Scalar Vs Vector Operators

<u>Vector operators</u> transform like vectors under rotation :

$$\delta \vec{V} = i \, \delta\theta \, [\hat{n} \cdot \vec{\hat{J}} , \vec{V}]$$

$$= \delta\theta \, \vec{n} \times \vec{\hat{V}} .$$

$$\Rightarrow \qquad [\hat{V}_i , \hat{J}_j] = i \, \varepsilon_{ijk} \hat{V}_k$$

Check that $\hat{x}$, $\hat{p}$, $\hat{J}$ are vector operators.

We will now show that vector operators satisfy

$$e^{i\theta \hat{J}_z} \hat{V}_x e^{-i\theta \hat{J}_z}$$

$$= \hat{V}_x \cos\theta - \hat{V}_y \sin\theta .$$

$$e^{i\theta \hat{J}_z} \hat{V}_y e^{-i\theta \hat{J}_x}$$

$$= \hat{V}_y \cos\theta + \hat{V}_x \sin\theta .$$

How to derive finite rotations from infinitesimal,

$$\hat{V}_x(\theta) = e^{i\theta \hat{J}_z} \hat{V}_x e^{-i\theta \hat{J}_z}$$

$$\frac{d\hat{V}_x(\theta)}{d\theta} = i\, e^{i\theta \hat{J}_z} [J_z, \hat{V}_x] e^{-i\theta \hat{J}_z}$$

$$= -\hat{V}_y(\theta)$$

$$\frac{d\hat{V}_y(\theta)}{d\theta} = \hat{V}_x(\theta)$$

Note that these can also be thought of as Heisenberg's E.O.M. with θ = time, and J_z = Hamiltonian

$$\Rightarrow \frac{d^2 V_x}{d\theta^2} + \hat{V}_x = 0 \, , \quad \frac{d^2 \hat{V}_y}{d\theta^2} = \hat{V}_y$$

Solving these with the boundary condition

$$\hat{V}_x(\theta = 0) = \hat{V}_x \, , \quad \hat{V}_y(\theta = 0) = \hat{V}_y .$$

$$\frac{d\hat{V}_x}{d\theta}(\theta = 0) = -\hat{V}_y \, , \quad \frac{d\hat{V}_y}{d\theta}(\theta = 0) = \hat{V}_x$$

gives the above expression of $\hat{V}_x(\theta), \hat{V}_y(\theta)$.

In contrast to vector operators, <u>scalar operators</u> $\hat{S}$ transform trivially under rotations:

$$[\hat{S}, \hat{J}_i] = 0$$

An example is $\hat{S} = \sum_i \hat{V}_i \hat{V}_i \equiv V_i V_i$

where $\hat{V}_i$ is a vector operator [heuristically $\hat{S}$ is the squared magnitude of $\vec{\hat{V}}$ and hence does not change as $\vec{\hat{V}}$ is rotated.

Check: $[\hat{S}, \hat{J}_i]$

$$= [\hat{V}_k \hat{V}_k, \hat{J}_i]$$

$$= \hat{V}_k \, i \, \varepsilon_{kij} \hat{V}_j + i \varepsilon_{kij} \hat{V}_j \hat{V}_k$$

$$= -i \, \hat{V}_j \hat{V}_k \, \varepsilon_{kij} + i \varepsilon_{kij} \hat{V}_j \hat{V}_k$$

(recall that ε_{ijk} is fully antisym.)

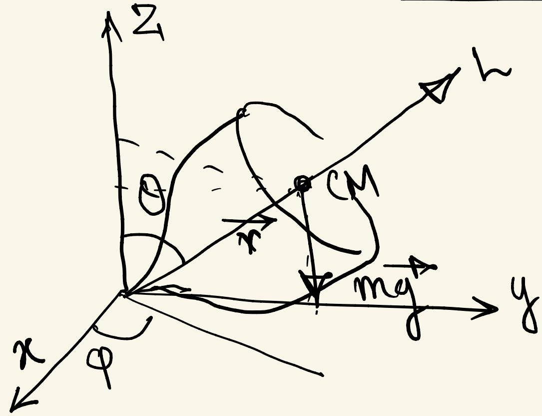
$$= 0.$$

Precession of Angular Momentum

Let's recall the precession of a classical top.

$$H = \frac{L^2}{2I} + mgz$$

(z = z-coord. of the center of mass).



L_z is conserved since the torque is in the x-y plane $\Rightarrow \theta$ independent of time, only φ changes.

$$\frac{dL_x}{dt} = (\vec{r} \times \vec{Force})_x$$
$$= -r_y mg$$
$$= -r \sin(\theta) \sin(\varphi) mg$$

$$L_x = L \sin\theta \cos(\varphi(t)), \quad L_y = L \sin\theta \sin(\varphi(t))$$

$$-L \cancel{\sin\theta} \cancel{\sin(\varphi)} \dot{\varphi} = -mg \cancel{\sin(\theta)} r \cancel{\sin(\varphi)}$$

$$\Rightarrow \dot{\varphi} = \frac{mgr}{L}$$

$$h_z = h\cos(\theta)$$

$$\Rightarrow \quad mgz = mgr\cos(\theta)$$

$$= \left(\frac{mgr}{L}\right) L_z$$

Therefore, one may write,

$$H = \frac{L^2}{2I} + \alpha L_z \qquad \left[\alpha = \frac{mgr}{L} \text{ is } \underline{\text{time-independent}}\right]$$

and $\dot{\varphi} = \alpha$

$$\Rightarrow \quad L_x(t) = L_x(t=0)\cos(\alpha t) - L_y(t=0)\sin(\alpha t)$$

$$L_y(t) = L_y(t=0)\cos(\alpha t) + L_x(t=0)\sin(\alpha t)$$

Quantum Mechanical top.

$$H = \frac{\hat{J}^2}{2I} + \vec{J} \cdot \vec{B}$$

One may chose $\vec{B}$ along the z-direction.

so that $H = \frac{\hat{J}^2}{2I} + \alpha J_z \quad (\alpha = |B|)$

$[J_z, H] = 0 \Rightarrow \hat{J}_z$ a constant of motion

$$i \frac{dJ_k}{dt} = [J_k, H] = [J_k, J_l B_l] = i \varepsilon_{klm} J_m B_l$$

$$\Rightarrow \frac{d\vec{J}}{dt} = \underbrace{\vec{B} \times \vec{J}}_{\text{torque}}$$

Same as $\frac{d(\text{Angular mom.})}{dt} = \text{Torque}$

Heisenberg's Eq. of motion:

$$\hat{J}_{x/y}(t) = e^{i\hat{H}t} \hat{J}_{x/y}(t=0) e^{-i\hat{H}(t)}$$
$$= e^{i\alpha \hat{J}_z t} \hat{J}_{x/y} e^{-i\alpha \hat{J}_z t}$$

Using above discussion:

$$\hat{J}_x(t) = \hat{J}_x(0) \cos(\alpha t) - \hat{J}_y(0) \sin(\alpha t)$$
$$\hat{J}_y(t) = \hat{J}_y(0) \cos(\alpha t) + \hat{J}_x(0) \sin(\alpha t)$$

Derivation only relies on $\vec{J}$ being a vector operator i.e. $[J_i, J_j] = i\varepsilon_{ijk} J_k$.

A specific way to get the above H :

Consider a quantum mechanical particle coupled to external, constant magnetic field.

$$\hat{H} = \frac{(\hat{p} - e\hat{A})^2}{2m} \qquad \vec{A} = \frac{\vec{B}}{2}(-y, x, 0)$$

$$= \frac{\hat{p}^2}{2m} - \frac{e}{2m}(\hat{p}\cdot\hat{A} + \hat{A}\cdot\hat{p}) + \underbrace{\frac{e^2\vec{A}^2}{2m}}_{\text{constant.}}$$

Since $\nabla\cdot A = 0$ by gauge choice,

$$\vec{p}\cdot\vec{A}\,|\psi\rangle = -i\vec{\nabla}\cdot\vec{A}\,|\psi\rangle$$

$$= -i(\vec{\nabla}\cdot\vec{A})|\psi\rangle - i\vec{A}\cdot\vec{\nabla}|\psi\rangle$$

$$= -i(\vec{A}\cdot\vec{\nabla})|\psi\rangle = (\vec{A}\cdot\vec{p})|\psi\rangle$$

$$\Rightarrow \hat{H} = \frac{p^2}{2m} - \frac{e}{m}(\vec{A}\cdot\vec{p}) + \text{const.}$$

$$= \frac{p^2}{2m} - \frac{e}{m}[A_x p_x + A_y p_y]$$

$$= \frac{p^2}{2m} - \frac{e}{m}BL_z = \frac{p^2}{2m} - \frac{e}{m}\vec{B}\cdot\vec{L}$$

In the above derivation for precession of the angular momentum, we only relied on the commutation relations $[J_i, J_j] = i\varepsilon_{ijk} J_k$, and never had to write down an explicit form of $\vec{J}$ operators in a chosen basis.

As we will soon discuss, there exist an infinite number of possibilities for matrices that satisfy $[J_i, J_j] = i\varepsilon_{ijk} J_k$ where each choice corresponds to a different sized matrix. Here are two possibilities,

- 2×2 matrices: $J_i = \dfrac{\sigma_i}{2}$ where σ_i are Pauli matrices

- 3×3 matrices: $L_x = \dfrac{1}{2}\begin{bmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{bmatrix}$, $L_y = \dfrac{i}{2}\begin{bmatrix} 0 & -\sqrt{2} & 0 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 0 & \sqrt{2} & 0 \end{bmatrix}$

$$L_z = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

(We will soon derive these)

Wave-f^n approach to Precession

Let's specialize to 2X2 matrices, so that $\vec{\tau} = \frac{\vec{\sigma}}{2}$ ← Pauli matrices

Above we considered the operator approach to precession, where to calculate $\langle\psi(0)| e^{iHt} \frac{\vec{\sigma}}{2} e^{-iHt} |\psi(0)\rangle$ we evaluated $\vec{\sigma}(t) = e^{iHt} \frac{\vec{\sigma}}{2} e^{-iHt}$. One can also consider the Schrodinger's approach where we instead evaluate $|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$ and calculate $\langle\psi(t)| \frac{\vec{\sigma}}{2} |\psi(t)\rangle$.

At $t=0$, let's say $\langle\sigma^z\rangle = \cos(\theta) \equiv n_z$

$\langle\sigma^x\rangle = \sin(\theta)\cos(\varphi) \equiv n_x$, $\langle\sigma^y\rangle = \sin\theta \sin\varphi \equiv n_y$.

i.e. $\langle\psi(0)|\vec{\sigma}|\psi(0)\rangle = \vec{n}$

The corresponding state is the eigenvector of $\vec{\sigma}\cdot\hat{n}$ with eigenvalue $+1$. One finds

$$|\psi\rangle \equiv |\hat{n}+\rangle = \begin{bmatrix} \cos(\theta/2)\, e^{-i\varphi/2} \\ \sin(\theta/2)\, e^{i\varphi/2} \end{bmatrix}$$

Check: $\vec{\sigma} \cdot \hat{n} \, |\hat{n}+\rangle$

$$= \begin{bmatrix} \cos\theta & \sin\theta \, e^{-i\varphi} \\ \sin\theta \, e^{i\varphi} & -\cos\theta \end{bmatrix} \begin{bmatrix} \cos(\theta/2) e^{-i\varphi/2} \\ \sin(\theta/2) e^{i\varphi/2} \end{bmatrix}$$

$$= \begin{bmatrix} \cos(\theta/2) e^{-i\varphi/2} \\ \sin(\theta/2) e^{i\varphi/2} \end{bmatrix} = |\hat{n}_+\rangle$$

Similarly,

$$\langle \sigma^x \rangle = \langle \hat{n}_+ | \sigma^x | \hat{n}_+ \rangle$$

$$= \begin{bmatrix} \cos(\theta/2) e^{i\varphi/2} & \sin(\theta/2) e^{-i\varphi/2} \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \cos(\theta/2) e^{-i\varphi/2} \\ \sin(\theta/2) e^{i\varphi/2} \end{bmatrix}$$

$$= \sin(\theta) \cos(\varphi) = n_x$$

Similarly $\langle \sigma^y \rangle = n_y$ and $\langle \sigma^z \rangle = n_z$.

Therefore $|\hat{n}+\rangle$ is indeed the correct initial state.

Now, we time evolve $|\hat{n}+\rangle$ with respect to $H = \alpha J_z = \frac{\alpha \sigma^z}{2}$

$$|\psi(t)\rangle = e^{-i\hat{H}t} |\psi(t=0)\rangle$$

$$= \begin{bmatrix} e^{-i\alpha t/2} & 0 \\ 0 & e^{i\alpha t/2} \end{bmatrix} \begin{bmatrix} \cos(\theta/2)\, e^{-i\varphi/2} \\ \sin(\theta/2)\, e^{i\varphi/2} \end{bmatrix}$$

$$= \begin{bmatrix} \cos(\theta/2)\, e^{-i[\varphi+\alpha t]/2} \\ \sin(\theta/2)\, e^{i[\varphi+\alpha t]/2} \end{bmatrix}$$

Therefore, under time-evolution, the state corresponds to $\theta \to \theta$, $\varphi \to \varphi + \alpha t$ i.e. $\langle \sigma^z \rangle$ remains unchanged, while the vector $(\langle \sigma^x \rangle, \langle \sigma^y \rangle)$ rotates at an angular velocity α exactly in agreement with the result in the operator (Heisenberg) picture.

Spin Resonance

As discussed above, if one applies a static field only along the z-axis, then the angular-momentum will precess around the z-axis. Therefore, if one goes to a new frame of reference that is rotating at the angular velocity corresponding to the precession about z-axis, then $\langle \vec{J} \rangle_{\text{rot. frame}}$ will be independent of time. This change of frame is implemented via a unitary transformation. To see this, if there is a static field only along the z-axis,

then $$|\psi(t)\rangle_{Lab} = e^{-i L_z B_0 t} |\psi(0)\rangle_{Lab}$$

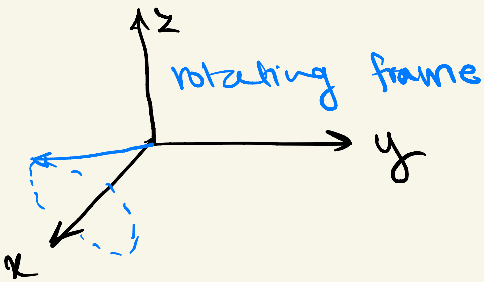
Let's define $$|\psi(t)\rangle_{\text{rot. frame}} = \underbrace{e^{i L_z B_0 t}}_{\text{Unitary } \mathcal{U}} |\psi(t)\rangle_{Lab}$$

then $$|\psi(t)\rangle_{\text{rot-frame}} = |\psi(0)\rangle_{Lab}$$

$$= \text{independent of time}$$

Therefore, in the rotating frame, there is **no** magnetic field along the z-direction (in fact, the Hamiltonian is exactly zero in the rotating frame).

Now, let's apply a field B_1 along x-direction in the rotating frame. Based on our discussion of precession, one now expects that *in the rotating frame*, the angular momentum will precess around the x-axis



$$\Rightarrow \quad H_{rot} = J_x B_1 .$$

To find the Hamiltonian in the lab-frame, we write down the

Schrodinger's equation in the lab frame:

$$i \frac{d|\psi\rangle_{lab}(t)}{dt} = i \frac{d}{dt}\left[U^{-1}(t)\, |\psi\rangle_{rot}(t) \right]$$

where $U(t) = e^{i \hat{J}_z B_0 t}$ as defined above.

$$\Rightarrow i \frac{d|\psi\rangle_{lab}(t)}{dt} = i \left(\frac{dU^{-1}}{dt}(t) \right) |\psi_{rot}\rangle$$

$$+ i\, U^{-1}(t) \left(\frac{d|\psi_{rot}\rangle}{dt} \right)$$

By definition $i \frac{d|\psi_{rot}\rangle}{dt} = H_{rot} |\psi_{rot}\rangle$

$$= \hat{J}_x B_1 |\psi_{rot}\rangle$$

$$\Rightarrow i \frac{d|\psi_{lab}(t)\rangle}{dt} = i \frac{dU^{-1}}{dt}(t)\, U(t) |\psi_{lab}\rangle$$

$$+ U^{-1}(t) \hat{J}_x B_1 U |\psi_{lab}\rangle.$$

$$\Rightarrow H_{lab}(t) = i \frac{dU^{-1}}{dt} U + B_1 U^{-1} \hat{J}_x U$$

$$= i - i \hat{J}_z B_0 + B_1 e^{-i\hat{J}_z B_0 t} \hat{J}_x e^{i \hat{J}_z B_0 t}$$

$$= B_0 \hat{J}_z + B_1 \hat{J}_x \cos(B_0 t) + B_1 \hat{J}_y \sin(B_0 t).$$

Therefore, we conclude that if one applies a time-dependent field

$$B(t) = (B_1 \cos(B_0 t), B_1 \sin(B_0 t), B_0),$$

in the <u>lab frame</u>, then

in the <u>rotating frame</u>, the angular momentum will precess along x-axis.

In the lab frame, $\langle \hat{J}_z \rangle$ would oscillate at frequency B_0. For example, if at $t = 0$, $\langle \hat{J}_z \rangle = m$, then at time $T = \frac{\pi}{B_0}$, $\langle \hat{J}_z \rangle = -m$.

From an experimental standpoint, applying the above time-dependent field that oscillates both along the x and the y axis is a bit inconvenient. It's easier to apply a field that in the lab frame oscillates only along the x-direction in addition to a static component along the z-direction. For example,

$$\vec{B}_{lab} = (2B_1 \cos(\omega t), 0, B_0),$$

where ω is some frequency. We will now show that when $B_1 \ll B_0$, and $\omega \simeq B_0$, then such a field produces an effect quite similar to the one discussed above.

We will see below that the amplitude of oscillation in $\langle \hat{J}_z \rangle_{lab} = \langle \hat{J}_z \rangle_{rot}$ will be maximum, when $\omega = B_0$.

This has practical implications: Suppose one has a material in their lab in which there exists an unknown magnetic field $B_0 \hat{z}$. By applying an oscillating field along the x-direction, and by maximizing $\langle \hat{J}_z \rangle$, one can deduce B_0.

To find $\langle \hat{J}_z \rangle$, let's write down the schrodinger's eqn in the lab:

$$i \frac{d|\psi\rangle_{lab}}{dt} = \left[B_0 \hat{L}_z + 2B_1 \cos(\omega t) \hat{L}_x \right] |\psi\rangle_{lab}$$

Let's define $|\psi\rangle_{rot} = e^{i\omega t \hat{L}_z} |\psi\rangle_{lab}$.

$$\Rightarrow i \frac{d|\psi_{rot}\rangle}{dt} =$$

$$- \omega \hat{L}_z e^{i\omega t \hat{L}_z} |\psi\rangle_{lab}$$

$$+ e^{i\omega t \hat{L}_z} (B_0 \hat{L}_z + 2B_1 \cos(\omega t) \hat{L}_x) |\psi\rangle_{lab}$$

$$= -\omega \hat{L}_z |\psi_{rot}\rangle + B_0 \hat{L}_z |\psi_{rot}\rangle$$

$$+ 2B_1 e^{i\omega t \hat{L}_z} \hat{L}_x e^{-i\omega t \hat{L}_z} \cos(\omega t) |\psi_{rot}\rangle$$

The second term contains the factor

$$\cos(\omega t)\, e^{i\omega t \hat{L}_z} \hat{L}_x e^{-i\omega t \hat{L}_z}$$

$$= \cos(\omega t) [\hat{L}_x \cos(\omega t) - \hat{L}_y \sin(\omega t)]$$

$$= \frac{\hat{L}_x [1 + \cos(2\omega t)]}{2} - \hat{L}_y \frac{\sin(2\omega t)}{2}$$

We will be interested in the case when $\omega \simeq B_0 \gg B_1$. Therefore, the terms such as $\cos(2\omega t)$ and $\sin(2\omega t)$ average out to zero on time-scale of order B_1^{-1} and one may approximate

$$\cos(\omega t)\left[\hat{L}_x \cos(\omega t) - \hat{L}_y \sin(\omega t)\right] \simeq \frac{\hat{L}_x}{2} = \text{time-independent.}$$

This is called 'rotating-wave approximation'. Physically, in the lab frame, $\vec{B} = (2B_1 \cos(\omega t), 0, B_0)$

$$= (B_1 \cos(\omega t), B_1 \sin(\omega t), B_0)$$
$$+ (B_1 \cos(\omega t), -B_1 \sin(\omega t), 0)$$

When $\omega = B_0$, the first term in

this expression is precisely the term that leads to field only along x-direction in the rotating frame.

The second term corresponds to a field that is rotating at the opposite frequency $-\omega \simeq -B_0$ and doesn't change the physics much.

Completely neglecting the second term then reproduces the effect of a field along x-direction in the rotating frame.

Therefore, in the rotating wave approximation,

$$i \frac{d|\psi_{rot}\rangle}{dt} = \left[(B_0 - \omega)\hat{L}_z + B_1 \hat{L}_x\right]|\psi_{rot}\rangle$$

$\equiv$ independent of time.

$$\Rightarrow |\psi_{rot}(t)\rangle = e^{-i\left[(B_0-\omega)\hat{L}_z + B_1 \hat{L}_x\right]t} |\psi_{rot}(t=0)\rangle$$

$$\Rightarrow |\psi_{lab}(t)\rangle = e^{-i\omega t \hat{L}_z} |\psi_{rot}(t)\rangle$$

$$= e^{-i\omega t \hat{L}_z} e^{-i[(B_0-\omega)\hat{L}_z + B_1 \hat{L}_x]t} |\psi_{lab}(t=0)\rangle,$$

Let's specialize to spin-1/2 system, so that $\hat{L}_z = \frac{\hat{Z}}{2}$, $\hat{L}_x = \frac{\hat{X}}{2}$ where $\hat{X}, \hat{Z}$ are Pauli operators,

$$\Rightarrow |\psi_{lab}(t)\rangle = e^{-i\omega t \frac{\hat{Z}}{2}} e^{-i\left[\hat{Z}\frac{(B_0-\omega)}{2} + B_1 \frac{\hat{X}}{2}\right]t} |\psi_{lab}(t=0)\rangle$$

$$= e^{-i\omega t \frac{\hat{Z}}{2}} e^{-i B_{eff}\left[\frac{\vec{\sigma}}{2}\cdot\hat{n}\right]} |\psi_{lab}(t=0)\rangle$$

where $B_{eff} = \sqrt{(B_0-\omega)^2 + B_1^2}$, $\vec{\sigma} = (\hat{X}, \hat{Y}, \hat{Z})$

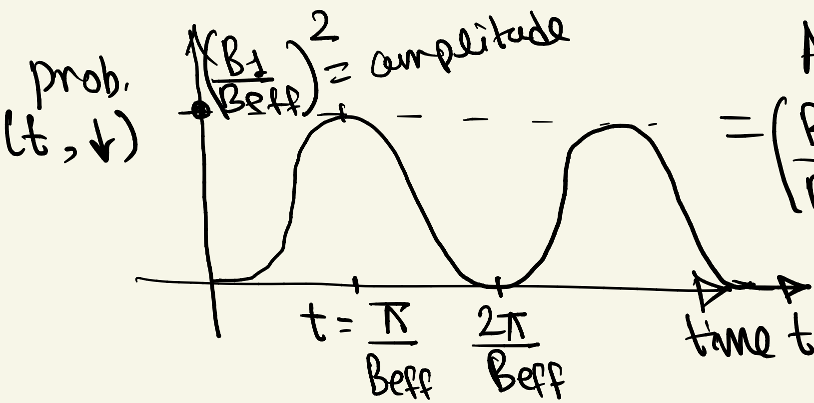
and $\hat{n} = \left(\frac{B_1}{B_{eff}}, 0, \frac{B_0-\omega}{B_{eff}}\right)$ is a unit vector.

Let's assume that at time $t=0$, the state is $|0\rangle$ i.e. the spin points up. (recall $\hat{z}|0\rangle = |0\rangle$). Let's find the probability for the spin to point down at time t:

$$\text{prob.}(t,\downarrow) = |\langle 1 | \psi(t)\rangle|^2$$

$$= \left|\langle 1 | \cos\left(\frac{B_{eff}\, t}{2}\right) - i\,\vec{\sigma}\cdot\hat{n}\,\sin\left(\frac{B_{eff}\, t}{2}\right) |0\rangle\right|^2$$

$$= \left(\frac{B_1}{B_{eff}}\right)^2 \sin^2\left(\frac{B_{eff}\, t}{2}\right)$$



Amplitude $= \left(\frac{B_1}{B_{eff}}\right)^2 \rightarrow 1$ as $\omega \rightarrow B_0$.

"Parametric resonance".