Effective Hamiltonians in Two-Level Quantum Dynamics

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Abstract

The time evolution of two-level quantum systems such as spin-1/2 particles in magnetic fields are introduced in major textbooks by immediately casting the time-dependent Schrödinger equation as a set of coupled differential equations. This is a dry approach, which leaves out a great deal of physics insight that is critical for understanding the time evolution of the system. A more useful alternative is to explore fully the richness of dynamics observed from rotating frames—with which students may already be familiar from classical mechanics—via effective Hamiltonians. The advantage stems from spotlighting the wealth of information contained in effective fields and Hamiltonians rather than solving a system of differential equations from the outset.

I. INTRODUCTION

In 1954 Rabi, Ramsey, and Schwinger[1] introduced the use of rotating coordinates for the quantum mechanical treatment of magnetic resonance. This approach marked a turning point in understanding quantum resonance phenomena. Its importance stemmed from the fact that the effective Hamiltonian governing the evolution of the "rotated" state becomes *independent* of time. This property considerably simplifies calculations of amplitudes, probabilities, and expectation values. Conceptually, this simplification is rooted in the possibility of describing the spin-field interaction dynamics from the rotating frame, via an effective magnetic field. Moreover, the authors introduced the new paradigm largely without resorting to a specific basis. Soon afterward, the technique became well established in the research community. For example, Carver and Partridge[2] used it in conjunction with the density matrix to obtain monitoring operators for optical transitions; more recently Hanson *et al.*[3] resorted to effective fields and Hamiltonians to discuss phase decoherence of a single spin immersed in a "spin bath." Over the years, some authors saw the educational potential of the effective-field approach, used to describe a range of educational aids such as classical analogs[4] and numerical simulations[5] of magnetic resonance.

Despite the conceptual potential of the original basis-free treatment, the effective-field description has been given short shrift as a pedagogical method. It is mentioned in select "classic" [6,7] and newer textbooks,[8] as well as the quantum computing book of Nielsen and Chuang[9]. In particular, Refs. 7 and 8 point to the concept of an effective magnetic field responsible for placing the analysis in the rotating coordinate system. On the other hand, many widely-adopted textbooks[10–13] opt for the more technical way of introducing spin resonance, sometimes to the detriment of concept. Thus, in what has become the traditional approach, the time-dependent Schrödinger equation (TDSE) is cast in matrix form *at the outset*. In the basis formed by $\{|\uparrow\rangle \equiv |+z\rangle, |\downarrow\rangle \equiv |-z\rangle\}$—the eigenstates of $\widehat{S}_z$ (the z component of the spin operator)—the state at time t is $|\psi(t)\rangle = a(t)|\uparrow\rangle + b(t)|\downarrow\rangle$. The coefficients a and b are then obtained by solving the TDSE matrix as a set of coupled differential equations in the rotating frame, subject to the initial condition $|\psi(0)\rangle = |\psi_0\rangle = a_0|\uparrow\rangle + b_0|\downarrow\rangle$. Although it is correct from a practical viewpoint (e.g. easily amenable to numerical simulations), the matrix approach is not as efficient in conveying a clear understanding of quantum dynamics in rotating frames. This conclusion is drawn based on student feedback received over the years of teaching quantum mechanics from a variety of texts combined with written notes.

Here we advocate for introducing quantum spin resonance by following and expanding on the original framework of Ref. 1. The central argument is that one can defer specifying a basis toward the very end, emphasizing instead all aspects of the physics "seen" from rotating frames, via effective Hamiltonians. This approach resonates better with students because it keeps phenomenology in focus for a longer time, rather than delving into a system of differential equations right away.

II. THE PREMISE

Consider a spin-$\frac{1}{2}$ particle of charge q, mass m, and g-factor g placed in a magnetic field having a constant component B_0 along the z axis and a weaker component $B_1 \cos\omega t$ oscillating with angular frequency ω along direction x; assume $B_1 \ll B_0$. The total field is thus $\boldsymbol{B}(t) = \boldsymbol{e_z} B_0 + \boldsymbol{e_x} B_1 \cos\omega t$. The spin-field interaction Hamiltonian (in SI) is

$$\begin{aligned} \widehat{H} &= -\widehat{\boldsymbol{\mu}} \cdot \boldsymbol{B} = -g\frac{q}{2m}\widehat{\boldsymbol{S}} \cdot \boldsymbol{B} = -\gamma \widehat{\boldsymbol{S}} \cdot \boldsymbol{B} \\ &= \omega_0 \widehat{S}_z + \omega_1 \widehat{S}_x \cos\omega t = \frac{\hbar}{2}(\omega_0 \widehat{\sigma}_z + \omega_1 \widehat{\sigma}_x \cos\omega t) \\ &\equiv \widehat{H}_0 + \widehat{H}_1(t). \end{aligned} \tag{1}$$

where $\widehat{\boldsymbol{\mu}}$ is the magnetic moment operator, $\gamma = gq/2m$ is the gyromagnetic ratio of the particle (ratio of magnetic moment to angular momentum), and $\omega_0 \equiv -\gamma B_0$ and $\omega_1 \equiv -\gamma B_1$ are the frequencies of spin precession about the z and x axes, respectively, positive for $q < 0$ and negative for $q > 0$. There are three time scales in the system, represented by the three characteristic frequencies appearing in the Hamiltonian: ω_0−precession about the z axis (set by B_0), ω_1−precession about the x axis (set by B_1), and ω−oscillation along the x axis (tunable). The goal is to solve the time-dependent Schrödinger equation (TDSE)

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = \widehat{H}|\psi(t)\rangle, \tag{2}$$

subject to an initial condition $|\psi(0)\rangle = |\psi_0\rangle$.

III. PERTURBATION OFF ($B_1 = 0$)

This case corresponds to the interaction of the spin magnetic moment with the uniform magnetic field $\boldsymbol{B_0}$, leading to spin precession about the z axis with angular frequency ω_0.

The Schrödinger equation is

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = \widehat{H}_0|\psi(t)\rangle, \tag{3}$$

subject to an initial condition $|\psi_0\rangle = a_0|\uparrow\rangle + b_0|\downarrow\rangle$. Owing to the simplicity of this scenario, we compare here the "regular" solution relying on the $\widehat{S}_z$-basis formulation to the effective-field method. In the $\widehat{S}_z$ basis, the Schrödinger equation is

$$(a\,\omega_0)|\uparrow\rangle + (-b\,\omega_0)|\downarrow\rangle = 2i\,(\dot{a}|\uparrow\rangle + \dot{b}|\downarrow\rangle),$$

This particular form of the TDSE is obtained using the representation of the Pauli matrices, namely $\widehat{\sigma}_z = |\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|$ and $\widehat{\sigma}_x = |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|$. Since the Hamiltonian is time-independent, the solution is readily found as

$$\begin{aligned} |\psi(t)\rangle &= \widehat{U}(t)|\psi_0\rangle = \widehat{\mathbb{R}}_z(\omega_0 t)|\psi_0\rangle = e^{-i(\omega_0 t)\widehat{\sigma}_z}|\psi_0\rangle \\ &= a_0 e^{-i\omega_0 t/2}|\uparrow\rangle + b_0 e^{+i\omega_0 t/2}|\downarrow\rangle. \end{aligned} \tag{4}$$

Note that unitary time evolution governed by the constant Hamiltonian $\widehat{H}_0 = \omega_0\widehat{S}_z$ is equivalent to a rotation about the z axis by instantaneous phase angle $\omega_0 t$. The rotation is counter-clockwise (ccw) for $\omega_0 > 0$ and clockwise (cw) for $\omega_0 < 0$.

The effective-field method allows for a more insightful solution by showing explicitly what the switch to the precession frame entails. In the precession frame, one seeks a state $|\psi(t)\rangle'$ obtained by "unwinding" $|\psi(t)\rangle$ through an opposite angle $-\omega_0 t$ i.e. $|\psi(t)\rangle' = \widehat{\mathbb{R}}_z(-\omega_0 t)|\psi(t)\rangle$. Consequently, the TDSE (Eq. 3) becomes

$$\begin{aligned} i\hbar\frac{d}{dt}\left[\widehat{\mathbb{R}}_z(+\omega_0 t)|\psi(t)\rangle'\right] &= i\hbar\widehat{\mathbb{R}}_z(+\omega_0 t)\frac{d}{dt}|\psi(t)\rangle' + \frac{\hbar\omega_0}{2}\widehat{\sigma}_z\,\widehat{\mathbb{R}}_z(+\omega_0 t)|\psi(t)\rangle' \\ &= i\hbar\widehat{\mathbb{R}}_z(+\omega_0 t)\frac{d}{dt}|\psi(t)\rangle' + \widehat{H}_0\,\widehat{\mathbb{R}}_z(+\omega_0 t)|\psi(t)\rangle' \\ &= \widehat{H}_0\,\widehat{\mathbb{R}}_z(+\omega_0 t)|\psi(t)\rangle' \end{aligned}$$

hence

$$\widehat{\mathbb{R}}_z(+\omega_0 t)\frac{d}{dt}|\psi(t)\rangle' = 0.$$

By acting with $\widehat{\mathbb{R}}_z(-\omega_0 t)$ from the left, one obtains

$$i\hbar\frac{d}{dt}|\psi(t)\rangle' = 0, \tag{5}$$

subject to $|\psi(0)\rangle' = |\psi(0)\rangle = |\psi_0\rangle$, whose solution is $|\psi(t)\rangle' = |\psi_0\rangle$. Despite its disarming simplicity, Eq. 5 holds a wealth of conceptual information. It is the TDSE in the precession frame, governed by the *effective* Hamiltonian $\widehat{H}_{\text{eff}} = 0$. The latter can be seen as arising from an *effective magnetic field* $\boldsymbol{B}_{\text{eff}} = \boldsymbol{B_0} + (-\boldsymbol{B_0}) = 0$, i.e. the field "felt" in the rotating frame. Switching back to the non-rotating frame, the state $|\psi(t)\rangle$ is determined by "unwinding" $|\psi(t)\rangle'$ through a rotation by angle $+\omega_0 t$:

$$|\psi(t)\rangle = \widehat{\mathbb{R}}_z(+\omega_0 t)|\psi(t)\rangle' = a_0 e^{-i\omega_0 t/2}|\uparrow\rangle + b_0 e^{+i\omega_0 t/2}|\downarrow\rangle$$

which is the same as Eq. 4, in the $\widehat{S}_z$ basis.

IV. PERTURBATION ON ($B_1 \neq 0$)

The Schrödinger equation now involves the perturbed Hamiltonian,

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = \left[\widehat{H}_0 + \widehat{H}_1(t)\right]|\psi(t)\rangle.$$

A. In the frame rotating with ω_0 about the z axis (precession frame)

This is the usual choice of a rotating frame, commonly used with the matrix formulation. Here, however, it is treated basis-free, through the effective-field concept. We first calculate the state evolution with respect to a coordinate system rotating with angular frequency ω_0—the "precession frame." The rotated state is

$$|\psi(t)\rangle' = \widehat{\mathbb{R}}_z(-\omega_0 t)|\psi(t)\rangle \equiv c(t)|\uparrow\rangle + d(t)|\downarrow\rangle, \tag{6}$$

where $c(t) = a(t)e^{+i\omega_0 t/2}$ and $d(t) = b(t)e^{-i\omega_0 t/2}$, in the $\widehat{S}_z$ basis. For an observer in the precession frame, the magnetic field $\boldsymbol{B_1}$ appears to be rotating in the xy plane with nonzero x and y components. We therefore expect that the effective Hamiltonian $\widehat{H}_{\text{eff}}$, seen from the rotating frame, will include terms oscillating at $\omega_0 \pm \omega$ despite having no $\widehat{H}_0$ component. The evolution of the state $|\psi(t)\rangle'$ in the precession frame is found by solving the TDSE governed by $\widehat{H}_{\text{eff}}$:

$$i\hbar\frac{d}{dt}|\psi(t)\rangle' = \widehat{H}_{\text{eff}}|\psi(t)\rangle'. \tag{7}$$

To find $\widehat{H}_{\text{eff}}$, start with the original TDSE (Eq. 2) using $|\psi(t)\rangle = \widehat{\mathbb{R}}_z(+\omega_0 t)|\psi(t)\rangle'$:

- *LHS* of (7):

$$\begin{aligned} i\hbar\frac{d}{dt}|\psi(t)\rangle &= \frac{\hbar\omega_0}{2}\widehat{\sigma}_z\widehat{\mathbb{R}}_z(\omega_0 t)|\psi(t)\rangle' + i\hbar\widehat{\mathbb{R}}_z(\omega_0 t)\frac{d}{dt}|\psi(t)\rangle' \\ &= \widehat{\mathbb{R}}_z(\omega_0 t)\left(\frac{\hbar\omega_0}{2}\widehat{\sigma}_z|\psi(t)\rangle' + i\hbar\frac{d}{dt}|\psi(t)\rangle'\right) \\ &= \widehat{\mathbb{R}}_z(\omega_0 t)\left(\widehat{H}_0|\psi(t)\rangle' + i\hbar\frac{d}{dt}|\psi(t)\rangle'\right) \\ &= \widehat{H}_0\widehat{\mathbb{R}}_z(\omega_0 t)|\psi(t)\rangle' + i\hbar\widehat{\mathbb{R}}_z(\omega_0 t)\frac{d}{dt}|\psi(t)\rangle'. \end{aligned}$$

- *RHS* of (7):

$$\widehat{H}|\psi(t)\rangle = \left[\widehat{H}_0 + \widehat{H}_1(t)\right]\widehat{\mathbb{R}}_z(\omega_0 t)|\psi(t)\rangle'.$$

The first terms on either side of Eq. 7 thus cancel out, leaving

$$\widehat{\mathbb{R}}_z(\omega_0 t)\, i\hbar\frac{d}{dt}|\psi(t)\rangle' = \widehat{H}_1\widehat{\mathbb{R}}_z(\omega_0 t)|\psi(t)\rangle' \tag{8}$$

To obtain the TDSE for $|\psi(t)\rangle'$ we apply $\widehat{\mathbb{R}}_z^\dagger(\omega_0 t) = \widehat{\mathbb{R}}_z(-\omega_0 t)$ to the left of Eq. 8:

$$i\hbar\frac{d}{dt}|\psi(t)\rangle' = \widehat{\mathbb{R}}_z(-\omega_0 t)\widehat{H}_1\widehat{\mathbb{R}}_z(\omega_0 t)|\psi(t)\rangle' \equiv \widehat{H}_{\text{eff}}|\psi(t)\rangle'. \tag{9}$$

Note that Eq. 9 is the TDSE in the Interaction Picture, in which the (known) effects of the unperturbed Hamiltonian, $\widehat{H}_0$, are removed. The effective Hamiltonian can be expressed as follows:

$$\begin{aligned} \widehat{H}_{\text{eff}} &\equiv \widehat{\mathbb{R}}_z(-\omega_0 t)\widehat{H}_1\widehat{\mathbb{R}}_z(\omega_0 t) && \text{(10a)} \\ &= \widehat{H}_1(t)\cos\omega_0 t - \frac{\hbar\omega_1}{2}\widehat{\sigma}_y\cos\omega t\sin\omega_0 t && \text{(10b)} \\ &= \frac{\hbar\omega_1}{2}(\widehat{\sigma}_x\cos\omega_0 t - \widehat{\sigma}_y\sin\omega_0 t)\,\cos\omega t && \text{(10c)} \\ &= \frac{\hbar\omega_1}{2}(\widehat{\sigma}_+ e^{i\omega_0 t} + \widehat{\sigma}_- e^{-i\omega_0 t})\,\cos\omega t && \text{(10d)} \\ &= \frac{\hbar\omega_1}{4}\left[\widehat{\sigma}_+(e^{i(\omega_0+\omega)t} + e^{i(\omega_0-\omega)t}) + \widehat{\sigma}_-(e^{-i(\omega_0+\omega)t} + e^{-i(\omega_0-\omega)t})\right]. && \text{(10e)} \end{aligned}$$

The above expressions for $\widehat{H}_{\text{eff}}$ are obtained using the commutation and multiplication rules for Pauli matrices, and the definitions of the Pauli ladder operators, $\widehat{\sigma}_\pm$, given in the Appendix. Furthermore, the effective Hamiltonian can be shown to arise from an effective magnetic field $\boldsymbol{B}_{\text{eff}}$, apparent from Eq. 10c:

$$\widehat{H}_{\rm eff} = -\gamma \boldsymbol{B}_{\rm eff}(t) \cdot \widehat{\boldsymbol{S}},$$

where

$$\boldsymbol{B}_{\rm eff} = B_1 \left(\boldsymbol{e_x} \cos\omega_0 t - \boldsymbol{e_y} \sin\omega_0 t\right) \cos\omega t \equiv B_1\, \boldsymbol{e}_-(t) \cos\omega t \tag{11a}$$

$$= \frac{B_1}{2} \left[(\boldsymbol{e_x} + i\boldsymbol{e_y})e^{i\omega_0 t} + (\boldsymbol{e_x} - i\boldsymbol{e_y})e^{-i\omega_0 t}\right] \cos\omega t \tag{11b}$$

$$= \frac{B_1}{4} \left[(\boldsymbol{e_x} + i\boldsymbol{e_y})(e^{i(\omega_0+\omega)t} + e^{i(\omega_0-\omega)t}) + (\boldsymbol{e_x} - i\boldsymbol{e_y})(e^{-i(\omega_0+\omega)t} + e^{-i(\omega_0-\omega)t})\right]. \tag{11c}$$

In Eq. 11a, $\boldsymbol{e}_-(t) \equiv \boldsymbol{e_x} \cos\omega_0 t - \boldsymbol{e_y} \sin\omega_0 t = \boldsymbol{e_x} \cos(-\omega_0 t) + \boldsymbol{e_y} \sin(-\omega_0 t)$ is a unit vector rotating *negatively* (clockwise for $\omega_0 > 0$, counter-clockwise for $\omega_0 < 0$) about the z axis. Thus, in order to study the dynamics from the precession frame, one has to apply the magnetic field of Eq. 11 rotating in the xy plane with phase angle $-\omega_0 t$. Its role is to counter the precession with angle $+\omega_0 t$, in the presence of the perturbing time-dependent field. In the *rotating-wave approximation* (*RWA*), the rapid oscillations at $\omega_0+\omega$ are neglected hence the TDSE is approximated by

$$i\hbar \frac{d}{dt}|\psi(t)\rangle' \approx \frac{\hbar\omega_1}{4} \left[\widehat{\sigma}_+ e^{i(\omega_0-\omega)t} + \widehat{\sigma}_- e^{-i(\omega_0-\omega)t}\right] |\psi(t)\rangle'. \tag{12}$$

When $\omega \neq \omega_0$ Eq. 12 yields the Rabi oscillations. At resonance ($\omega = \omega_0$), the TDSE becomes

$$i\hbar \frac{d}{dt}|\psi(t)\rangle' = \frac{\hbar\omega_1}{4} \left(\widehat{\sigma}_+ + \widehat{\sigma}_-\right) |\psi(t)\rangle' = \frac{\hbar\omega_1}{4} \widehat{\sigma}_x |\psi(t)\rangle'. \tag{13}$$

Since the Hamiltonian is independent of time, the evolved state is simply

$$|\psi(t)\rangle' = e^{-i(\omega_1 t/4)\,\widehat{\sigma}_x} |\psi_0\rangle = \left(\cos\frac{\omega_1 t}{4} - i\,\widehat{\sigma}_x \sin\frac{\omega_1 t}{4}\right) |\psi_0\rangle.$$

The required state at time t is obtained by "jumping" off the rotating frame back to the laboratory system through a *positive* rotation of angle $+\omega_0 t$:

$$|\psi(t)\rangle = \widehat{\mathbb{R}}_z(+\omega_0 t)|\psi(t)\rangle' = e^{-i\,[(\omega_0 t/2)\,\widehat{\sigma}_z + (\omega_1 t/4)\,\widehat{\sigma}_x]}\, |\psi_0\rangle.$$

B. In the frame oscillating at the external (tunable) frequency ω

This method has the advantage that it leads to a time-independent effective Hamiltonian *even in the off-resonance case*, upon applying the rotating-wave approximation. When seen from the oscillating frame (with instantaneous phase angle ωt), the rotated state is

$$|\psi(t)\rangle' = \widehat{\mathbb{R}}_z(-\omega t)\, |\psi(t)\rangle. \tag{14}$$

1. Impose the RWA on the high-frequency oscillations.

The mathematical formalism follows, to some degree, the one developed in the previous section, with $\omega_0 t$ replaced by ωt. The most notable difference is in the new TDSE for $|\psi(t)\rangle'$ in the oscillating frame:

$$\begin{aligned} i\hbar\frac{d}{dt}|\psi(t)\rangle' &= \frac{\hbar}{2}\left[(\omega_0-\omega)\,\widehat{\sigma}_z + \omega_1\left(\widehat{\sigma}_x\cos\omega t - \widehat{\sigma}_y\sin\omega t\right)\cos\omega t\right]|\psi(t)\rangle' \\ &= \frac{\hbar}{2}\left\{(\omega_0-\omega)\,\widehat{\sigma}_z + \frac{\omega_1}{2}\left[\widehat{\sigma}_x(1+\cos 2\omega t) - \widehat{\sigma}_y\sin 2\omega t\right]\right\}|\psi(t)\rangle' \end{aligned} \tag{15}$$

The effective Hamiltonian governing Eq. 15 is

$$\begin{aligned} \widehat{H}_{\text{eff}} &= \frac{\hbar\Delta\omega}{2}\,\widehat{\sigma}_z + \widehat{\mathbb{R}}_z(-\omega t)\widehat{H}_1\widehat{\mathbb{R}}_z(\omega t) \\ &= \frac{\hbar\Delta\omega}{2}\,\widehat{\sigma}_z + \frac{\hbar\omega_1}{4}\left[\,\widehat{\sigma}_x(1+\cos 2\omega t) - \widehat{\sigma}_y\sin 2\omega t\right]. \end{aligned} \tag{16}$$

where $\Delta\omega = \omega_0 - \omega$ is the field detuning. The corresponding effective field giving rise to $\widehat{H}_{\text{eff}}$ is

$$\boldsymbol{B}_{\text{eff}} = \boldsymbol{e_x}\frac{B_1}{2}(1+\cos 2\omega t) - \boldsymbol{e_y}\frac{B_1}{2}\sin 2\omega t - \boldsymbol{e_z}\frac{\Delta\omega}{\gamma}. \tag{17}$$

In the rotating-wave approximation, fast oscillations at frequency 2ω are neglected. This yields the Schrödinger equation

$$i\hbar\frac{d}{dt}|\psi(t)\rangle' \approx \left(\frac{\hbar\omega_1}{4}\,\widehat{\sigma}_x + \frac{\hbar\Delta\omega}{2}\,\widehat{\sigma}_z\right)|\psi(t)\rangle', \tag{18}$$

associated with the time-*independent* Hamiltonian

$$\widehat{H}_{\text{eff}} = \frac{\hbar\omega_1}{4}\,\widehat{\sigma}_x + \frac{\hbar\Delta\omega}{2}\,\widehat{\sigma}_z. \tag{19}$$

2. Impose the RWA in a co-rotating frame.

The premise of this method is that the direction of the fluctuating field $\boldsymbol{B_1}$ can be seen as the superposition of two rotations of frequency ω in the xy plane: a positive one (*ccw* for $\omega > 0$, *cw* for $\omega < 0$) and a negative one (*cw* for $\omega > 0$, *ccw* for $\omega < 0$), defined respectively by unit vectors $\boldsymbol{e}_+$ and $\boldsymbol{e}_-$:

$$\begin{aligned} \boldsymbol{e_x}\cos\omega t &= \tfrac{1}{2}\left[(\cos\omega t + \sin\omega t)\,\boldsymbol{e_x} + (\cos\omega t - \sin\omega t)\,\boldsymbol{e_y}\right] \\ &\equiv \tfrac{1}{2}[\boldsymbol{e}_+(t) + \boldsymbol{e}_-(t)] \end{aligned} \tag{20}$$

The main spin precession (imposed by the constant field $\boldsymbol{B_0}$) is in the xy plane. Therefore the decomposition shown in Eq. 20 suggests that the only way to achieve resonance is when the two rotations (with ω_0 and ω) are *co-rotating* i.e. the counter-rotating component is neglected,

$$\boldsymbol{e_x}\cos\omega t \approx \tfrac{1}{2}(\cos\omega t + \sin\omega t)\,\boldsymbol{e_x} \equiv \tfrac{1}{2}\,\boldsymbol{e}_+(t). \tag{21}$$

Eq. 21 is the rotating-wave approximation—it states that the oscillating field $\boldsymbol{e_x}B_1\cos\omega t$ is a viable approximation for a field co-rotating with the precession imposed by $\boldsymbol{B_0}$.[6,7] The Hamiltonian then becomes

$$\begin{aligned}\widehat{H} &\approx \frac{\hbar\omega_0}{2}\,\widehat{\sigma}_z + \frac{\hbar\omega_1}{4}\,\boldsymbol{e}_+(t)\cdot\widehat{\boldsymbol{\sigma}} \\ &= \frac{\hbar\omega_0}{2}\,\widehat{\sigma}_z + \frac{\hbar\omega_1}{4}\,\widehat{\mathbb{R}}_z(\omega t)\,\widehat{\sigma}_x\,\widehat{\mathbb{R}}_z(-\omega t).\end{aligned} \tag{22}$$

Switching to the oscillating frame via Eq. 14 leads directly to Eq. 18, governed by the time-independent effective Hamiltonian of Eq. 19. The corresponding effective magnetic field is easily found as

$$\boldsymbol{B}_{\text{eff}} = \boldsymbol{e_x}\frac{B_1}{2} - \boldsymbol{e_z}\frac{\Delta\omega}{\gamma}.$$

With respect to the rotating frame, the solution of the Schrödinger equation (18) can be obtained via the unitary operation $\widehat{U}_t = \exp\left(-i\widehat{H}_{\text{eff}}\,t/\hbar\right)$ on the initial state:

$$|\psi(t)\rangle' = \widehat{U}_t|\psi_0\rangle = e^{-i\,[(\omega_1/2)\,\widehat{\sigma}_x + \Delta\omega\,\widehat{\sigma}_z]\,t/2}\,|\psi_0\rangle. \tag{23}$$

Despite the apparent simplicity of Eq. 23, the action of the unitary operator on $|\psi_0\rangle$ is not straightforward. The complications arise because the Hamiltonian is of the form $e^{\widehat{X}+\widehat{Z}}$, which has no closed form for non-commuting $\widehat{X}$ and $\widehat{Z}$.[14] Gottfried and Yan[6] provide an elegant solution as follows. Let $c_x \equiv \omega_1/2$ and $c_z \equiv \Delta\omega$ be the components of a vector $\boldsymbol{c}$ in the xz plane along direction $\boldsymbol{n}$ such that $(\omega_1/2)\,\widehat{\sigma}_x + \Delta\omega\,\widehat{\sigma}_z = c_x\widehat{\sigma}_x + c_z\widehat{\sigma}_z$. We seek an equivalent expression for $\widehat{U}_t$ in Eq. 23 in terms of a single rotation angle ξ_t and $\widehat{\sigma}_n = \boldsymbol{n}\cdot\widehat{\boldsymbol{\sigma}}$, the Pauli operator along direction $\boldsymbol{n}$. Thus we impose

$$\widehat{U}_t = e^{-i(c_x\widehat{\sigma}_x + c_z\widehat{\sigma}_z)t/2} \overset{!}{=} e^{-i\,\xi_t\widehat{\sigma}_n\,t/2}. \tag{24}$$

To find ξ_t and $\widehat{\sigma}_n$ we start with

$$c_x\widehat{\sigma}_x + c_z\widehat{\sigma}_z = \boldsymbol{c}\cdot\widehat{\boldsymbol{\sigma}} = (c\cos\phi)\widehat{\sigma}_x + (c\sin\phi)\widehat{\sigma}_z. \tag{25}$$

Hence $\boldsymbol{c} = c\,\boldsymbol{n}$ and ϕ an angle measured from the x axis in the xz plane. They satisfy

$$\begin{aligned} c_x &\equiv c\cos\phi = \omega_1/2, \\ c_z &\equiv c\sin\phi = \Delta\omega, \\ c &= \sqrt{c_x^2 + c_z^2} = \sqrt{(\Delta\omega)^2 + (\omega_1/2)^2}. \end{aligned} \tag{26}$$

From the above, one obtains the following expressions for $\widehat{\sigma}_n$ and ξ_t:

$$\begin{aligned} \widehat{\sigma}_n &= \frac{\widehat{\sigma}_x\,(\omega_1/2) + \widehat{\sigma}_z\,(\Delta\omega)}{\sqrt{(\Delta\omega)^2 + (\omega_1/2)^2}}, \\ \xi_t &\equiv t\,c = t\,\sqrt{(\Delta\omega)^2 + (\omega_1/2)^2}. \end{aligned} \tag{27}$$

The problem is now solved: Eq. 24 with relations (27) and (26) can be easily applied to the initial state $|\psi_0\rangle$. As an example, if $|\psi_0\rangle = |\uparrow\rangle$, the rotated state at time t is

$$\begin{aligned} |\psi(t)\rangle' &= \widehat{U}_t\,|\psi_0\rangle \\ &= e^{-i\,\xi_t\widehat{\sigma}_n\,t/2}\,|\uparrow\rangle = \left(\cos\frac{\xi_t}{2} - i\,\widehat{\sigma}_n \sin\frac{\xi_t}{2}\right)|\uparrow\rangle \\ &= \cos\frac{\xi_t}{2}|\uparrow\rangle - i\,\sin\frac{\xi_t}{2}\,\frac{c_x\widehat{\sigma}_x + c_z\widehat{\sigma}_z}{c}|\uparrow\rangle \\ &= \cos\frac{\xi_t}{2}|\uparrow\rangle - i\,\sin\frac{\xi_t}{2}\,\left(\frac{c_x}{c}|\downarrow\rangle + \frac{c_z}{c}|\uparrow\rangle\right) \\ &= \left(\cos\frac{\xi_t}{2} - i\,\frac{c_z}{c}\,\sin\frac{\xi_t}{2}\right)|\uparrow\rangle - i\,\frac{c_x}{c}\,\sin\frac{\xi_t}{2}|\downarrow\rangle. \end{aligned}$$

Alternatively, one can evaluate Eq. 23 through the spectral decomposition of $\widehat{U}_t$, regarded as a function of $\widehat{H}_{\text{eff}}$:

$$\widehat{U}_t = e^{(-it/\hbar)\lambda_+}|\lambda_+\rangle\langle\lambda_+| + e^{(-it/\hbar)\lambda_-}|\lambda_-\rangle\langle\lambda_-|,$$

where $\lambda_\pm$ and $|\lambda_\pm\rangle$ are the eigenvalues and eigenstates, respectively, of $\widehat{H}_{\text{eff}}$. This method, however, is more laborious and will not be detailed here.

Finally, the state in the fixed frame can be obtained by applying a rotation by angle $+\omega t$ about the z axis to $|\psi(t)\rangle'$:

$$\begin{aligned} |\psi(t)\rangle &= \widehat{\mathbb{R}}_z(+\omega t)\,|\psi(t)\rangle' = e^{-i(\omega t/2)\,\widehat{\sigma}_z}|\psi(t)\rangle' \\ &= \left(\cos\frac{\xi_t}{2} - i\,\frac{c_z}{c}\,\sin\frac{\xi_t}{2}\right)e^{-i(\omega t/2)}|\uparrow\rangle - i\,\frac{c_x}{c}\,\sin\frac{\xi_t}{2}\,e^{+i(\omega t/2)}|\downarrow\rangle \end{aligned} \tag{28}$$

The state in Eq. 28 can be used to obtain the Rabi Formula directly—the probability of spin flip at time t:

$$\begin{aligned}\mathcal{P}_{|\uparrow\rangle\to|\downarrow\rangle}(t) &= |\langle\downarrow|\psi(t)\rangle|^2 = \left(\frac{c_x}{c}\right)^2 \sin^2\frac{\xi_t}{2} \\ &= \frac{(\omega_1/2)^2}{(\Delta\omega)^2+(\omega_1/2)^2}\,\sin^2\frac{t\,\sqrt{(\Delta\omega)^2+(\omega_1/2)^2}}{2}.\end{aligned}$$

V. CONCLUSIONS

The article presents the advantages of using effective Hamiltonians instead of the traditional method of casting the problem as a system of differential equations at the outset, when introducing quantum dynamics in senior-level quantum mechanics courses. The analysis does not require the specification of an orthonormal basis set except at the very end, when the initial conditions have to be implemented. The advantage of this approach—applied here to the treatment of a spin in a time-dependent magnetic field biased by a constant field—lies in keeping the physics of the spin-field interaction in focus, unlike the usual method of expressing the Schrödinger equation in matrix form and solving a differential set early on.

We derive various expressions for the effective Hamiltonians associated with implementing the Rotating Wave Approximation in the frames rotating at the precession frequency (set by the constant magnetic field), and at the external frequency of the fluctuating field component. In both cases, we derive sets of expressions for the *effective magnetic fields* that can be used in practice to counter the rotation of the respective frame—essentially, to implement the effective Hamiltonians.

Appendix: Pauli-operator relations

$$\begin{aligned}&[\widehat{\sigma}_i,\widehat{\sigma}_j] = 2\,i\,\epsilon_{ijk}\widehat{\sigma}_k, \qquad \widehat{\sigma}_i\,\widehat{\sigma}_j = i\,\epsilon_{ijk}\widehat{\sigma}_k, \\ &\widehat{\sigma}_\pm \equiv \tfrac{1}{2}(\widehat{\sigma}_x \pm i\,\widehat{\sigma}_y), \quad \widehat{\sigma}_\pm|\pm z\rangle = 0, \quad \widehat{\sigma}_\pm|\mp z\rangle = |\pm z\rangle.\end{aligned} \tag{A.1}$$

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[1] I. I. Rabi, N. F. Ramsey, and J. Schwinger, Reviews of Modern Physics **26**, 167 (1954).

[2] T. R. Carver and R. B. Partridge, American Journal of Physics **34**, 339 (1966).

[3] R. Hanson, V. V. Dobrovitski, A. E. Feiguin, O. Gywat, and D. D. Awschalom, Science **320**, 352 (2008), https://science.sciencemag.org/content/320/5874/352.full.pdf.

[4] V. Leroy, J.-C. Bacri, T. Hocquet, and M. Devaud, European Journal of Physics **31**, 157 (2009).

[5] J.-P. Grivet, American Journal of Physics **61**, 1133 (1993).

[6] K. Gottfried and T. Yan, *Quantum Mechanics: Fundamentals*, Graduate Texts in Contemporary Physics (Springer New York, 2003).

[7] G. Baym, *Lectures on Quantum Mechanics Quantum Mechanics*, Lecture notes and supplements in physics (Addison-Wesley, 1990).

[8] R. Shankar, *Principles of Quantum Mechanics* (Springer US, 2011).

[9] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information: 10th Anniversary Edition* (Cambridge University Press, 2010).

[10] J. S. Townsend, *A Modern Approach to Quantum Mechanics* (University Science Books, New Jersey, 2013).

[11] S. Gasiorowicz, *Quantum Physics* (John Wiley & Sons, New York, 2003).

[12] J. J. Sakurai and J. Napolitano, *Modern Quantum Mechanics* (Cambridge University Press, London, 2017).

[13] R. Liboff and L. Davis, *Introductory Quantum Mechanics* (Addison-Wesley, 1998).

[14] R. Achilles and A. Bonfiglioli, Archive for History of Exact Sciences **66**, 295 (2012).