previous lemma this implies that $u = 0$. One therefore has $h = k + \alpha(t)a$, which can be written as (27). □

Since $\rho_s(t)$ and $H(t)$ are known, the Proposition ensures that the difference between $H(t)$ and $K(t)$ is proportional to the special solution $\rho_s(t)$ minus a constant operator. Then, (16) implies

$$\begin{aligned} \frac{d}{dt} f_t(\rho_s(0)) &= V^*(t)\{K(t) - H(t)\}V(t) \\ &= -\alpha(t)V^*(t)\{\rho_s(t) - C\}V(t) \\ &= -\alpha(t)\{\rho_s(0) - C\}. \end{aligned} \quad (30)$$

Therefore, one finds that $f_t(u)$ is the linear function given by

$$f_t(u) = \tau(t) u \quad \text{with} \quad \tau(t) = - \int_0^t ds \alpha(s). \quad (31)$$

Hence, (15) becomes

$$U(t) = e^{i\tau(t)(\rho_s(t)-C)}V(t) = V(t)e^{i\tau(t)(\rho_s(0)-C)}. \quad (32)$$

Inserting now (32) into the l.h.s. of (2) gives

$$\begin{aligned} i \left(\frac{d}{dt} U(t) \right) U^*(t) &= \left(i \left(\frac{d}{dt} V(t) \right) e^{i\tau(t)(\rho_s(0)-C)} - U(t)(\rho_s(0) - C) \frac{d\tau}{dt} \right) U^*(t) \\ &= K(t) + (\rho_s(t) - C)\alpha(t) \\ &= H(t). \end{aligned} \quad (33)$$

One concludes that $U(t)$, as given by (32), indeed solves (2). This completes the second step of the method. All it needs from the first step is the knowledge of $V(t)$ and the value of the Killing form $\langle k|a \rangle$.

Introduce coefficients $v_{mj}(t)$ defined by

$$V(t)S_jV^*(t) = \sum_m v_{mj}(t)S_m. \quad (34)$$

They satisfy

$$a_m(t) = \sum_j v_{mj}(t)a_j(0). \quad (35)$$

The $a_j(t)$ are known functions. We have to find $v_{mj}(t)$, solving (35), such that unitary operators $V(t)$ exist which solve (34).

Note that

$$\frac{d}{dt}\langle a|a\rangle = 2\langle h \times a|a\rangle = 2\langle h|a \times a\rangle = 0. \quad (36)$$

This means that $\langle a|a\rangle$ is constant in time. Hence, it is obvious to look for solutions $v_{kj}(t)$ of (35) which are matrix elements of a matrix $W(t)$ that leaves the Killing form invariant, in the sense that

$$\langle Wb|Wc\rangle = \langle b|c\rangle \quad \text{for all } b, c \in \mathbb{R}^n. \quad (37)$$

For the construction of a matrix $W(t)$ that leaves the Killing form invariant and that satisfies (35) one has to rely on the large amount of knowledge about automorphisms of Lie algebras (Note that automorphisms of the Lie algebra leave the Killing form invariant).

The next step is the construction of the operator $V(t)$. One can make use of the fact that the construction can be done in any faithful operator representation of the Lie algebra. Indeed, let \hat{S}_j be the generators in such a representation (the hat is used to distinguish the generators S_j from their representations \hat{S}_j) and assume that

$$\hat{\rho}_s(t) = \hat{V}(t)\hat{\rho}(0)\hat{V}^*(t) \quad (38)$$

with

$$\hat{\rho}_s(t) = \sum_{j=1}^n a_j(t)\hat{S}_j, \quad (39)$$

and

$$\hat{V}(t) = e^{ir_1(t)\hat{S}_1} e^{ir_2(t)\hat{S}_2} \dots e^{ir_n(t)\hat{S}_n}. \quad (40)$$

Choose for instance a $V(t)$ of the Wei-Norman form (12) [1]. Then the operators $V(t)$, defined by

$$V(t) = e^{ir_1(t)S_1} e^{ir_2(t)S_2} \dots e^{ir_n(t)S_n}, \quad (41)$$

satisfy

$$\rho_s(t) = V(t)\rho(0)V^*(t). \quad (42)$$

The argument is that, when calculating $V(t)\rho(0)V^*(t)$, using the Baker-Campbell-Hausdorff formula, one needs to know only the commutation relations between the generators S_j . Hence, the expressions for $V(t)$ and $\hat{V}(t)$ have the same form. Note that, if then the generators S_j are self-adjoint and the coefficients $r_j(t)$ are real, then $V(t)$ is unitary, as requested.

Factorisations of $V(t)$, other than that of Wei and Norman, will be used below as well. However, the above argument can be used in all cases.

4 SU(2)

Let be given operators S_1, S_2, S_3 that satisfy the commutation relations

$$[S_1, S_2] = iS_3 \quad \text{and cyclic permutations.} \quad (43)$$

The non-vanishing structure constants are $\omega_{123} = \omega_{231} = \omega_{312} = 1$ and $\omega_{132} = \omega_{213} = \omega_{321} = -1$. The Lie bracket is

$$(a \times b)_3 = a_1 b_2 - a_2 b_1 \quad \text{and cyclic permutations.} \quad (44)$$

The Killing form is

$$\langle a|b \rangle = -2 \sum_j a_j b_j. \quad (45)$$

A well-known identity is

$$2x \times (x \times y) = \langle x|y \rangle x - \langle x|x \rangle y. \quad (46)$$

This implies that the conditions of the Proposition 1 are satisfied, provided that $a(0) \neq 0$. Indeed, assume $\langle b|a(0) \rangle = 0$. Then (46) implies that $b = a(0) \times c$ with

$$c = -2 \frac{a(0) \times b}{\langle a(0)|a(0) \rangle}. \quad (47)$$

Let be given a special solution $\rho_s(t)$ of the von Neumann equation. Then we have to construct automorphisms $W(t)$ of the Lie algebra such that (13) holds. In addition, we have to calculate $\langle k|a \rangle$. The rotations of \mathbb{R}^3 are the natural candidates for the $W(t)$. Several parametrisations are possible and are treated below.

4.1 Magnus expansion

Any rotation of \mathbb{R}^3 can be denoted $R(n, \phi)$, meaning a rotation around an axis determined by the vector n , satisfying $|n| = 1$, and by an angle ϕ . One has

$$R(n, \phi)u = \cos(\phi)u - \sin(\phi)a \times u + (1 - \cos(\phi))(u \cdot n)n. \quad (48)$$

A well-known projective representation of the group $SO(3)$ in $SU(2)$ is

$$\hat{V}(n, \phi) = \exp \left(-i \frac{\phi}{2} \sum_{\alpha=1}^3 n_\alpha \sigma_\alpha \right), \quad (49)$$

where the σ_α are the Pauli spin matrices. It satisfies

$$\begin{aligned} \hat{V}(n, \phi)(a \cdot \sigma) \hat{V}(n, -\phi) &= \cos(\phi)a \cdot \sigma - \sin(\phi)(a \times n) \cdot \sigma \\ &\quad + (1 - \cos(\phi))(a \cdot n)n \cdot \sigma \\ &= (R(n, \phi)a) \cdot \sigma. \end{aligned} \quad (50)$$

Hence, the map $a \rightarrow \frac{1}{2}a \cdot \sigma$ is an operator representation of the Lie algebra $SU(2)$ (note that $\sigma_j = 2\hat{S}_j$).

Let $n(t)$ and $\phi(t)$ be smooth functions such that $a(t) = R(n, \phi)a(0)$. Then (49) is an explicitly constructed representation, satisfying our requirements. One concludes that

$$V(t) = \exp \left(-i\phi \sum_{\alpha=1}^3 n_\alpha S_\alpha \right). \quad (51)$$

This ends the first step of the method. The disadvantage of the Magnus expansion is that the expression for the operator K is rather complicated. The expansion is therefore less useful and further application of the method is omitted here.

4.2 Wei-Norman expansion

A rotation in \mathbb{R}^3 can also be described as a sequence of rotations about each of the principal axes. Let

$$\begin{aligned} R_1(q_1) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(q_1) & \sin(q_1) \\ 0 & -\sin(q_1) & \cos(q_1) \end{pmatrix} \\ R_2(q_2) &= \begin{pmatrix} \cos(q_2) & 0 & -\sin(q_2) \\ 0 & 1 & 0 \\ \sin(q_2) & 0 & \cos(q_2) \end{pmatrix} \\ R_3(q_3) &= \begin{pmatrix} \cos(q_3) & \sin(q_3) & 0 \\ -\sin(q_3) & \cos(q_3) & 0 \\ 0 & 0 & 1 \end{pmatrix}. \end{aligned} \quad (52)$$

Then one has

$$e^{iq_1\sigma_1/2} e^{iq_2\sigma_2/2} e^{iq_3\sigma_3/2} (u \cdot \sigma) e^{-iq_3\sigma_3/2} e^{-iq_2\sigma_2/2} e^{-iq_1\sigma_1/2} = (R_1 R_2 R_3 u) \cdot \sigma. \quad (53)$$

One concludes that

$$V(t) = e^{iq_1 S_1} e^{iq_2 S_2} e^{iq_3 S_3}, \quad (54)$$

with time-dependent angles $q_j(t)$ determined by $a(t) = R_1(q_1)R_2(q_2)R_3(q_3)a(0)$. The Hamiltonian K is found to be

$$\begin{aligned} K &= -\dot{q}_1 S_1 - \dot{q}_2 \{ \cos(q_1) S_2 - \sin(q_1) S_3 \} \\ &\quad + \dot{q}_3 \{ \sin(q_2) S_1 + \sin(q_1) \cos(q_2) S_2 - \cos(q_1) \cos(q_2) S_3 \}. \end{aligned} \quad (55)$$

Given a special solution of the form (26), the functions $a_j(t)$ are known. The time-dependent angles $q_j(t)$ can then be determined by the requirement that the vector $a(t)$ is obtained from $a(0)$ by three successive rotations. Hence the Hamiltonian K can be computed explicitly. From the difference with the given Hamiltonian H one can determine the function $\alpha(t)$ — see Proposition 1. The full unitary time evolution $U(t)$ is then obtained from (31, 32). This is surely a viable approach. However, the equations determining the time-dependent angles can be rather complicated. Therefore, some alternatives are given below.

4.3 Euler angles

Another well-known parametrisation of rotations is that of Euler. It describes the rotation of a reference frame. When describing a rotation in \mathbb{R}^3 the first rotation can be used to bring the initial vector in the plane orthogonal to direction 1. Let

$$a(t) = R_3(\psi) R_1(\theta) R_3(\phi) a(0). \quad (56)$$

Then one has for arbitrary $u \in \mathbb{R}^3$

$$e^{\frac{i}{2}\psi\sigma_3} e^{\frac{i}{2}\theta\sigma_1} e^{\frac{i}{2}\phi\sigma_3} (u \cdot \sigma) e^{-\frac{i}{2}\phi\sigma_3} e^{-\frac{i}{2}\theta\sigma_1} e^{-\frac{i}{2}\psi\sigma_3} = (R_3(\psi) R_1(\theta) R_3(\phi) u) \cdot \sigma.$$

(57)

One concludes that

$$V(t) = e^{i\psi S_3} e^{i\theta S_1} e^{i\phi S_3}, \quad (58)$$

with time-dependent Euler angles determined by $a(t) = R_3(\psi)R_1(\theta)R_3(\phi)a(0)$.

The Hamiltonian K is found to be

$$K = -\dot{\psi}S_3 - \dot{\theta}(\cos(\psi)S_1 - \sin(\psi)S_2) - \dot{\phi}\{\cos(\theta)S_3 + \sin(\theta)\cos(\psi)S_2 + \sin(\theta)\sin(\psi)S_1\}. \quad (59)$$

Note that one can replace (58) by the alternative expressions

$$V(t) = e^{i(\psi+\phi)S_3} e^{i\theta(\cos(\phi)S_1 + \sin(\phi)S_2)} \quad (60)$$

or

$$V(t) = e^{i\theta(\cos(\psi)S_1 - \sin(\psi)S_2)} e^{i(\phi+\psi)S_3}. \quad (61)$$

These expressions might be more convenient in certain applications.

4.4 Calculation of the time-dependent angles

The calculation of the time-dependent angles ψ, θ, ϕ may involve complicated expressions. It is therefore noteworthy that one can redefine the Euler angles in such a way that (58) may be replaced by

$$V(t) = e^{i\phi(t)S_3} e^{i\theta(t)S_1} e^{-i\theta(0)S_1} e^{-i\phi(0)S_3}. \quad (62)$$

This expression involves only two angles $\phi(t)$ and $\theta(t)$, determined by

$$\begin{aligned} \sin(\phi) &= \frac{a_1}{z}, & \cos(\phi) &= \frac{a_2}{z}, \\ \sin(\theta) &= -\frac{a_3}{\lambda}, & \cos(\theta) &= \frac{z}{\lambda}, \end{aligned} \quad (63)$$

where $z(t) = \sqrt{a_1(t)^2 + a_2(t)^2}$ and $\lambda = \sqrt{z(t)^2 + a_3(t)^2}$. To see this, note that $R_1(-\theta)R_3(-\phi)$ rotates the arbitrary vector a into the fixed vector $\lambda(0, 1, 0)^T$.

Using $\dot{\phi} = \frac{a_2\dot{a}_1 - a_1\dot{a}_2}{z^2}$ and $\dot{\theta} = -\frac{\dot{a}_3}{z}$ the Hamiltonian $K(t)$ can be calculated as follows

$$\begin{aligned} K(t) &= i\frac{dV}{dt}V^*(t) \\ &= -\dot{\theta}\{\cos(\phi)S_1 - \sin(\phi)S_2\} - \dot{\phi}S_3 \\ &= \frac{a_2\dot{a}_3}{z^2}S_1 - \frac{a_1\dot{a}_3}{z^2}S_2 + \frac{a_1\dot{a}_2 - a_2\dot{a}_1}{z^2}S_3. \end{aligned} \quad (64)$$

Using $\dot{a} = h \times a$ one sees that this expression is of the form $k = h - \alpha(t)a$ with the function $\alpha(t)$ given by

$$\alpha = \frac{a_1h_1 + a_2h_2}{z^2}. \quad (65)$$

The final result is then (see (32))

$$U(t) = V(t) \exp \left(i\tau(t) \sum_j a_j(0) S_j \right), \quad (66)$$

with $V(t)$ given by (62) and with

$$\tau(t) = - \int_0^t ds \alpha(s) \quad (67)$$

4.5 General solution of the equation $\dot{x} = h \times x$

For the applications, discussed later on, it is of interest that one can now write down the general solution of the equations $\dot{x} = h \times x$ in terms of the special solution a and the effective time $\tau(t)$. Indeed, one has

$$x(t) = A \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} - \frac{\lambda B}{z} \cos(\lambda\tau + C) \begin{pmatrix} a_2 \\ -a_1 \\ 0 \end{pmatrix} + \frac{B}{z} \sin(\lambda\tau + C) \begin{pmatrix} a_3 a_1 \\ a_3 a_2 \\ -z^2 \end{pmatrix}, \quad (68)$$

with A, B, C arbitrary constants. The verification of this results is a matter of a straightforward calculation.

5 SU(1,1)

Consider operators S_1, S_2, S_3 satisfying the commutation relations

$$\begin{aligned} [S_1, S_2] &= iS_3 \\ [S_2, S_3] &= -iS_1 \\ [S_3, S_1] &= -iS_2. \end{aligned} \quad (69)$$

Introduce $S'_1 = iS_1$, $S'_2 = iS_2$, and $S'_3 = -S_3$. Then S'_1, S'_2, S'_3 satisfy the commutation relations of SU(2). Hence, the results of the previous Sections can be used to solve step 1 of our method. However, in step 2 the assumption is made that the generators S_1, S_2, S_3 are self-adjoint. Therefore, the results of Section 4 have to be rederived here for SU(1,1).

The non-vanishing structure constants are $\omega_{123} = \omega_{321} = \omega_{132} = 1$ and $\omega_{213} = \omega_{231} = \omega_{312} = -1$. The Lie bracket for vectors in \mathbb{R}^3 is

$$\begin{aligned} (a \times b)_1 &= a_3 b_2 - a_2 b_3, \\ (a \times b)_2 &= a_1 b_3 - a_3 b_1, \\ (a \times b)_3 &= a_1 b_2 - a_2 b_1. \end{aligned} \quad (70)$$

The Killing form is

$$\langle a|b \rangle = -2a_1 b_1 - 2a_2 b_2 + 2a_3 b_3. \quad (71)$$

The identity (46) still holds. Hence, the Proposition 1 predicts the form of the relation between the unitary operators $V(t)$ and $U(t)$.

5.1 Representation in \mathbb{R}^3

Note that the cyclic permutation symmetry of $SU(2)$ is lost. Hence, from the Wei-Norman expansion (54) and the expansion based on Euler angles (58) one can derive two times three different expansions. Let us consider just one of these, corresponding with the choice of signs $(-, -, +)$ in the Killing form, as found in (71). Then the rotations around the third axis $R_3(\phi)$ and $R_3(\psi)$ remain automorphisms. But $R_1(\theta)$ must be replaced by

$$P_1(\chi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cosh(\chi) & \sinh(\chi) \\ 0 & \sinh(\chi) & \cosh(\chi) \end{pmatrix}. \quad (72)$$

Assume now that the coefficients $a_j(t)$ are written as $a(t) = R_3(\psi)P_1(\chi)R_3(\phi)a(0)$. Then the unitary operators $V(t)$ are given by

$$V(t) = e^{-i\psi S_3} e^{-i\chi S_1} e^{-i\phi S_3}. \quad (73)$$

Indeed, for arbitrary u in \mathbb{R}^3 is

$$e^{i\psi S_3} e^{i\theta S_1} e^{i\phi S_3} (u \cdot \sigma) e^{-i\phi S_3} e^{-i\theta S_1} e^{-i\psi S_3} = (R_3(-\psi)P_1(-\theta)R_3(-\phi)u) \cdot \sigma. \quad (74)$$

The corresponding Hamiltonian is

$$K = i \frac{dV}{dt} V^*(t) = \dot{\psi} S_3 + \dot{\chi} (\cos(\psi) S_1 - \sin(\psi) S_2) + \dot{\phi} \{ \cosh(\chi) S_3 + \sinh(\chi) \cos(\psi) S_2 + \sinh(\chi) \sin(\psi) S_1 \}. \quad (75)$$

As before in the $SU(2)$ case one can rewrite the automorphism in such a way that only two angles are involved

$$a(t) = R_3(\phi(t))P_1(\chi(t) - \chi(0))R_3(-\phi(0)). \quad (76)$$

The corresponding unitary operators are

$$V(t) = e^{-i\phi(t)S_3} e^{-i\chi(t)S_1} e^{i\chi(0)S_1} e^{i\phi(0)S_3} \quad (77)$$

The angles $\phi(t)$ and $\chi(t)$ must satisfy

$$\begin{aligned} \sin(\phi) &= \frac{a_1}{z} & \cos(\phi) &= \frac{a_2}{z} \\ \sinh(\chi) &= \frac{\dot{a}_3}{\mu} & \cosh(\chi) &= \frac{z}{\mu}, \end{aligned} \quad (78)$$

where $z(t) = \sqrt{a_1(t)^2 + a_2(t)^2}$ and $\mu = \sqrt{z(t)^2 - a_3(t)^2}$. The fixed vector is

$$P_1(-\chi(0))R_3(-\phi(0))a(0) = \mu(0, 1, 0)^T. \quad (79)$$

Using $\dot{\chi} = \dot{a}_3/z$ and $\dot{\phi} = (a_2\dot{a}_1 - a_1\dot{a}_2)/z^2$ the Hamiltonian K can be calculated as follows

$$\begin{aligned} K = i \frac{dV}{dt} V^*(t) &= \dot{\chi} \{ \cos(\phi(t)) S_1 - \sin(\phi(t)) S_2 \} + \dot{\phi} S_3 \\ &= \frac{\dot{a}_3 a_2}{z^2} S_1 - \frac{\dot{a}_3 a_1}{z^2} S_2 + \frac{a_2 \dot{a}_1 - a_1 \dot{a}_2}{z^2} S_3. \end{aligned} \quad (80)$$

Using $\dot{a} = h \times a$ one sees that this expression is of the form $k = h - \alpha a$ with the function $\alpha(t)$ given by

$$\alpha = \frac{a_1 h_1 + a_2 h_2}{z^2}. \quad (81)$$

The final result is then (see (32))

$$U(t) = V(t) \exp \left(i\tau(t) \sum_j a_j(0) S_j \right), \quad (82)$$

with $V(t)$ given by (77) and with

$$\tau(t) = - \int_0^t ds \alpha(s) \quad (83)$$

If the initial conditions satisfy $a_3^2 = a_1^2 + a_2^2$ then $\mu = 0$ and the angle $\chi(t)$ cannot be determined by (78). In that case $R_3(-\phi(0))a(0)$ equals $z(0, 1, 1)^T$ (we assume that $a_3(0) > 0$). The angle $\chi(0)$ can be taken equal to zero. The corresponding expression for the time-dependent angle $\chi(t)$ is then

$$e^{\chi(t)} = \frac{a_3(t)}{a_3(0)}. \quad (84)$$

Using $\dot{\chi} = \dot{a}_3/a_3$ and $\dot{\phi} = (a_2\dot{a}_1 - a_1\dot{a}_2)/a_3^2$ the Hamiltonian K becomes

$$K = \frac{\dot{a}_3}{a_3^2}(a_2 S_1 - a_1 S_2) + \frac{a_2\dot{a}_1 - a_1\dot{a}_2}{a_3^2} S_3. \quad (85)$$

One then verifies that $k = h - \alpha a$ still holds with the function $\alpha(t)$ given by (81), in spite of the fact that in this case the conditions of the Proposition 1 are not satisfied.

Note that slightly different choices have to be made in the case that the initial conditions satisfy $a_3^2 > a_1^2 + a_2^2$ instead of $a_3^2 < a_1^2 + a_2^2$. Because $a_3(t)$ does not change sign, and is assumed to be positive, one can take

$$\sinh(\chi) = \frac{z}{\mu} \quad \cosh(\chi) = \frac{a_3}{\mu}, \quad (86)$$

with $\mu = \sqrt{a_3(t)^2 - z(t)^2}$. Then $P_1(-\chi(0))R_3(-\phi(0))a$ equals $\mu(0, 0, 1)^T$.

5.2 General solution of the equation $\dot{x} = h \times x$

In the same way as for the SU(2) symmetry one can now write down the general solution of the equation $\dot{x} = h \times x$. One finds, assuming $a_1^2 \neq a_2^2 + a_3^2$,

$$x(t) = A \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} + \frac{\mu B}{z} \cosh(\mu\tau + C) \begin{pmatrix} a_2 \\ -a_1 \\ 0 \end{pmatrix} + \frac{B}{z} \sinh(\mu\tau + C) \begin{pmatrix} a_3 a_1 \\ a_3 a_2 \\ z^2 \end{pmatrix}, \quad (87)$$

with A, B, C arbitrary constants. In the case that $a_1^2 = a_2^2 + a_3^2$ then one finds

$$x(t) = (A + B\tau + C\tau^2) \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} + \frac{a_3}{z^2} (B + 2C\tau) \begin{pmatrix} a_2 \\ -a_1 \\ 0 \end{pmatrix} + \frac{1}{z^2} C \begin{pmatrix} -a_1 \\ -a_2 \\ a_3 \end{pmatrix}. \quad (88)$$

6 The Bloch equations

A well-known application of $SU(2)$ concerns the Bloch equations — see [9]. It is treated in the present Section. The modification obtained by considering phase modulation is treated in the next Section.

Note that the incorporation of the Bloch equations into the Maxwell-Bloch equations have been studied by many authors, including [14, 36].

More general applications of $SU(2)$ symmetry have been considered in the literature as well. Campolieti and Sanctuary [10] applied the Wei-Norman technique to field modulation in NMR. Zhou and Ye [16] study the case where all coefficients are time-dependent. They introduce Euler angles with the same purpose as in the present work. Finally, Dasgupta [24] studies the Jaynes-Cummings model with time-dependent coupling between the spin and the photon field.

6.1 The Bloch equations

A magnetic spin in a magnetic field is usually described by a Hamiltonian of the form

$$H = \frac{1}{2}\epsilon\sigma_3 - \frac{1}{2}\xi\sigma_1. \quad (89)$$

The Pauli matrices $\sigma_1, \sigma_2, \sigma_3$ are related to the generators of the Lie algebra by $\sigma_\alpha = 2S_\alpha$. One has $h = (-\xi, 0, \epsilon)^T$. The equations of motion $\dot{a} = h \times a$ are known as the Bloch equations — see [9]. Written explicitly, they are

$$\begin{aligned} \dot{a}_1 &= -\epsilon a_2, \\ \dot{a}_2 &= \epsilon a_1 + \xi a_3 \\ \dot{a}_3 &= -\xi a_2. \end{aligned} \quad (90)$$

6.2 Special solutions

Assume that the constant ϵ does not depend on time. If $\xi(t)$ does not depend on time then any solution $x(t)$ of the harmonic oscillator equation $\ddot{x} + (\epsilon^2 + \xi^2)x = 0$ determines a solution of (90), given by

$$\begin{aligned} a_1 &= \frac{\epsilon \dot{x}}{\epsilon^2 + \xi^2} + \xi C \\ a_2 &= x, \\ a_3 &= \frac{\xi \dot{x}}{\epsilon^2 + \xi^2} - \epsilon C, \end{aligned} \quad (91)$$

with integration constant C .

When $\xi(t)$ is time-dependent then a solution is known only in very specific cases. One such case involves Jacobi's elliptic functions sn , cn , and dn , with elliptic modulus k . Let

$$\xi(t) = 2\omega k \text{cn}(\omega t; k). \quad (92)$$

Then a solution of (90) exists of the form

$$\begin{aligned} a_1(t) &= \epsilon \text{cn}(\omega t; k), \\ a_2(t) &= \omega \text{sn}(\omega t; k) \text{dn}(\omega t; k), \\ a_3(t) &= -\omega k \text{sn}^2(\omega t; k) + \gamma, \end{aligned} \quad (93)$$

with

$$\gamma = -\frac{\epsilon^2 - \omega^2}{2\omega k}. \quad (94)$$

In the limit $k = 1$ these expressions lead to the well-known result (see Eq. 4.21 of [9])

$$\begin{aligned} \xi(t) &= 2\omega \operatorname{sech}(\omega t), \\ a_1(t) &= \epsilon \operatorname{sech}(\omega t), \\ a_2(t) &= \omega \tanh(\omega t) \operatorname{sech}(\omega t), \\ a_3(t) &= -\omega \tanh^2(\omega t) + \gamma. \end{aligned} \quad (95)$$

When $\omega = \epsilon$ then the limit $k = 0$ can be taken. The rather trivial result is

$$\begin{aligned} \xi(t) &= 0, \\ a_1(t) &= \omega \cos(\omega t), \\ a_2(t) &= \omega \sin(\omega t), \\ a_3(t) &= 0. \end{aligned} \quad (96)$$

6.3 General solution of the Bloch equations

The general solution of the Bloch equations, given arbitrary initial conditions and with time-dependent Hamiltonian determined by (92), is derived in the Appendix A. The three independent solutions $a^{(1)}, a^{(2)}, a^{(3)}$ of $\dot{a} = h \times a$ are obtained from (A.10). They are

$$\begin{aligned} a^{(1)} &= \frac{\epsilon}{\lambda} \begin{pmatrix} \sin(\phi) \cos(\theta) \\ \cos(\phi) \cos(\theta) \\ -\sin(\theta) \end{pmatrix} - \frac{\gamma}{\lambda} \cos(\lambda\tau) \begin{pmatrix} \sin(\phi) \sin(\theta) \\ \cos(\phi) \sin(\theta) \\ \cos(\theta) \end{pmatrix} + \frac{\gamma}{\lambda} \sin(\lambda\tau) \begin{pmatrix} \cos(\phi) \\ -\sin(\phi) \\ 0 \end{pmatrix} \\ a^{(2)} &= -\sin(\theta) \sin(\lambda\tau) \begin{pmatrix} \sin(\phi) \\ \cos(\phi) \\ 0 \end{pmatrix} - \cos(\lambda\tau) \begin{pmatrix} \cos(\phi) \\ -\sin(\phi) \\ 0 \end{pmatrix} - \cos(\theta) \sin(\lambda\tau) \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \\ a^{(3)} &= \frac{\gamma}{\lambda} \begin{pmatrix} \sin(\phi) \cos(\theta) \\ \cos(\phi) \cos(\theta) \\ -\sin(\theta) \end{pmatrix} + \frac{\epsilon}{\lambda} \cos(\lambda\tau) \begin{pmatrix} \sin(\phi) \sin(\theta) \\ \cos(\phi) \sin(\theta) \\ \cos(\theta) \end{pmatrix} - \frac{\epsilon}{\lambda} \sin(\lambda\tau) \begin{pmatrix} \cos(\phi) \\ -\sin(\phi) \\ 0 \end{pmatrix} \end{aligned} \quad (97)$$

The special solution (93) satisfies $a = \epsilon a^{(1)} + \gamma a^{(3)}$. The general solution of the Bloch equations $\dot{x} = h \times x$ is given by expression (68), with $a(t)$ given by (97). The equations determining the angles ϕ and θ are given in the appendix.

The solution $a^{(2)}$ has the initial condition $a^{(2)}(t = 0) = (0, 1, 0)^T$. The other new solution is

$$\gamma a^{(1)} - \epsilon a^{(3)} = -\lambda \cos(\lambda\tau) \begin{pmatrix} \sin(\phi) \sin(\theta) \\ \cos(\phi) \sin(\theta) \\ \cos(\theta) \end{pmatrix} + \lambda \sin(\lambda\tau) \begin{pmatrix} \cos(\phi) \\ -\sin(\phi) \\ 0 \end{pmatrix}. \quad (98)$$

Its initial condition is $a(t = 0) = -\lambda(\sin\theta(0), 0, \cos\theta(0))^T$. Both new solutions are characterised by the appearance of the angle $\tau(t)$ describing a nutation of the rotation axis.

In the limit $k = 1$ the formulas simplify. The relevant expressions become

$$\sin(\phi) = \frac{a_1}{z} = \frac{\epsilon}{\sqrt{\epsilon^2 + \omega^2 \tanh^2(\omega t)}},$$



$$\begin{aligned}
\cos(\phi) &= \frac{a_2}{z} = \frac{\omega \tanh(\omega t)}{\sqrt{\epsilon^2 + \omega^2 \tanh^2(\omega t)}}, \\
\sin(\theta) &= -\frac{a_3}{\lambda} = \frac{\omega \tanh^2(\omega t) - \gamma}{\sqrt{\epsilon^2 + \gamma^2}}, \\
\cos(\theta) &= \frac{z}{\lambda} = \operatorname{sech}(\omega t) \sqrt{\frac{\epsilon^2 + \omega^2 \tanh^2(\omega t)}{\epsilon^2 + \gamma^2}}, \\
z &= \sqrt{a_1^2 + a_2^2} = \operatorname{sech}(\omega t) \sqrt{\epsilon^2 + \omega^2 \tanh^2(\omega t)}, \\
\lambda &= \sqrt{z^2 + a_3^2} = \sqrt{\epsilon^2 + \gamma^2} = \frac{\epsilon^2 + \omega^2}{2\omega}, \\
\alpha &= -\frac{a_1}{z^2} \xi = -\frac{2\epsilon\omega}{\epsilon^2 + \omega^2 \tanh^2(\omega t)},
\end{aligned} \tag{99}$$

with $\gamma = (\omega^2 - \epsilon^2)/2\omega$. The integral of $\alpha(t)$ can be done analytically. It yields

$$\tau(t) = -\int_0^t ds \alpha(s) = \frac{2\omega}{\epsilon^2 + \omega^2} \left\{ \epsilon t + \arctan\left(\frac{\omega}{\epsilon} \tanh(\omega t)\right) \right\}. \tag{100}$$

6.4 The Bloch equations at resonance

The resonant condition is $\epsilon = \omega$. In that case, γ , as given by (94), vanishes. The equations (A.19) can be used to obtain the general solution of $\dot{a} = h \times a$ at resonance

$$\begin{aligned}
a_1^{\text{gen}}(t) &= a_1^{\text{gen}}(0) \cos(\theta) \sin(\phi) \\
&\quad + \sin(\theta) \sin(\phi) [a_3^{\text{gen}}(0) \cos(\omega\tau) - a_2^{\text{gen}}(0) \sin(\omega\tau)] \\
&\quad - \cos(\phi) [a_2^{\text{gen}}(0) \cos(\omega\tau) + a_3^{\text{gen}}(0) \sin(\omega\tau)] \\
a_2^{\text{gen}}(t) &= a_1^{\text{gen}}(0) \cos(\theta) \cos(\phi) \\
&\quad + \sin(\theta) \cos(\phi) [a_3^{\text{gen}}(0) \cos(\omega\tau) - a_2^{\text{gen}}(0) \sin(\omega\tau)] \\
&\quad + \sin(\phi) [a_2^{\text{gen}}(0) \cos(\omega\tau) + a_3^{\text{gen}}(0) \sin(\omega\tau)] \\
a_3^{\text{gen}}(t) &= -a_1^{\text{gen}}(0) \sin(\theta) \\
&\quad + [a_3^{\text{gen}}(0) \cos(\omega\tau) - a_2^{\text{gen}}(0) \sin(\omega\tau)] \cos(\theta).
\end{aligned} \tag{101}$$

The correction angle α , given by (A.5), simplifies to

$$\alpha(t) = -\frac{a_1}{z^2} \xi = -k\omega (1 + \operatorname{cn}(2\omega t; k)). \tag{102}$$

This expression can be integrated analytically. The result is

$$\tau(t) = -\int_0^t ds \alpha(s) = kt - \frac{1}{\omega} \arctan \frac{\operatorname{dn}(\omega t; k)}{k \operatorname{sn}(\omega t; k) \operatorname{cn}(\omega t; k)}. \tag{103}$$

With some effort, (101) can now be written as

$$\begin{aligned}
a_1^{\text{gen}}(t) &= a_1^{\text{gen}}(0) \operatorname{cn}(\omega t; k) \\
&\quad + a_2^{\text{gen}}(0) \operatorname{sn}(\omega t; k) \cos(k\omega t) \\
&\quad + a_3^{\text{gen}}(0) \operatorname{sn}(\omega t; k) \sin(k\omega t), \\
a_2^{\text{gen}}(t) &= a_1^{\text{gen}}(0) \operatorname{sn}(\omega t; k) \operatorname{dn}(\omega t; k) \\
&\quad + a_2^{\text{gen}}(0) (\operatorname{cn}(\omega t; k) \operatorname{dn}(\omega t; k) \cos(k\omega t) - k \operatorname{sn}(\omega t; k) \sin(k\omega t)) \\
&\quad + a_3^{\text{gen}}(0) (\operatorname{cn}(\omega t; k) \operatorname{dn}(\omega t; k) \sin(k\omega t) + k \operatorname{sn}(\omega t; k) \cos(k\omega t)),
\end{aligned}$$

$$\begin{aligned}
a_3^{\text{gen}}(t) &= -a_1^{\text{gen}}(0)k \operatorname{sn}^2(\omega t; k) \\
&\quad + a_2^{\text{gen}}(0) (k \operatorname{cn}(\omega t; k) \operatorname{sn}(\omega t; k) \cos(k\omega t) + \operatorname{dn}(\omega t; k) \sin(k\omega t)) \\
&\quad + a_3^{\text{gen}}(0) (k \operatorname{cn}(\omega t; k) \operatorname{sn}(\omega t; k) \sin(k\omega t) - \operatorname{dn}(\omega t; k) \cos(k\omega t)). \quad (104)
\end{aligned}$$

The three independent solutions are therefore

$$\begin{aligned}
a^{(1)} &= \begin{pmatrix} \operatorname{cn}(\omega t; k) \\ \operatorname{sn}(\omega t; k) \operatorname{dn}(\omega t; k) \\ -k \operatorname{sn}^2(\omega t; k) \end{pmatrix}, \\
a^{(2)} &= \begin{pmatrix} \operatorname{sn}(\omega t; k) \cos(k\omega t) \\ \operatorname{cn}(\omega t; k) \operatorname{dn}(\omega t; k) \cos(k\omega t) - k \operatorname{sn}(\omega t; k) \sin(k\omega t) \\ k \operatorname{cn}(\omega t; k) \operatorname{sn}(\omega t; k) \cos(k\omega t) + \operatorname{dn}(\omega t; k) \sin(k\omega t) \end{pmatrix}, \\
a^{(3)} &= \begin{pmatrix} \operatorname{sn}(\omega t; k) \sin(k\omega t) \\ \operatorname{cn}(\omega t; k) \operatorname{dn}(\omega t; k) \sin(k\omega t) + k \operatorname{sn}(\omega t; k) \cos(k\omega t) \\ k \operatorname{cn}(\omega t; k) \operatorname{sn}(\omega t; k) \sin(k\omega t) - \operatorname{dn}(\omega t; k) \cos(k\omega t) \end{pmatrix}. \quad (105)
\end{aligned}$$

One clearly has $a = \omega a^{(1)}$, the special solution we started with. It is easy to verify that also $a^{(2)}$ and $a^{(3)}$ are solutions of $\dot{a} = a \times h$.

7 Bloch equations continued

7.1 Including phase modulation

A slightly different solution is obtained when the parameter ϵ in (90) is made time dependent in the following way

$$\epsilon = \epsilon_0 \tanh(\omega t). \quad (106)$$

In [9], the resulting equations are called the Bloch equations including phase modulation. Also in this case a special solution is known. The generalisation to Jacobi's elliptic functions, as given below, can be done in two different ways.

7.2 Special solutions

Assume that

$$\begin{aligned}
\xi(t) &= \xi_0 \operatorname{cn}(\omega t; k), \\
\epsilon(t) &= \epsilon_0 \operatorname{sn}(\omega t; k). \quad (107)
\end{aligned}$$

or

$$\begin{aligned}
\xi(t) &= \xi_0 \operatorname{dn}(\omega t; k), \\
\epsilon(t) &= \epsilon_0 \operatorname{sn}(\omega t; k). \quad (108)
\end{aligned}$$

Both assumptions reduce to $\xi(t) = \xi_0 \operatorname{sech}(\omega t)$ and (106) in the limit $k = 1$.

A solution of the equations (90) is given by

$$\begin{aligned}
a_1(t) &= \epsilon_0 \operatorname{cn}(\omega t; k), \\
a_2(t) &= \omega \operatorname{dn}(\omega t; k), \\
a_3(t) &= -\xi_0 \operatorname{sn}(\omega t; k). \quad (109)
\end{aligned}$$

or

$$\begin{aligned} a_1(t) &= \omega \operatorname{cn}(\omega t; k), \\ a_2(t) &= \epsilon_0 \operatorname{dn}(\omega t; k), \\ a_3(t) &= -\xi_0 \operatorname{sn}(\omega t; k). \end{aligned} \quad (110)$$

provided that $\xi_0^2 = \epsilon_0^2 + \omega^2 k^2$, respectively $\xi_0^2 = \epsilon_0^2 k^2 + \omega^2$, is satisfied.

Only the first of the cases is treated below. The other case is completely analogous.

Note that in the limit $k = 1$ the solution (109) reduces to the well-known solution

$$\begin{aligned} a_1(t) &= \epsilon_0 \operatorname{sech}(\omega t), \\ a_2(t) &= \omega \operatorname{sech}(\omega t), \\ a_3(t) &= -\xi_0 \tanh(\omega t). \end{aligned} \quad (111)$$

In the limit $k = 0$ it reduces to a harmonic precession

$$\begin{aligned} \xi(t) &= \xi_0 \cos(\omega t), \\ \epsilon(t) &= \epsilon_0 \sin(\omega t), \\ a_1(t) &= \epsilon_0 \cos(\omega t), \\ a_2(t) &= \omega, \\ a_3(t) &= -\xi_0 \sin(\omega t). \end{aligned} \quad (112)$$

7.3 General solution including phase modulation

It is now possible to obtain the general solution of the Bloch equations including phase modulation, with driving fields of the form (107).

The three independent solutions of $\dot{a} = h \times a$, obtained from (B.6), are

$$\begin{aligned} a^{(1)}(t) &= \frac{\epsilon_0}{\lambda} \begin{pmatrix} \sin(\phi) \cos(\theta) \\ \cos(\phi) \cos(\theta) \\ -\sin(\theta) \end{pmatrix} \\ &\quad + \frac{\omega}{\lambda} \sin(\lambda \tau) \begin{pmatrix} \sin(\phi) \sin(\theta) \\ \cos(\phi) \sin(\theta) \\ \cos(\theta) \end{pmatrix} + \frac{\omega}{\lambda} \cos(\lambda \tau) \begin{pmatrix} \cos(\phi) \\ -\sin(\phi) \\ 0 \end{pmatrix}, \\ a^{(2)}(t) &= \frac{\omega}{\lambda} \begin{pmatrix} \sin(\phi) \cos(\theta) \\ \cos(\phi) \cos(\theta) \\ -\sin(\theta) \end{pmatrix} \\ &\quad - \frac{\epsilon_0}{\lambda} \sin(\lambda \tau) \begin{pmatrix} \sin(\phi) \sin(\theta) \\ \cos(\phi) \sin(\theta) \\ \cos(\theta) \end{pmatrix} - \frac{\epsilon_0}{\lambda} \cos(\lambda \tau) \begin{pmatrix} \cos(\phi) \\ -\sin(\phi) \\ 0 \end{pmatrix}, \\ a^{(3)}(t) &= \cos(\lambda \tau) \begin{pmatrix} \sin(\phi) \sin(\theta) \\ \cos(\phi) \sin(\theta) \\ \cos(\theta) \end{pmatrix} - \sin(\lambda \tau) \begin{pmatrix} \cos(\phi) \\ -\sin(\phi) \\ 0 \end{pmatrix}. \end{aligned} \quad (113)$$

The equations determining the angles ϕ and θ are found in the Appendix B. The special solution (109) satisfies $a = \epsilon_0 a^{(1)} + \omega a^{(2)}$. The general solution of the equations $\dot{x} = h \times x$ has been given in Section 4.5 and can be rederived from the knowledge of $a^{(1)}, a^{(2)}, a^{(3)}$.

7.4 The $k = 1$ -limit

In this limit the existence of the special solution requires that $\xi_0 = \lambda$. The angle ϕ and the phase α become constants

$$\sin(\phi) = \frac{\epsilon_0}{\lambda} \quad \text{and} \quad \cos(\phi) = \frac{\omega}{\lambda} \quad (114)$$

and $\alpha = -\epsilon_0 \xi_0 / \lambda^2$. Hence one has $\lambda \tau(t) = \epsilon_0 t$. The angle θ satisfies

$$\sin(\theta) = -\tanh(\omega t) \quad \text{and} \quad \cos(\theta) = \text{sech}(\omega t). \quad (115)$$

The three independent solutions are

$$\begin{aligned} a^{(1)}(t) &= \frac{\epsilon_0}{\lambda^2} \begin{pmatrix} \epsilon_0 \text{sech}(\omega t) \\ \omega \text{sech}(\omega t) \\ \lambda \tanh(\omega t) \end{pmatrix} + \frac{\omega}{\lambda^2} \sin(\epsilon_0 t) \begin{pmatrix} -\epsilon_0 \tanh(\omega t) \\ -\omega \tanh(\omega t) \\ \lambda \text{sech}(\omega t) \end{pmatrix} + \frac{\omega}{\lambda^2} \cos(\epsilon_0 t) \begin{pmatrix} \omega \\ -\epsilon_0 \\ 0 \end{pmatrix} \\ a^{(2)}(t) &= \frac{\omega}{\lambda^2} \begin{pmatrix} \epsilon_0 \text{sech}(\omega t) \\ \omega \text{sech}(\omega t) \\ \lambda \tanh(\omega t) \end{pmatrix} - \frac{\epsilon_0}{\lambda^2} \sin(\epsilon_0 t) \begin{pmatrix} -\epsilon_0 \tanh(\omega t) \\ -\omega \tanh(\omega t) \\ \lambda \text{sech}(\omega t) \end{pmatrix} - \frac{\epsilon_0}{\lambda^2} \cos(\epsilon_0 t) \begin{pmatrix} \omega \\ -\epsilon_0 \\ 0 \end{pmatrix} \\ a^{(3)}(t) &= \frac{1}{\lambda} \cos(\epsilon_0 t) \begin{pmatrix} -\epsilon_0 \tanh(\omega t) \\ -\omega \tanh(\omega t) \\ \lambda \text{sech}(\omega t) \end{pmatrix} - \frac{1}{\lambda} \sin(\epsilon_0 t) \begin{pmatrix} \omega \\ -\epsilon_0 \\ 0 \end{pmatrix}. \end{aligned} \quad (116)$$

8 The generalised harmonic oscillator

Consider creation and annihilation operators b^\dagger and b satisfying the canonical commutation relations $[b, b^\dagger] = \mathbb{I}$. Then the operators

$$\begin{aligned} S_1 &= \frac{1}{4}((b^\dagger)^2 + b^2), \\ S_2 &= \frac{i}{4}((b^\dagger)^2 - b^2), \\ S_3 &= \frac{1}{4}(b^\dagger b + b b^\dagger) \end{aligned} \quad (117)$$

satisfy (69). Hamiltonians which can be written as a linear combination of these generators are the generalised harmonic oscillators.

8.1 Time-dependent frequency

Consider the harmonic oscillator with arbitrary time-dependent frequency $\omega(t)$

$$H = \frac{1}{2m} P^2 + \frac{1}{2} m \omega^2(t) Q^2. \quad (118)$$

Here, Q is the position operator and P the momentum operator. They satisfy $[Q, P] = i$. This problem was studied by Lewis and Riesenfeld [3]. See also [5, 13, 17, 27, 28, 33, 34, 37, 40]. Also here we use the known analytical solutions to derive the general solution with arbitrary initial conditions.

Introduce an annihilation operator defined by

$$b = \frac{1}{r\sqrt{2}} Q + i \frac{r}{\sqrt{2}} P, \quad (119)$$

with $r = \frac{1}{\sqrt{m\omega_0}}$ and ω_0 some constant frequency. Then the generators equal

$$S_1 = \frac{1}{4r^2}Q^2 - \frac{r^2}{4}P^2 \quad (120)$$

$$S_2 = \frac{1}{4}(QP + PQ) \quad (121)$$

$$S_3 = \frac{1}{4r^2}Q^2 + \frac{r^2}{4}P^2. \quad (122)$$

Introduce the function $\gamma(t)$, modulating the frequency ω_0 , defined by $\omega(t) = \gamma(t)\omega_0$. The Hamiltonian becomes

$$\begin{aligned} H(t) &= -\frac{1}{4}\omega_0(b - b^\dagger)^2 + \frac{1}{4}\omega_0\gamma^2(t)(b + b^\dagger)^2 \\ &= \omega_0(\gamma^2(t) - 1)S_1 + \omega_0(\gamma^2(t) + 1)S_3. \end{aligned} \quad (123)$$

Hence one has $h = \omega_0(\gamma^2(t) - 1, 0, \gamma^2(t) + 1)^\top$.

8.2 Special solution

The time evolution equation reads (see the definition (70) of the Lie bracket)

$$\begin{aligned} \dot{a} &= h \times a \\ &= (h_3a_2, h_1a_3 - h_3a_1, h_1a_2)^\top \\ &= \omega_0(\gamma^2(t) + 1)(a_2, -a_1, 0)^\top + \omega_0(\gamma^2(t) - 1)(0, a_3, a_2)^\top. \end{aligned} \quad (124)$$

Proposition 2 *Let $x(t)$ be a solution of the classical oscillator equation*

$$\ddot{x} + \omega^2(t)x = 0. \quad (125)$$

Then a , defined by

$$a = \frac{1}{2}(\dot{x})^2(1, 0, 1)^\top + \frac{1}{2}\omega_0^2x^2(-1, 0, 1)^\top - \omega_0x\dot{x}(0, 1, 0)^\top, \quad (126)$$

is a solution of (124).

The proof is done by explicit calculation. One concludes that, to find a special solution of the von Neumann equation, it suffices to find a special solution of the classical equation (125). Note that the latter problem is equivalent with solving Riccati's equation

$$\dot{g} - g^2 = \omega^2(t). \quad (127)$$

The corresponding solution of (125) is

$$x = C \exp\left(-\int dt g(t)\right), \quad (128)$$

with integration constant C . In the case that $\omega(t)$ is constant one finds

$$g(t) = \omega \tan(\omega t) \quad (129)$$

so that $x(t) = C \cos(\omega t)$. With $C = 1$ and $\omega_0 = \omega$ one obtains the special solution

$$a = \frac{1}{2}\omega^2(-\cos(2\omega t), \sin(2\omega t), 1)^T. \quad (130)$$

If $\omega(t)$ is of the form $\omega(t) = \omega_0(1 + \epsilon \cos(2\lambda t))$ then the equation (125) is related to Mathieu's equation. The solution $x = \text{cn}(\omega_0 t; k)$, involving Jacobi's elliptic function with $0 < k < 1/\sqrt{2}$, is obtained when

$$\omega(t) = \omega_0 \sqrt{2 \text{dn}^2(\omega_0 t; k) - 1}. \quad (131)$$

8.3 Automorphisms

Note that the special solution (126) satisfies $\langle a|a \rangle = 0$ (using the metric with signature $-, -, +$). Hence, we have to apply the exceptional case discussed at the end of Section 5.1.

Write $a(t)$ into the form

$$a(t) = R_3(\phi)P_1(\chi)R_3(-\phi(0))a(0). \quad (132)$$

From (78) follows

$$\begin{aligned} \sin(\phi) &= \frac{a_1}{a_3} = \frac{(\dot{x})^2 - \omega_0^2 x^2}{(\dot{x})^2 + \omega_0^2 x^2}, \\ \cos(\phi) &= \frac{a_2}{a_3} = \frac{2\omega_0 x \dot{x}}{(\dot{x})^2 + \omega_0^2 x^2}. \end{aligned} \quad (133)$$

From (84) follows

$$\chi = \ln \frac{a_3(t)}{a_3(0)} = \ln \frac{(\dot{x})^2 + \omega_0^2 x^2}{[(\dot{x})^2 + \omega_0^2 x^2]_{t=0}}. \quad (134)$$

Note that $\phi(0)$ simplifies if either $x(0) = 0$ or $\dot{x}(0) = 0$.

From the general theory now follows that (see (77))

$$V(t) = e^{-i\phi(t)S_3} e^{-i\chi(t)S_1} e^{i\phi(0)S_3}. \quad (135)$$

The corresponding Hamiltonian is

$$K = \dot{\chi} \{ \cos(\phi)S_1 - \sin(\phi)S_2 \} + \dot{\phi}S_3. \quad (136)$$

Note that

$$\dot{\chi} = \frac{\dot{a}_3}{a_3} = h_1 \frac{a_2}{a_3} \quad \text{and} \quad \dot{\phi} = \frac{a_2 \dot{a}_1 - a_1 \dot{a}_2}{a_3^2} = h_3 - h_1 \frac{a_1}{a_3}. \quad (137)$$

Hence K can be written as

$$\begin{aligned} K &= (\cos(\phi)\dot{\chi}, -\sin(\phi)\dot{\chi}, \dot{\phi})^T \\ &= \frac{1}{a_3^2} (h_1 a_2^2, -h_1 a_1 a_2, h_3 a_3^2 - h_1 a_1 a_3)^T. \end{aligned} \quad (138)$$

One obtains $h - k = \alpha a$, with

$$\alpha = h_1 \frac{a_1}{a_3}. \quad (139)$$

The final result is

$$U(t) = V(t) e^{if_t(\rho_s(0)-C)} = e^{-i\phi(t)S_3} e^{-i\chi(t)S_1} e^{i\phi(0)S_3} e^{i\sum_j a_j(0)S_j \int_0^t ds \alpha(s)}. \quad (140)$$

It can be used to calculate the time evolution with arbitrary initial conditions. In particular, one can start with an initial state which does not satisfy the 'light cone condition' $\langle a|a\rangle = 0$.

9 More general oscillators

More general time-dependent harmonic oscillators have been considered in the literature [7, 11, 12, 21, 30, 32, 37]. Even damped oscillators have been studied — see for instance [15, 18, 31]. Some of them can be treated by the present method. An example not yet considered in the literature is $H = \sum_{j=1}^3 h_j(t)S_j$ with

$$h_1(t) = a \operatorname{cn}(\omega t; k) \quad (141)$$

$$h_2(t) = -a \operatorname{sn}(\omega t; k) \quad (142)$$

$$h_3(t) = c + \omega \operatorname{dn}(\omega t; k), \quad (143)$$

with constants ω , a , c , and $0 \leq k \leq 1$. A special solution of the von Neumann equation is given by (see [35]) $\rho_s(t) = \sum_{j=1}^3 a_j(t)S_j$ with

$$a_1(t) = a \operatorname{cn}(\omega t; k) \quad (144)$$

$$a_2(t) = -a \operatorname{sn}(\omega t; k) \quad (145)$$

$$a_3(t) = c. \quad (146)$$

Note that $\rho_s(t)$ is not a density operator. But this does not harm our method.

Introduce unitary operators $V(t)$ by (see (77))

$$V(t) = e^{-i\phi(t)S_3} e^{-i\chi(t)S_1} e^{i\chi(0)S_1} e^{i\phi(0)S_3} \quad (147)$$

with angles $\phi(t)$ and $\chi(t)$ satisfying (see (78))

$$\sin(\phi) = \operatorname{cn}(\omega t; k), \quad \cos(\phi) = \operatorname{sn}(\omega t; k) \quad (148)$$

$$\sinh(\chi) = \frac{c}{\sqrt{a^2 - c^2}}, \quad \cosh(\chi) = \frac{a}{\sqrt{a^2 - c^2}}. \quad (149)$$

Note that we assume that $a^2 > c^2$. Also, note that $\phi(0) = \pi/2$. Because $\chi(t)$ turns out to be independent of time t , (147) simplifies to

$$V(t) = e^{-i(\phi(t)-\phi(0))S_3}. \quad (150)$$

Next calculate

$$\alpha(t) = \frac{a_1 h_1 + a_2 h_2}{a^2} = 1. \quad (151)$$

Hence, the time evolution is described by the unitary operators

$$U(t) = V(t)e^{-i\rho_s(0)t} = e^{-i(\phi(t)-\phi(0))S_3} e^{-it(aS_1+cS_3)}. \quad (152)$$

It is now possible to calculate the time evolution of the generators in the Heisenberg picture. For simplicity take $c = 0$. Then one obtains

$$\begin{aligned} S_1(t) &= U(t)^* S_1 U(t) \\ &= \cos(\phi(t) - \phi(0)) S_1 + \sin(\phi(t) - \phi(0)) S_2 \\ &= \sin(\phi(t)) S_1 - \cos(\phi(t)) S_2 \\ &= \operatorname{cn}(\omega t; k) S_1 - \operatorname{sn}(\omega t; k) S_2. \end{aligned} \quad (153)$$

Similarly is

$$\begin{aligned} S_2(t) &= U(t)^* S_2 U(t) \\ &= \cosh(at) [\cos(\phi(t) - \phi(0)) S_2 - \sin(\phi(t) - \phi(0)) S_1] - \sinh(at) S_3 \\ &= \cosh(at) [\sin(\phi(t)) S_2 + \cos(\phi(t)) S_1] - \sinh(at) S_3 \\ &= \cosh(at) [\operatorname{cn}(\omega t; k) S_2 + \operatorname{sn}(\omega t; k) S_1] - \sinh(at) S_3, \end{aligned} \quad (154)$$

and

$$\begin{aligned} S_3(t) &= U(t)^* S_3 U(t) \\ &= \cosh(at) S_3 - \sinh(at) [\cos(\phi(t) - \phi(0)) S_2 - \sin(\phi(t) - \phi(0)) S_1] \\ &= \cosh(at) S_3 - \sinh(at) [\sin(\phi(t)) S_2 + \cos(\phi(t)) S_1] \\ &= \cosh(at) S_3 - \sinh(at) [\operatorname{cn}(\omega t; k) S_2 + \operatorname{sn}(\omega t; k) S_1]. \end{aligned} \quad (155)$$

Note that S_3 is the energy of the unperturbed harmonic oscillator. Clearly, this quantity explodes for large times. Hence, the time-dependent harmonic oscillator described by (143) is at resonance.

10 Discussion

We present a general method of constructing unitary operators $U(t)$ that solve a quantum time evolution in the case of a time-dependent Hamiltonian $H(t)$. The method starts from a special solution of the von Neumann equation. It differs from the approach of [3], where the special solution is called a time-dependent invariant, by using an explicit solution instead of defining it by means of a classical differential equation and an asymptotic procedure. The method is worked out in detail for the case that $H(t)$ can be written as a linear combination of generators S_1, \dots, S_n of a Lie algebra, with time-dependent coefficients. Most studied in the literature is the case of $SU(2)$. The explicit expressions for the operators $U(t)$, known as Magnus expansion, respectively Wei-Norman expansion, are shown to be special instances of a more general theory and correspond to specific representations of the rotation group in \mathbb{R}^3 . A simpler expression for the operators $U(t)$ is obtained when the rotations are described in terms of Euler angles – see (62) and (66). Also the case of $SU(1,1)$ has been discussed often. The representation of the rotation group involving Euler angles can be adapted to this case. The result is given by (77, 82).

The generator corresponding to the special solution is denoted by $K(t)$. The result of Proposition 1 is very convenient because it proves that the difference between the Hamiltonians $H(t)$ and $K(t)$ is a linear function of the special solution $\rho_s(t)$. The conditions of

this Proposition may not always be fulfilled. But one can fall back on the general method described in Section 2. It suffices that the special solution $\rho_s(0)$ is multiplicity free. Then the left side of (16) is an element of a commutative algebra generated by $\rho_s(0)$, and at the same time an element of a Lie algebra. The degree of difficulty of determining the form of $f_t(x)$ depends on how many different functions of $\rho_s(0)$ are Lie-algebra valued. Nevertheless, in all cases the procedure just reduces to integration of ordinary functions. The expression $e^{if_t(\rho_s(0))}$ in (15) is easy to calculate as an exponent of a sum of commuting operators.

Initially [1, 2], the Wei-Norman method translated the problem of obtaining explicit expressions for the operators $U(t)$ into sets of differential equations with time-dependent coefficients. In the Lie-algebraic context these equations can be written into the form $\dot{x} = h \times x$, where we use the notation $h \times x$ for the Lie bracket of h and x . The main result of the present approach is that we obtain the general solution x of these equations, starting from a special solution – see (68) and (87, 88).

The method depends on the knowledge of a special solution. Note that the Schrödinger and von Neumann equations with time-dependent Hamiltonian are related to the non-linear Schrödinger and von Neumann equations. In particular, a solution of the non-linear equation

$$\frac{d}{dt}\rho(t) = i[\rho(t)^2, H] \quad (156)$$

can be used as a special solution of the von Neumann equation (4) with time-dependent Hamiltonian $H(t) = \rho(t)H + H\rho(t)$. See for instance [26]. The theory of finding special solutions for non-linear von Neumann equations can be found in [25].

We apply our method to two well-known cases, one corresponding with $SU(2)$ symmetry, the other with $SU(1,1)$. In both cases the method is shown to reproduce known results and to produce some new results as well.

We did not try to reproduce the most general results found in the literature. We are confident that we could do so, at the expense of writing a more technical and less pedagogical paper. Of more interest is the application of our method to other Lie algebras.

In [21], the Lie algebra that we used in Section 4 is extended to contain 6 elements $\frac{1}{2}P^2$, $\frac{1}{2}Q^2$, $\frac{1}{2}(PQ + QP)$, P , Q , \mathbb{I} . With this extension it becomes possible to calculate the time evolution in the Heisenberg picture of physically interesting quantities such as the position Q and the momentum P . One then can calculate the classical phase portrait by studying the orbit $t \rightarrow \langle \psi|Q(t)|\psi \rangle, \langle \psi|P(t)|\psi \rangle$ for an arbitrary wavefunction ψ . This will be done in a future work.

Weigert [23] has considered the general case of $SU(N)$ symmetry. Lopez and Suslov [38] used the Heisenberg-Weyl group $N(3)$ to describe a forced harmonic oscillator. Finally, Cariñena et al [39], among others, are interested in developing a superposition principle for nonlinear equations by mapping the solutions onto the solutions of linear equations with time-dependent coefficients.

Appendix A

Here, our method is applied to find the general solution of the Bloch equations starting from the special solution (93).

Following the general method of Section 4.4 the transformation $V(t)$ is determined by two angles $\phi(t), \theta(t)$. The special solution $a(t)$ at time $t = 0$ reads

$$a(0) = (\epsilon, 0, \gamma)^T. \quad (\text{A.1})$$

It is rotated into the fixed vector $\lambda(0, 1, 0)^T$. One has

$$\begin{aligned} z(t) &= \sqrt{a_1^2(t) + a_2^2(t)} = \sqrt{\epsilon^2 \text{cn}^2(\omega t; k) + \omega^2 \text{sn}^2(\omega t; k) \text{dn}^2(\omega t; k)}, \\ z(0) &= \epsilon, \\ \lambda &= \sqrt{z^2(t) + a_3^2(t)} = \sqrt{\epsilon^2 + \gamma^2}. \end{aligned} \quad (\text{A.2})$$

The angles $\phi(t)$ and $\theta(t)$ are determined by (62). In particular, at $t = 0$ is

$$\begin{aligned} \sin(\phi(0)) &= \frac{a_1(0)}{z(0)} = 1 & \text{and} & \quad \cos(\phi(0)) = \frac{a_2(0)}{z(0)} = 0, \\ \sin(\theta(0)) &= -\frac{a_3(0)}{\lambda} = -\frac{\gamma}{\lambda} & \text{and} & \quad \cos(\theta(0)) = \frac{z(0)}{\lambda} = \frac{\epsilon}{\lambda}. \end{aligned} \quad (\text{A.3})$$

One can understand these values as follows. By a rotation of $-\phi(0) = -\pi/2$ around the third axis the initial vector $a(0)$ becomes $(0, \epsilon, \gamma)^T$. Then by a rotation with angle $-\theta(0)$ around the first axis it becomes $(0, \lambda, 0)^T$. Next, the rotation $R_1(\theta(t))$, followed by the rotation $R_3(\phi(t))$ maps this fixed vector onto the time-dependent $a(t)$.

The Hamiltonian $K(t)$ equals (see (64))

$$\begin{aligned} K(t) &= \frac{a_2 \dot{a}_3}{z^2} S_1 - \frac{a_1 \dot{a}_3}{z^2} S_2 + \frac{a_1 \dot{a}_2 - a_2 \dot{a}_1}{z^2} S_3 \\ &= \frac{\xi(t)}{z^2(t)} [-a_2^2(t) S_1 + a_1(t) a_2(t) S_2 + a_1(t) a_3(t) S_3] + \epsilon S_3. \end{aligned} \quad (\text{A.4})$$

The difference between this $K(t)$ and the Hamiltonian $H(t)$ as given by (89) makes an extra rotation necessary. It involves the function $\alpha(t)$, given by (65). It evaluates to

$$\alpha(t) = -\frac{a_1(t)}{z^2(t)} \xi(t) = -\frac{2\epsilon\omega k \text{cn}^2(\omega t; k)}{\epsilon^2 \text{cn}^2(\omega t; k) + \omega^2 \text{sn}^2(\omega t; k) \text{dn}^2(\omega t; k)}. \quad (\text{A.5})$$

The final result then becomes

$$U(t) = e^{i\phi(t)S_3} e^{i(\theta(t)-\theta(0))S_1} e^{-i(\pi/2)S_3} e^{-i(\int_0^t ds \alpha(s))(\epsilon S_1 + \gamma S_3)}. \quad (\text{A.6})$$

Note that this expression can be simplified to

$$U(t) = e^{i(\phi(t)-\pi/2)S_3} e^{-i(\theta(t)-\theta(0))S_2} e^{i\lambda\tau X}. \quad (\text{A.7})$$

with $\tau \equiv \tau(t) = -\int_0^t ds \alpha(s)$ and $X = \frac{\epsilon S_1 + \gamma S_3}{\lambda}$. For further use note that

$$e^{i\lambda\tau X} S_j e^{-i\lambda\tau X} = S_j + i \sin(\lambda\tau) [X, S_j] + (\cos(\lambda\tau) - 1) [X, [X, S_j]]. \quad (\text{A.8})$$

Note that (omitting time dependences and denoting $\theta_0 \equiv \theta(0)$)

$$\epsilon \cos(\theta - \theta_0) - \gamma \sin(\theta - \theta_0) = \frac{\epsilon^2 - \gamma^2}{\lambda} \cos(\theta) - 2\frac{\epsilon\gamma}{\lambda} \sin(\theta)$$

$$\begin{aligned}
\gamma \cos(\theta - \theta_0) + \epsilon \sin(\theta - \theta_0) &= 2\frac{\epsilon\gamma}{\lambda} \cos(\theta) + \frac{\epsilon^2 - \gamma^2}{\lambda} \sin(\theta) \\
\gamma \cos(\theta - \theta_0) - \epsilon \sin(\theta - \theta_0) &= -\lambda \sin(\theta) \\
\epsilon \cos(\theta - \theta_0) + \gamma \sin(\theta - \theta_0) &= \lambda \cos(\theta).
\end{aligned} \tag{A.9}$$

These relations can be used to calculate

$$\begin{aligned}
U(t)(\epsilon S_1 + \gamma S_3)U(t)^* &= -\lambda \sin(\theta)S_3 + \lambda \cos(\theta)S_+, \\
\lambda U(t)(\epsilon S_1 - \gamma S_3)U(t)^* &= [(\epsilon^2 - \gamma^2) \cos(\theta) - 2\epsilon\gamma \sin(\theta) \cos(\lambda\tau)] S_+ \\
&\quad + 2\gamma\epsilon \sin(\lambda\tau)S_- \\
&\quad - [2\epsilon\gamma \cos(\theta) \cos(\lambda\tau) + (\epsilon^2 - \gamma^2) \sin(\theta)] S_3 \\
U(t)S_2U(t)^* &= -\sin(\lambda\tau) \cos(\theta)S_3 - \cos(\lambda\tau)S_- - \sin(\theta) \sin(\lambda\tau)S_+,
\end{aligned} \tag{A.10}$$

with

$$S_+ = \sin(\phi)S_1 + \cos(\phi)S_2 \quad \text{and} \quad S_- = \cos(\phi)S_1 - \sin(\phi)S_2. \tag{A.11}$$

Note further that

$$\begin{aligned}
\dot{\phi} &= -\epsilon + \xi \sin(\phi) \tan(\theta) \\
\dot{\theta} &= \xi \cos(\phi) \\
\dot{\tau} &= \frac{\xi \sin(\phi)}{\lambda \cos(\theta)}.
\end{aligned} \tag{A.12}$$

Using these equations one can verify explicitly that the time-dependent operators (A.10) satisfy indeed the von Neumann equation of motion.

Let us finally consider the situation when the resonance condition $\epsilon = \omega$ is satisfied. The normalisations $z(t)$ and λ , given by (A.2) and appearing in the expressions for the angles ϕ and θ (see (62)), become

$$z(t) = \omega \sqrt{\text{cn}^2(\omega t; k) + \text{sn}^2(\omega t; k) \text{dn}^2(\omega t; k)}, \tag{A.13}$$

$$\lambda = \omega. \tag{A.14}$$

There follows

$$\sin(2\phi) = \frac{2a_1a_2}{z^2} = \text{sn}(2\omega t; k) \tag{A.15}$$

$$\cos(2\phi) = \frac{a_2^2 - a_1^2}{z^2} = -\text{cn}(2\omega t; k) \tag{A.16}$$

$$\sin(\theta) = -\frac{a_3}{\lambda} = k \text{sn}^2(\omega t; k), \tag{A.17}$$

$$\cos(\theta) = \frac{z}{\lambda} = \sqrt{\text{cn}^2(\omega t; k) + \text{sn}^2(\omega t; k) \text{dn}^2(\omega t; k)}. \tag{A.18}$$

In particular is $\theta(0) = 0$. The equations (A.10) become

$$\begin{aligned}
U(t)S_1U(t)^* &= -\sin(\theta)S_3 + \cos(\theta)S_+, \\
U(t)S_3U(t)^* &= \sin(\theta) \cos(\omega\tau)S_+ - \sin(\omega\tau)S_- + \cos(\omega\tau) \cos(\theta)S_3 \\
U(t)S_2U(t)^* &= -\sin(\omega\tau) \cos(\theta)S_3 - \cos(\omega\tau)S_- - \sin(\theta) \sin(\omega\tau)S_+.
\end{aligned} \tag{A.19}$$

Appendix B

Here, our method is applied to find the general solution of the Bloch equations including phase modulation.

Consider the special solution (109). The angles $\phi(t)$ and $\theta(t)$ are determined by (62). In particular, at $t = 0$ is

$$\sin(\phi(0)) = \frac{\epsilon_0}{\lambda}, \quad \cos(\phi(0)) = \frac{\omega}{\lambda}, \quad (\text{B.1})$$

and $\theta(0) = 0$, with $\lambda = \sqrt{\epsilon_0^2 + \omega^2}$. This means that by a rotation $R_3(-\phi(0))$ around the third axis the initial vector $a(0)$ is rotated into the fixed vector $\lambda(0, 1, 0)^T$. Next, the rotation $R_1(\theta(t))$, followed by the rotation $R_3(\phi(t))$ maps this fixed vector onto the time-dependent $a(t)$.

The Hamiltonian $K(t)$ equals (see (64))

$$\begin{aligned} K(t) &= \frac{a_2 \dot{a}_3}{z^2} S_1 - \frac{a_1 \dot{a}_3}{z^2} S_2 + \frac{a_1 \dot{a}_2 - a_2 \dot{a}_1}{z^2} S_3 \\ &= \frac{\xi(t)}{z^2(t)} [-a_2^2(t) S_1 + a_1(t) a_2(t) S_2 + a_1(t) a_3(t) S_3] + \epsilon S_3. \end{aligned} \quad (\text{B.2})$$

This is the same expression as (A.4). The difference between this $K(t)$ and the Hamiltonian $H(t)$ as given by (89) makes an extra rotation necessary. It involves the function $\alpha(t)$, given by (65). It evaluates to

$$\alpha(t) = -\frac{a_1(t)}{z^2(t)} \xi(t) = -\frac{\epsilon_0 \xi_0 \operatorname{cn}(\omega t; k) \operatorname{dn}(\omega t; k)}{\epsilon_0^2 \operatorname{cn}^2(\omega t; k) + \omega^2 \operatorname{dn}^2(\omega t; k)}. \quad (\text{B.3})$$

The final result then becomes

$$U(t) = e^{i\phi(t)S_3} e^{i\theta(t)S_1} e^{-i\phi(0)S_3} e^{i\lambda\tau(t)X}, \quad (\text{B.4})$$

with $\tau(t) = -\int_0^t ds \alpha(s)$ and $X = \frac{\epsilon_0 S_1 + \omega S_2}{\lambda}$. Note that (B.3) can be integrated analytically. The result is

$$\tau(t) = \frac{\epsilon_0 \xi_0}{2\omega \lambda \mu} \ln \frac{\lambda + \mu \operatorname{sn}(\omega t; k)}{\lambda - \mu \operatorname{sn}(\omega t; k)} \quad (\text{B.5})$$

with $\mu = \sqrt{\epsilon_0^2 + k^2 \omega^2}$.

One further calculates (again omitting time dependencies and denoting $\phi_0 \equiv \phi(0)$)

$$\begin{aligned} U(t)(\epsilon_0 S_1 + \omega S_2)U(t)^* &= \lambda \cos(\theta) S_+ - \lambda \sin(\theta) S_3 \\ \lambda U(t)(\epsilon_0 S_1 - \omega S_2)U(t)^* &= [(\epsilon_0^2 - \omega^2) \cos(\theta) + 2\epsilon_0 \omega \sin(\theta) \sin(\lambda\tau)] S_+ \\ &\quad + 2\epsilon_0 \omega \cos(\lambda\tau) S_- \\ &\quad + [2\epsilon_0 \omega \cos(\theta) \sin(\lambda\tau) - (\epsilon_0^2 - \omega^2) \sin(\theta)] S_3 \\ U(t)S_3U(t)^* &= \cos(\lambda\tau) \sin(\theta) S_+ - \sin(\lambda\tau) S_- + \cos(\lambda\tau) \cos(\theta) S_3, \end{aligned} \quad (\text{B.6})$$

with

$$S_+ = \sin(\phi) S_1 + \cos(\phi) S_2 \quad \text{and} \quad S_- = \cos(\phi) S_1 - \sin(\phi) S_2. \quad (\text{B.7})$$

This result can be used to derive the general solution of $\dot{a} = h \times a$.

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