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Dynamics of Quantum State and Effective Hamiltonian with Vector Differential Form of Motion Method

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Effective Hamiltonians in periodically driven systems have received widespread attention for realization of novel quantum phases, non-equilibrium phase transition, and Majorana mode. Recently, the study of effective Hamiltonian using various methods has gained great interest. We consider a vector differential equation of motion to derive the effective Hamiltonian for any periodically driven two-level system, and the dynamics of the spin vector are an evolution under the Bloch sphere. Here, we investigate the properties of this equation and show that a sudden change of the effective Hamiltonian is expected. Furthermore, we present several exact relations, whose expressions are independent of the different starting points. Moreover, we deduce the effective Hamiltonian from the high-frequency limit, which approximately equals the results in previous studies. Our results show that the vector differential equation of motion is not affected by a convergence problem, and thus, can be used to numerically investigate the effective models in any periodic modulating system. Finally, we anticipate that the proposed method can be applied to experimental platforms that require time-periodic modulation, such as ultracold atoms and optical lattices.

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Periodic modulation systems have become an important concern in ultracold atoms, atomic and molecular physics, and quantum optics recently because they can produce exotic phases[1–12] and spin-orbit coupling.[13–17] Thus, they have paved the way for research of some fundamental principles in modern physics, such as many-body localization,[18–22] time crystals, and ergodicity.[23–27]

For an arbitrary time-depending Hamiltonian, $H(t+T)=H(t)$, where $T=2\pi/\omega$ is the time period. We can define $H(t)=H_0+\sum_n H_n e^{itn\omega}$. Then, in the high-frequency limit, the effective Floquet Hamiltonian, in analogy to the Bloch theorem in a spatially periodic system,[28] can be written as

$$H_{\rm eff}=H_0+\sum_{n>0}\frac{[H_n,H_{-n}]}{n\omega}+\mathcal{O}(\omega^{-2}). \tag{1}$$

Here, the high-frequency ω ensures that higher-order terms are negligible.[29–37] Various methods have been used to derive the above Hamiltonian. In the Magnus expansion method,[38–41] a necessary but not sufficient condition for convergence is given by

$$\int_0^T ||H(t)||_2\,dt\le\pi, \tag{2}$$

where $||\cdot||_2$ is the norm-2 of the Hamiltonian. The same criteria are applied to the Floquet expansion in Eq. (1), regarding the equivalence between both methods in deriving the effective Hamiltonians.

Due to the non-commuting relations between H_n and H_{-n}, the above effective Hamiltonian can acquire some new terms excluded in the original Hamiltonian, which are essential for their novel applications. The modulating method provides a new way to explore and discover fundamental physics in the areas of many Majorana modes, Floquet topological insulator, and time crystal.

Vector Differential Form of Motion Method. We study the effective Hamiltonian for a periodically arbitrary Hamiltonian using the equation-of-motion method, and discuss the generic features and interesting results. Here, we consider a two-level model subjected to the Schrödinger equation:[42–46]

$$i\hbar\frac{\partial}{\partial t}\psi(t)=H(t)\psi(t),\quad H(t)=\sum_{i=1}^{3}h_i\sigma^i=\boldsymbol{h}\cdot\boldsymbol{\sigma}, \tag{3}$$

where σ^i (for $i=x,y,z$) are the three traceless Pauli matrices; $\psi(t)=(\psi_1(t),\psi_2(t))^{\rm T}$ is the system wave function with two components and vector $\boldsymbol{h}=(h_1,h_2,h_3)$. The dynamics of the wave function can be described by the following unitary transformation:

$$\psi(t)=U(t,t_0)\psi(t_0),\quad iU_t(t,t_0)=H(t)U(t,t_0). \tag{4}$$

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Note that the unitary operator depends strongly on its initial value t_0. For this two-band model in Eq. (3), we assume[47]

$$U = \exp(-i\theta \boldsymbol{n}\cdot\boldsymbol{\sigma}) = \cos\theta - i\boldsymbol{n}\cdot\boldsymbol{\sigma}\sin\theta, \quad (5)$$

where $\boldsymbol{n}(t) = (n_1, n_2, n_3)$, $|\boldsymbol{n}| = 1$, and $\theta = \theta(t)$. Then, we derive the effective Hamiltonian using an equation of motion. By introducing Eq. (5) into the Schrodinger equation, we find

$$i(-\dot{\theta} - i\dot{\boldsymbol{n}}\cdot\boldsymbol{\sigma})\sin\theta + \boldsymbol{n}\cdot\boldsymbol{\sigma}(\cos\theta)\dot{\theta} = \boldsymbol{h}\cdot\boldsymbol{\sigma}U(t). \quad (6)$$

The real and imaginary parts of the above equation give the following two equations:

$$\dot{\theta} = \boldsymbol{n}\cdot\boldsymbol{h}, \quad \dot{\boldsymbol{n}} = \boldsymbol{n}\times\boldsymbol{\omega}, \quad (7)$$

where

$$\boldsymbol{\omega} = -\boldsymbol{h} - (\boldsymbol{n}\times\boldsymbol{h})\cot\theta. \quad (8)$$

The above Bloch equation limits the amplitude of the spin, thus $|\boldsymbol{n}| = 1$. Both different equations above are subjected to the boundary conditions $U(t_0, t_0) = 1$ and $U(pT + t_0, t_0) = (U(T + t_0, t_0))^p$, for $p \in \mathbb{Z}^+$. This constraint can be demonstrated by

$$\begin{aligned} &\boldsymbol{n}(pT + t_0, t_0) = \boldsymbol{n}(T + t_0, t_0), \quad (9)\\ &\theta(pT + t_0, t_0) = p\theta(T + t_0, t_0)\mathrm{mod}(2\pi). \end{aligned}$$

For different initial values, their expressions vary. The above equation of motion has a solution when $H(t) = H_0$ is independent of time. Thus, we can define $\boldsymbol{n} = \boldsymbol{h}_0//||\boldsymbol{h}_0||$ and $\theta = \boldsymbol{n}\cdot\boldsymbol{h}t$. Here, $\boldsymbol{n}\times\boldsymbol{h}_0 = 0$, then the singular point in the Cotangent function is negligible.

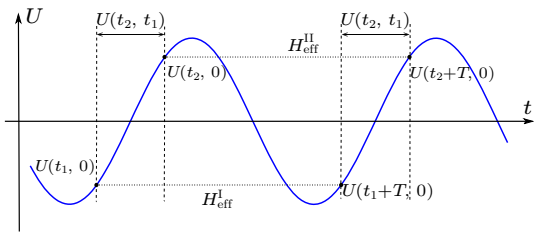

Fig. 1. Equivalence between the two effective Hamiltonians $H^i_{\rm eff}$ with different starting times t_i ($i = \mathrm{I}, \mathrm{II}$). Both Hamiltonians are connected by a unitary transformation determined using $U(t_2, t_1)$.

For a periodically modulating system with period T, the above unitary operator can be expressed using an effective Floquet Hamiltonian as follows:

$$U(t_0 + T, t_0) = \exp(-iH_{\rm eff}T). \quad (10)$$

The effective Floquet Hamiltonian[48–58] depends on the initial time t_0 and the time period T. The equivalence between these Floquet Hamiltonians is schematically presented in Fig. 1. Since both effective Hamiltonians are subject to two starting times, t_1 and t_2, the evolution from t_1 to $t_2 + T$ may have two trajectories if $t_1 < t_2$,

$$U(t_2 + T, t_2)U(t_2, t_1) = U(t_2 + T, t_1 + T)U(t_1 + T, t_1). \quad (11)$$

Due to the periodicity of the driving Hamiltonian, $U(t_2, t_1) = U(t_2 + T, t_1 + T)$, and results in the formula,

$$\exp(-iH^{\rm II}_{\rm eff}) = \exp[-iU(t_2, t_1)^\dagger H^{\rm I}_{\rm eff}U(t_2, t_1)]. \quad (12)$$

Hence, the Floquet system described by the effective Hamiltonian at any initial time is equivalent.

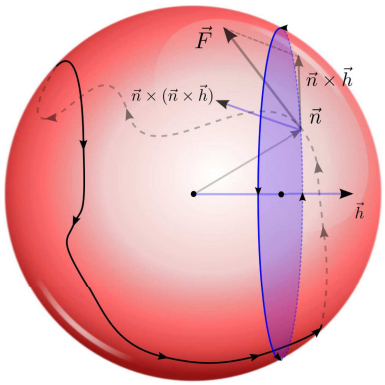

Fig. 2. Classical interpretation of a vector trajectory on the Bloch sphere. The evolution of the quantum state is an evolution of a spin vector evolving in an effective magnetic field. One term is made by the Hamiltonian due to the Bloch evolution, and the other due to the periodic oscillation of the magnetic field.

Some calculations consider the unitary transformations to the Hamiltonian, in which the vector $\boldsymbol{n}$ and angle θ need corresponding changes. We denote the unitary transformation operator as follows:

$$\mathcal{U} = e^{-iS}, \quad S = \phi\boldsymbol{m}\cdot\boldsymbol{\sigma}. \quad (13)$$

By this unitary transformation, we assume

$$\mathcal{U}^\dagger U(t)\mathcal{U} = e^{-i\theta'(t)\boldsymbol{n}'(t)\cdot\boldsymbol{\sigma}}. \quad (14)$$

Following the same procedure and after a few transformation, we find

$$\begin{aligned} &\theta' = \boldsymbol{n}(t)\cdot\boldsymbol{h} = \theta,\\ &\boldsymbol{n}' = \boldsymbol{n}(t) + \sin(2\phi)\boldsymbol{n}(t)\times\boldsymbol{m} + 2\sin^2\phi\,\boldsymbol{n}\times\boldsymbol{m}\times\boldsymbol{m},\\ &\boldsymbol{\omega}' = 1 + \sin(2\phi)\boldsymbol{m} + 2\sin^2\phi\,\boldsymbol{m}\times\boldsymbol{m}. \quad (15) \end{aligned}$$

Notably, these new variables still satisfy the equation of motion, i.e., $\dot{\boldsymbol{n}}'(t) = \boldsymbol{\omega}'\times\boldsymbol{n}'$. For a time-dependent unitary transformation, the expressions can still be solved similarly.

Time-Evolution Process. To gain a deep understanding of the dynamics for effective Hamiltonian and corresponding wave functions, $\boldsymbol{n}$ and θ are presented using the two-band model:

$$H = \begin{pmatrix} h_z + k\cos(\omega t) & g + k_1\sin(\omega t + \phi) \\ g + k_1\sin(\omega t + \phi) & -h_z - k\cos(\omega t) \end{pmatrix}, \quad (16)$$

where h_z, g, k, and k_1 are adjustable parameters. This model is relevant to qubits in various quantum systems, such as NV color centers, superconducting qubits, and trapped ions.

For $k = k_1 = 0$, the system degenerates to the time-independent case. Then, the following expression suffices:

$$\begin{aligned}\exp\Big(\int_0^{\mathrm{T}} iH dt\Big) &= \exp\Big(\int_0^{\mathrm{T}} i\boldsymbol{h}\cdot\boldsymbol{\sigma} dt\Big)\\ &= \exp(i\boldsymbol{h}\cdot\boldsymbol{\sigma}T) = \exp(-iH_{\mathrm{eff}}T)\\ &= \exp(-i\boldsymbol{n}\cdot\boldsymbol{\sigma}\theta). \end{aligned} \tag{17}$$

From Eq. (7), when the system is time-independent, the angle $\theta(t)$ increases linearly and its value reaches π, and its evolution is described by the black line in Fig. 5. The component of vector $\boldsymbol{n}$ remains constant. Moreover, our numerical calculation confirms this phenomenon. However, due to the influence of the time-dependent term, $\theta(t)$ fluctuates periodically, as exemplified in Figs. 3(a)–3(d). For the periodic modulation, the angle θ can be directly deduced from the differential equation and it is neither 0 nor π when $t > 0$. When θ approaches these two singular points, the terms $-\boldsymbol{n}\times(\boldsymbol{n}\times\boldsymbol{h})\cot\theta$ will dominate since $\cot\theta$ approaches infinity, which will quickly transform $\boldsymbol{n}\to-\boldsymbol{n}$. During the fluctuation of vector $\boldsymbol{n}$, θ shifts slightly, thus the unitary operator satisfies a smooth function of time. However, in weak modulation, as θ ranges from 0 to π, $\boldsymbol{n}(t)$ and $\boldsymbol{h}(t)$ are almost parallel to each other, and we have

$$\boldsymbol{n}\times\boldsymbol{h} = C\cdot\sin\phi \approx C\cdot\phi \approx 0, \tag{18}$$

where φ is the angle between $\boldsymbol{n}(t)$ and $\boldsymbol{h}(t)$. From Eq. (7), when $\theta(t)$ approaches π, we obtain

$$\cot\theta \approx \frac{1}{\theta-\pi}. \tag{19}$$

Hence, $(\boldsymbol{n}(t)\times\boldsymbol{h}(t))\cot(\theta(t))$ always remains finite, leading to the continuous fluctuation of $n(t)$ and $\theta(t)$ from perturbation. As long as there is a time-dependent term, the system will be quasi-periodic, which is consistent with the Floquet system. However, for the strong modulation, the upper and lower limits of θ significantly deviate from these two bounds (0 and π). As discussed before, both bounds are attained only when the Hamiltonian is time-independent and $\boldsymbol{n}\times\boldsymbol{h} = 0$, regarding that the effective equation of motion is exact.

Figure 5 shows that $\theta(t)$ translates with an interval of 2π. The first boundary condition is verified from results in Figs. 3(b)–3(d). In these calculations, the results were presented with an initial time $t_0 = 0$. In addition, we see that $\boldsymbol{n}(t,t_0) \neq \boldsymbol{n}(t+pT,t_0)$ for $t_0 \neq 0$ and $p \in \mathbb{Z}^+$. This result can be understood from the basic feature that $U(t+pT,t_0) = U(t,t_0)[U(t_0+T,t_0)]^p$, in which the time-evolution operator $U(t,t_0)$ breaks the periodicity of $\boldsymbol{n}(t+pT,t_0)$ for $t_0 \neq 0$. The intersection points of the black line and all colored lines can be described by the function

$$\theta(nT) = |2\,m\pi - n\theta(T)|, \tag{20}$$

where m is a positive integer and m does not equal n. Obviously, $\theta(nT)$ ranges from 0 to π.

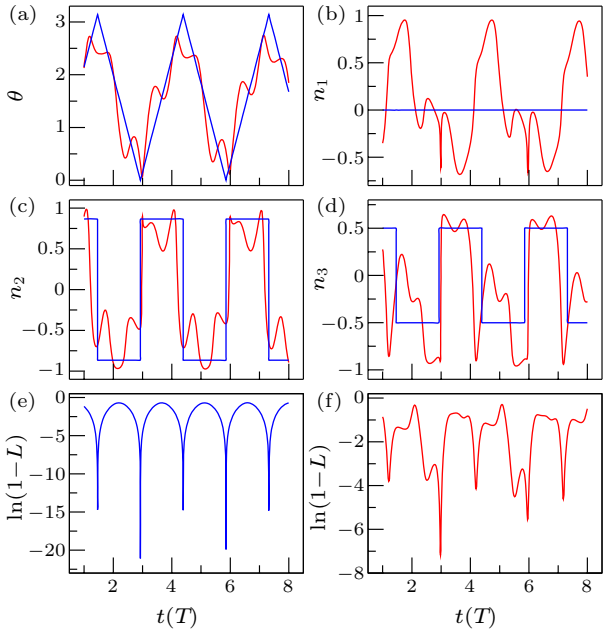

Fig. 3. Two parameter sets were used. The first set is $k = 0.7$, $k_1 = 0.6$ (red line), the second is $k = 6\times10^{-9}$, $k_1 = 6\times10^{-9}$ (blue line). It is obvious that the greater the amplitude of the time term, the more intense the fluctuation of the curve.

Notably, through a period of time evolution, the wave function never attains its initial value. We illustrate this result by calculating the Loschmidt echo $L = \langle\psi(t_0)|U(t,t_0)|\psi(t_0)\rangle$, and plot the value of $\ln(1-L)$ against time in Figs. 3(e) and 3(f). In the weak modulation, the wave function infinitesimally approaches but never attains the initial value.

Also, we demonstrate the dynamics of wave function in the Bloch sphere in Fig. 4. Suppose Bloch vectors $\boldsymbol{P} = (n_{x1}, n_{x2}, n_{x3})$, then we project the vector $\boldsymbol{n}(t) = (\boldsymbol{n}_1(t), \boldsymbol{n}_2(t), \boldsymbol{n}_3(t))$ onto the Bloch sphere as

$$\begin{aligned} &n_{x1} = \sin b_\theta\cos b_\phi, \quad n_{x2} = \sin b_\theta\sin b_\phi,\\ &n_{x3} = \cos b_\theta, \end{aligned} \tag{21}$$

with

$$b_\theta = \mathrm{Arccos}\, n_3, \quad b_\phi = i\ln\Big(\frac{n_1 - in_2}{\sqrt{(n_1)^2+(n_2)^2}}\Big).$$

Apparently, $n_{x3} = n_3$. We find that the dynamics exhibit some complex trajectories, and this vector almost goes through all points in the whole Bloch sphere in the long time limit. This is a general result, independent of whether the modulating Hamiltonian is trivial or topological.

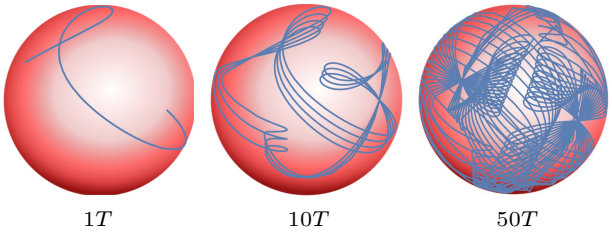

Fig. 4. Dynamics of a vector in a periodically driven system at $t = T$, $10T$, and $50T$. Since $\theta \neq \pi, 0$ in most cases, the quantum states cover the whole Bloch sphere after long periods. This feature is independent of whether the Hamiltonian is topological nontrivial or trivial.

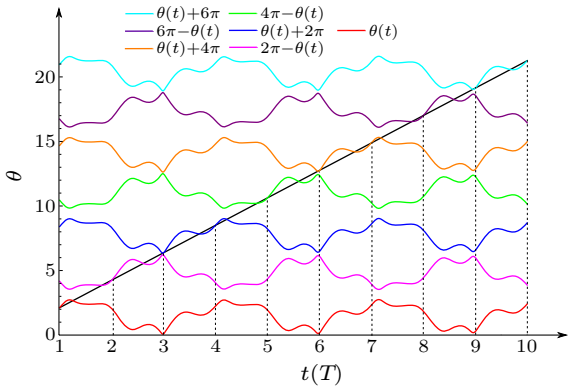

Fig. 5. Curves of $\theta(t)$ and $2m\pi \pm \theta(t)$ shown at nT. The black line indicates the fluctuation of $\theta(t)$.

Applications. The vector differential equation-of-motion method can be used to overcome the divergence existing in most high-frequency series expansions and to study the dynamics of some physical models in low-frequency regimes. Here, we discuss an interesting application of this equation-of-motion method. We try to derive the effective Hamiltonian in the high-frequency limit from our equation. Consider the following vector

$$\boldsymbol{h} = \boldsymbol{h}_0 + \sum_{p\geq 1} \boldsymbol{h}_p e^{ip\omega t} + \boldsymbol{h}_{-p} e^{-ip\omega t}. \tag{22}$$

The vector $\boldsymbol{n}$ is assumed as

$$\boldsymbol{n} = \boldsymbol{n}_0 + \sum_{p\geq 1} \boldsymbol{n}_p e^{ip\omega t} + \boldsymbol{n}_{-p} e^{-ip\omega t}. \tag{23}$$

Suppose h_p for $p \neq 0$ is much smaller than h_0, i.e., $|\boldsymbol{n}_p| \ll \boldsymbol{n}_0$ and $|\boldsymbol{n}_p| \ll 1$. Moreover, $\boldsymbol{n}_0 = \boldsymbol{h}_0//||\boldsymbol{h}_0||$. By substituting these expressions into the equation, we find

$$\theta(T) = \left(\boldsymbol{n}_0 \cdot \boldsymbol{h}_0 + \sum_{p\neq 0} \boldsymbol{n}_p \cdot \boldsymbol{h}_{-p}\right) \frac{2\pi}{\omega}. \tag{24}$$

Other terms, such as $\boldsymbol{n}_p \cdot \boldsymbol{h}_{p'}$, when $p + p' \neq 0$, disappear by integrating from 0 to T. Here, we only consider this initial condition since all Floquet Hamiltonians with different initial times are equivalent. The high-frequency limit ensures that $\theta(T)$ considered small enough, so that the limit can be derived as

$$\begin{aligned} \cot(\theta(T)) &= \frac{\omega}{2\pi \boldsymbol{n}_0 \cdot \boldsymbol{h}_0 + i\mathcal{Q}} \\ &\approx \frac{\omega}{2\pi^2 |\boldsymbol{h}_0|} - \frac{i\omega}{4\pi^2 |\boldsymbol{h}_0|^2} \mathcal{Q}, \end{aligned} \tag{25}$$

where

$$\mathcal{Q} = \sum_{p\geq 1} \boldsymbol{n}_0 \cdot \boldsymbol{h}_{-p} + \boldsymbol{n}_{-p} \cdot \boldsymbol{h}_0 - \boldsymbol{n}_0 \cdot \boldsymbol{h}_p - \boldsymbol{n}_p \cdot \boldsymbol{h}_0. \tag{26}$$

For the second vector differential equation of motion, we find

$$\begin{aligned} \dot{\boldsymbol{n}} = \sum_{p\geq 1} & ip\omega[\cos(p\omega t)(\boldsymbol{n}_p - \boldsymbol{n}_{-p}) \\ & - p\omega \sin(p\omega t)(\boldsymbol{n}_p + \boldsymbol{n}_{-p})]. \end{aligned} \tag{27}$$

Since the imaginary terms do not exist, $\boldsymbol{n}_p = \boldsymbol{n}_{-p}$. By substituting these results into the equation and keeping only the leading term, we obtain the formula

$$\begin{aligned} \dot{\boldsymbol{n}} &= -\boldsymbol{n}_0 \times \boldsymbol{h}_0 - \cot(\theta) \boldsymbol{n}_0 \times (\boldsymbol{n}_0 \times \boldsymbol{h}_0) \\ &= -\sum_{p\geq 1} p\omega \sin(p\omega t)(\boldsymbol{n}_p + \boldsymbol{n}_{-p}). \end{aligned} \tag{28}$$

From this result, we find

$$p\omega |\boldsymbol{h}_0| \boldsymbol{n}_p = i\epsilon_{ijk} \boldsymbol{h}_p \cdot \boldsymbol{h}_{-p}. \tag{29}$$

With these expressions, we can obtain the following Floquet Hamiltonian:

$$\begin{aligned} H_{\text{eff}} &= \frac{\boldsymbol{n}\theta}{T} \cdot \boldsymbol{\sigma} \\ &= \frac{[\boldsymbol{n}_0 + \sum_{p\geq 1}(\boldsymbol{n}_p + \boldsymbol{n}_{-p})](\boldsymbol{n}_0 \cdot \boldsymbol{h}_0)\frac{2\pi}{\omega}}{T} \cdot \boldsymbol{\sigma} \\ &= \boldsymbol{n}_0 + \sum_{p\geq 1} (\boldsymbol{n}_p + \boldsymbol{n}_{-p}) |\boldsymbol{h}_0| \cdot \boldsymbol{\sigma} \\ &= \boldsymbol{h}_0 \cdot \boldsymbol{\sigma} + \sum_{p\geq 1} \frac{[\boldsymbol{h}_p \cdot \boldsymbol{\sigma}, \boldsymbol{h}_{-p} \cdot \boldsymbol{\sigma}]}{p\omega}, \end{aligned} \tag{30}$$

which is identical to the first and second terms in Eq. (1) obtained in the literature.[28] Therefore, we are able to directly obtain the effective Floquet Hamiltonian from our vector differential equation-of-motion method.

Furthermore, this method can be generalized to Hamiltonians with greater orders. Noticeably, one representative work[59] found that a higher non-commuting term can produce the long-range hopping more easily in a periodical driving system. Specifically, the scheme uses a 1D periodic p-wave superconductor and provides good guidance for effectively generating long-range hopping in experiments. Thus, the generalization of our proposed method can be used to obtain higher-order non-commuting terms, giving a different perspective to the study of many Majorana mode problems.

Discussion and Conclusion. We have presented the vector differential equation of motion to study any periodically driven two-level system and deduced the effective Floquet Hamiltonian. Notably, evolution can be regarded as a spin vector evolving in an effective magnetic field. Furthermore, we discuss an interesting application of this method in the high-frequency limit of the effective Floquet Hamiltonian, corresponding to the results of the second-order Magnus. Finally, we expect that our method can provide some insights into degenerate structures and multi-level systems and that its generalization can give a different perspective to the study of many Majorana modes.

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