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# Classical Derivation of Frequency Shift and Berry's Phase

Cole Teander and Clark Hickman

# The Geometric Phase is expected to be the largest systematic uncertainty in the nEDM@SNS project

M.W. Ahmed et al. "A new cryogenic apparatus to search for the neutron electric dipole moment". In: *Journal of Instrumentation* 14.11 (Nov. 2019), P11017–P11017. DOI: 10.1088/1748-0221/14/11/p11017.

# Different Approaches Calculate Phase Shifts

- Explored in context of nEDM experiments
  - Pendlebury et al. (2004), Lamoreaux and Golub (2005), and Ignatovich (2008), *PSI (recent, 2015?)
- Quantum Parameter Space
  - Pancharatnam (1956) and Berry (1984)
- Rotation Matrices
  - Berry (1987) and Bliokh (2008)
- Bloch Siegert Shift
  - Bloch and Siegert (1940) and Ramsey (1955)
- Action Angle Variables and Differential Geometry
  - Hannay (1985) and Simon (1983)

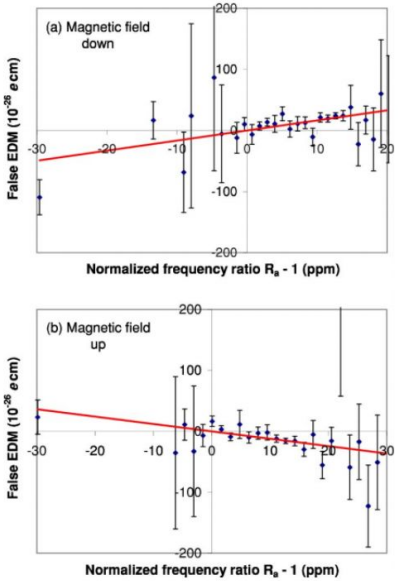



Image from Pendlebury (2004)

# Approaches to Calculating Shifts

Different approaches

Pendlebury, 2004

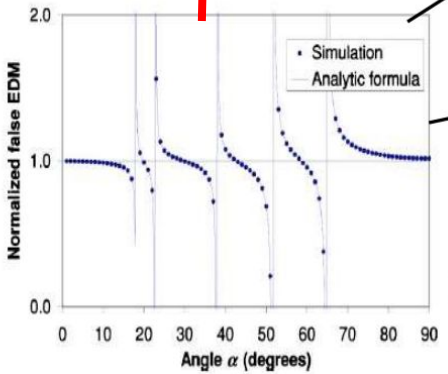
Classical Bloch equations

Quantum Density matrix or Torrey equation

Quantum Schroedinger equation (Steyerl)

Direct solution

Position-velocity correlation function




Single velocity
Cylinder
Specular wall reflections
No gas collisions

Pendlebury et al 2004

slide from Bob Golub

# Approaches to Calculating Shifts

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Our approach

Direct solution

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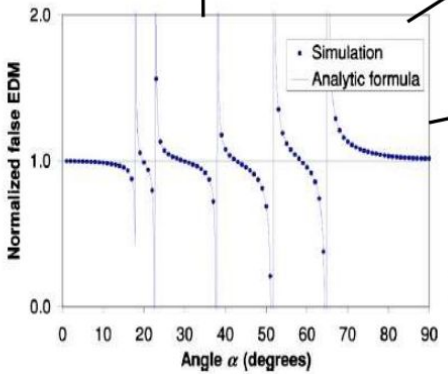


Single velocity
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Pendlebury et al 2004

# The nEDM@SNS Technique

For a spin-½ particle (spin vector given by $\vec{s}$) in electric and magnetic fields, the Hamiltonian is given by

$$H = -\frac{2ex}{\hbar}\left(\vec{s}\cdot\vec{E}\right) - \gamma\left(\vec{s}\cdot\vec{B}\right)$$



Ahmed et al. (2019)

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For a spin that is at an angle from the field axes (for parallel fields), the particle will precess with frequency

$$\omega_{\uparrow\uparrow} = \frac{2ex}{\hbar}|\vec{E}| + \gamma|\vec{B}|$$



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By flipping the direction of the electric field, the sign of the first term will change and the subsequent difference in frequencies is used to determine the nEDM (d)

$$\Delta\omega = \omega_{\downarrow\uparrow} - \omega_{\uparrow\uparrow} = \frac{4ex}{\hbar}|\vec{E}| = \frac{4d}{\hbar}|\vec{E}|$$

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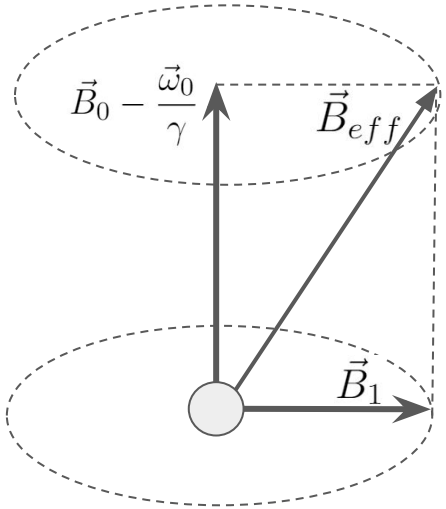
In order to reach the desired sensitivities of the nEDM@SNS experiment, we are very sensitive to any shifts in frequency that are proportional to the electric field (known as linear-in-E shifts) as they will present themselves as a ‘false EDM’

# Frequency Shift

Frequency shifts arise when a strong magnetic field ( $B_0\hat{z}$ ) is perturbed by a weak perpendicular field ( $B_1\hat{r}$ ) that's cycled around it

They interact to create a shifted effective field

$$\vec{B}_{eff}^2 = \vec{B}_1^2 + \left(\vec{B}_0 - \frac{\vec{\omega}_0}{\gamma}\right)^2$$

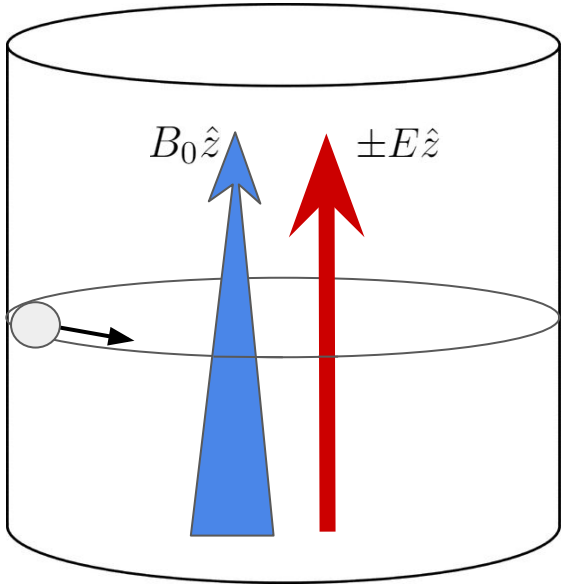



Magnetic fields seen by the particle in its rotating frame

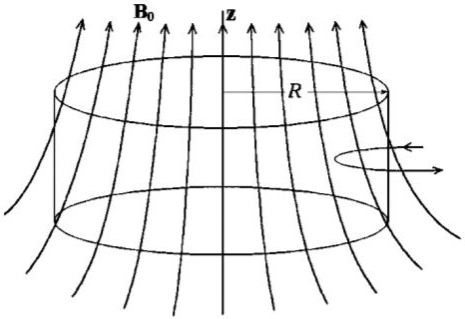
*Note: $B_1$ is greatly exaggerated in this and following diagrams

# Magnetic Field Contribution

There are two causes of the false EDM effect




Radial component to the gradient of the $B_z$ field




$$\vec{B}_r = -\frac{1}{2}\left(\frac{\partial B_z}{\partial z}\right)\vec{r}$$

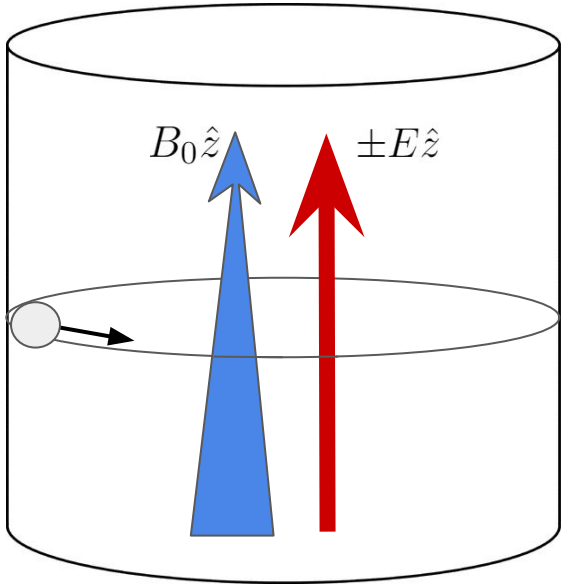
Note that $\vec{B}_r$ has no electric field dependence



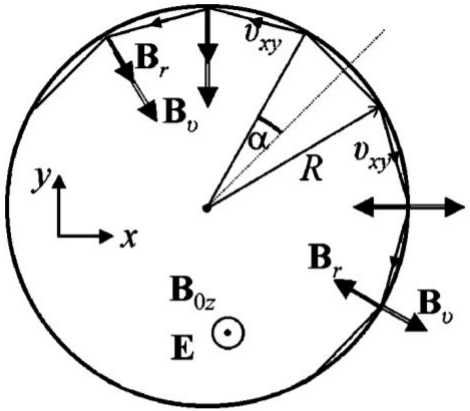
Right image from Pendlebury (2004)

# Electric Field contribution

There are two causes of the false EDM effect




Motional field due spins moving through electric field




$$\vec{B}_r = -\frac{1}{2}\left(\frac{\partial B_z}{\partial z}\right)\vec{r}$$

$$\vec{B}_v = \left(\vec{E} \times \frac{\vec{v}}{c^2}\right)$$

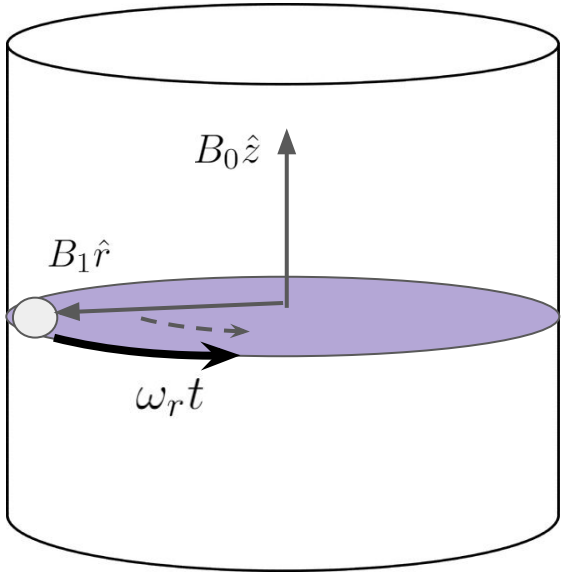
Note that $\vec{B}_v$ has linear electric field dependence



Right image from Pendlebury (2004)

# False EDM signal

The cross terms of $B_1$ linear in E present themselves as a false EDM




$$B_1^2 = \left|\vec{B}_v + \vec{B}_r\right|^2$$

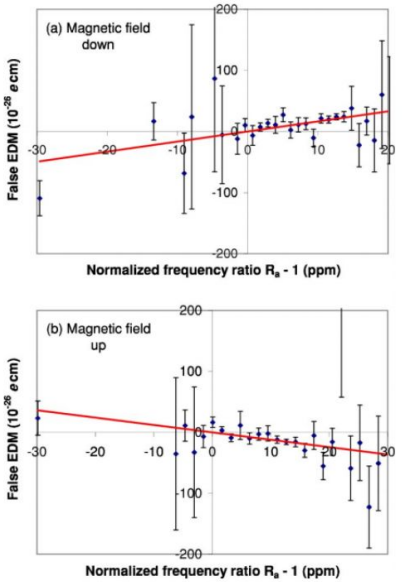
$$\vec{B}_r = -\frac{1}{2}\left(\frac{\partial B_z}{\partial z}\right)\vec{r}$$

$$\vec{B}_v = \left(\vec{E} \times \frac{\vec{v}}{c^2}\right)$$

# Frequency Shift and nEDM

In nEDM experiments, the false EDM was first encountered by ILL in the early 2000's

Pendlebury et al. (2004) gives a thorough description of how the frequency shift would be interpreted as a false EDM and gave a thorough analysis of the magnitude of such shifts for various cases




Golub and Lamoreaux (2005) added to this analysis in nEDM experiments with their solution using density matrices

However, nearly all derivations of the frequency shift have been done via quantum mechanics

Images from Pendlebury (2004)

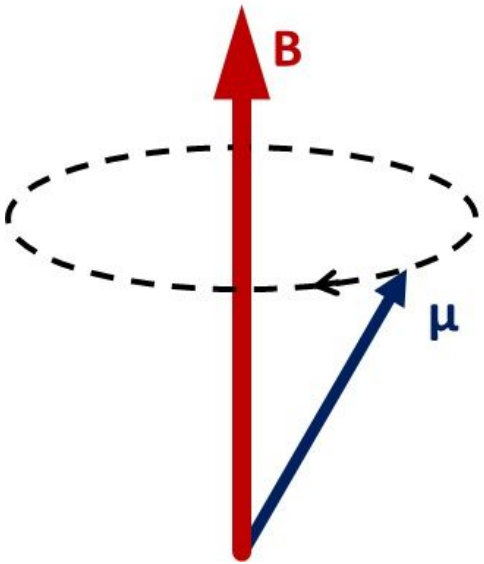
# Classically deriving frequency shift

Our starting point,

The Bloch Equation: $$\frac{d\vec{J}}{dt} = \gamma(\vec{B} \times \vec{J})$$

Or, in terms of ω: $$\vec{\omega} = -\gamma\vec{B}$$

$$\frac{d\vec{J}}{dt} = \vec{J} \times \vec{\omega}$$



$$\frac{d\vec{J}}{dt} = \vec{J} \times \vec{\omega}$$

$$\frac{dJ_z}{dt} = \omega_y J_x - \omega_x J_y$$
$$\frac{dJ_x}{dt} = \omega_z J_y - \omega_y J_z$$
$$\frac{dJ_y}{dt} = \omega_x J_z - \omega_z J_x$$

$$J_z = \cos\theta$$
$$J_x = \sin\theta\cos\phi$$
$$J_y = \sin\theta\sin\phi$$

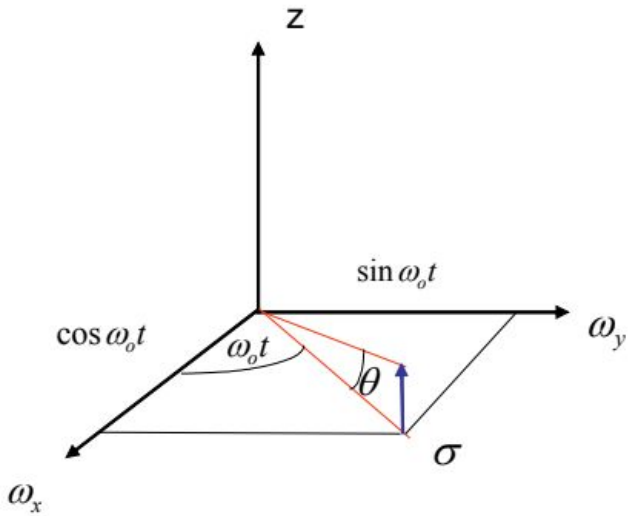
$$\frac{d}{dt}(\cos\theta) = \omega_y \sin\theta\cos\phi - \omega_x \sin\theta\sin\phi$$
$$\frac{d}{dt}(\sin\theta\cos\phi) = \omega_z \sin\theta\sin\phi - \omega_y \cos\theta$$
$$\frac{d}{dt}(\sin\theta\sin\phi) = \omega_x \cos\theta - \omega_z \sin\theta\cos\phi$$

Skipping some algebra…

$$-\dot{\theta} = \omega_y \cos\phi - \omega_x \sin\phi \qquad \tan\theta\left(\dot{\phi} + \omega_z\right) = \omega_y \sin\phi + \omega_x \cos\phi$$

Then changing our definition of theta:

$$\dot{\phi} + \omega_z = \left(\omega_y \sin\phi + \omega_x \cos\phi\right) \tan\theta$$

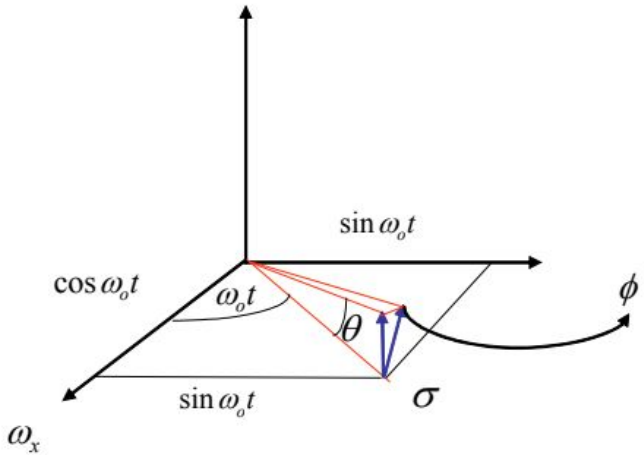


Then, redefining $\varphi = \phi + \omega_z t$

$$\dot{\theta} = \omega_y \cos(\varphi - \omega_z t) - \omega_x \sin(\varphi - \omega_z t)$$

and assuming small angle approximation for theta $tan(\theta) \approx \theta.$

$$\dot{\varphi} = (\omega_y \sin(\varphi - \omega_z t) + \omega_x \cos(\varphi - \omega_z t))\theta$$




*Reminder, theta in reality is much smaller than in image

Now we integrate to get a solution for $\theta$, and plug that in to determine the rate of change of $\varphi$

$$\theta(t) = \int_0^t dt' (\omega'_y \cos(\omega_0 t') + \omega'_x \sin(\omega_0 t'))$$

$$\dot{\varphi}(t) = \int_0^t d\tau \left[-\omega_y \sin(\omega_0 t) + \omega_x \cos(\omega_0 t)\right] \left[\omega'_y \cos(\omega_0 (t-\tau)) + \omega'_x \sin(\omega_0 (t-\tau))\right]$$

where we have made the substitution $t' = t - \tau$

Skipping some more algebra… We arrive at an expression to determine the instantaneous rate of the phase shift (*deviation from the larmor frequency*) as a function of time

$$\dot{\varphi}(t) = \int_0^t \frac{d\tau}{2} \begin{bmatrix} \cos(\omega_0\tau)[\omega'_y\omega_x - \omega'_x\omega_y] \\ -\sin(\omega_0\tau)[\omega'_x\omega_x + \omega'_y\omega_y] \\ +\sin(\omega_0[2t-\tau])[\omega'_x\omega_x - \omega'_y\omega_y] \\ +\cos(\omega_0[2t-\tau])[\omega'_y\omega_x + \omega'_x\omega_y] \end{bmatrix}$$

Now, in order to determine the frequency shift, we must take the time and ensemble average of all precessing particles

$$\delta\omega = \langle\dot{\varphi}\rangle = \left\langle \int_0^\infty \frac{d\tau}{2}[\cos(\omega_0\tau)(R_{yx}(\tau) - R_{xy}(\tau)) - \sin(\omega_0\tau)(R_{xx}(\tau) + R_{yy}(\tau))] \right\rangle$$

where $R_{ij}(\tau) = \langle\omega_i(t-\tau)\omega_j(t)\rangle$

Finally, recall the causes of the frequency shift

$$\omega_x = ax + bv_y \qquad a = \frac{\gamma}{2}\frac{\partial B_z}{\partial z} \qquad b = \gamma\frac{E}{c}.$$
$$\omega_y = ay + bv_x$$

Keeping the linear-in-E cross terms and noting that the sin term averages to 0

$$\delta\omega = \frac{ab}{2}\langle\int_0^\infty d\tau[\cos(\omega_0\tau)(G_{yv_y}(\tau) - G_{v_y y}(\tau) + G_{xv_x}(\tau) - G_{v_x x}(\tau))]\rangle$$

where $G_{fg}(\tau) = \langle f(t-\tau)g(t)\rangle$

Determining these correlation functions experimentally will be our next step

# Connection to Berry's Phase

Quantum phase: difference in phase of the two spin-½ eigenstates

Classical phase: azimuthal angle of the spin vector's expectation value

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Recall $$\dot{\varphi} = \int_0^t d\tau \left[-\omega_y \sin(\omega_0 t) + \omega_x \cos(\omega_0 t)\right] \left[\omega'_y \cos(\omega_0(t-\tau)) + \omega'_x \sin(\omega_0(t-\tau))\right]$$

Assuming now a rotating external field $\omega_x = \alpha \cos(\omega_r t)$ and $\omega_y = -\alpha \sin(\omega_r t)$

Our $\dot{\varphi}$ integral is transformed

$$\dot{\varphi} = \alpha^2 \left(\sin\omega_r t \sin\omega_0 t + \cos\omega_r t \cos\omega_0 t\right) \int_0^t dt' \left(-\sin\omega_r t' \cos\omega_0 t' + \cos\omega_r t' \sin\omega_0 t'\right)$$

$$\dot{\varphi} = \alpha^2 \cos((\omega_0 - \omega_r)t)[\frac{1 - \cos((\omega_0 - \omega_r)t)}{\omega_0 - \omega_r}]$$
$$= \frac{\alpha^2}{\omega_0 - \omega_r}\left[\cos((\omega_0 - \omega_r)t) - \tfrac{1}{2}\cos(2t(\omega_0 - \omega_r)) - \tfrac{1}{2}\right]$$

$$\langle\dot{\varphi}\rangle = -\frac{1}{2}\frac{\alpha^2}{\omega_0 - \omega_r}$$

This is the known Bloch-Siegert shift. Then, subtracting precession in the opposite direction $(\omega_r \to -\omega_r)$

$$\dot{\varphi}_B = \frac{1}{4}\alpha^2\left(\frac{1}{\omega_0 + \omega_r} - \frac{1}{\omega_0 - \omega_r}\right)$$
$$= -\frac{1}{2}\alpha^2\frac{\omega_r}{\omega_0^2 - \omega_r^2}$$

So that the phase accumulated over one rotation is $\phi_B = \dot{\varphi}_B\frac{2\pi}{\omega_r}$

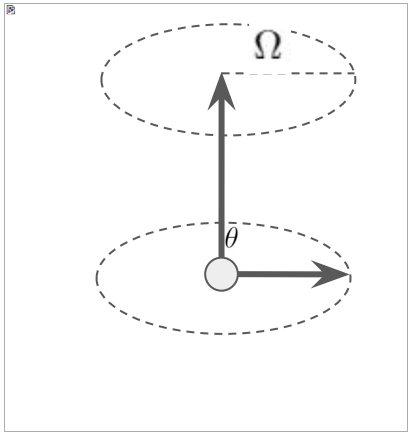
$$= -\frac{\pi\alpha^2}{\omega_0^2 - \omega_r^2}$$

# Berry's phase

In the adiabatic limit ($\omega_r \rightarrow 0$), this becomes

$$\phi_B = -\frac{\pi\alpha^2}{\omega_0^2 - \omega_r^2} \longrightarrow -\frac{\pi\alpha^2}{\omega_0^2} = -\Omega$$

which mirrors Berry's conclusion




While geometric phase had been a topic of discussion since the 1950's, Berry was the one to generalize it in his 1984 paper

He noted that, if an eigenstate adiabatically traverses a parameter space and forms a closed loop, the geometric phase will be equivalent to the solid angle enclosed by said loop

$$\exp\{i\gamma_n(C)\} = \exp\{-in\Omega(C)\},$$

# Conclusion

- A phase shift that is linear in E (due to radial field gradients and motional magnetic fields) can present itself as a false EDM. At the sensitivities at which the nEDM@SNS experiment hopes to reach, this is a significant systematic effect

- Here, we've derived a way to obtain this frequency shift using classical methods beginning with the classical Bloch equations and leading to the Fourier transform of the position-velocity correlation function

- We've also shown that in the adiabatic limit this leads to Berry's phase

# Acknowledgements

Thanks to Bob Golub for putting up with us while we took our time understanding everything

And to the rest of the nEDM@SNS collaboration

Thank you to US DOE for their funding support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# References


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# Skipped algebra

$$\frac{d}{dt}(\cos\theta) = \omega_y \sin\theta\cos\phi - \omega_x \sin\theta\sin\phi \rightarrow$$

$$-\sin\theta\dot{\theta} = \omega_y \sin\theta\cos\phi - \omega_x \sin\theta\sin\phi$$

$$-\dot{\theta} = \omega_y \cos\phi - \omega_x \sin\phi$$

$$\frac{d}{dt}(\sin\theta\cos\phi) = \omega_z \sin\theta\sin\phi - \omega_y \cos\theta \rightarrow$$

$$\cos\theta\dot{\theta}\cos\phi - \sin\theta\sin\phi\dot{\phi} = \omega_z \sin\theta\sin\phi - \omega_y \cos\theta$$

$$\tan\theta\sin\phi\left(\dot{\phi} + \omega_z\right) = \omega_y + \dot{\theta}\cos\phi$$

$$\frac{d}{dt}(\sin\theta\sin\phi) = \omega_x \cos\theta - \omega_z \sin\theta\cos\phi \rightarrow$$

$$\cos\theta\dot{\theta}\sin\phi + \sin\theta\cos\phi\dot{\phi} = \omega_x \cos\theta - \omega_z \sin\theta\cos\phi$$

$$\tan\theta\cos\phi\left(\dot{\phi} + \omega_z\right) = \omega_x - \dot{\theta}\sin\phi$$

# Second skipped algebra

$$\dot{\varphi} = \int_0^t d\tau \begin{bmatrix} \omega'_x \sin(\omega_0(t-\tau))\omega_x \cos(\omega_0 t) \\ -\omega'_y \cos(\omega_0(t-\tau))\omega_y \sin(\omega_0 t) \\ +\omega'_y \cos(\omega_0(t-\tau))\omega_x \cos(\omega_0 t) \\ -\omega'_x \sin(\omega_0(t-\tau))\omega_y \sin(\omega_0 t) \end{bmatrix}$$

$$\dot{\varphi} = \int_0^t \frac{d\tau}{2} \begin{bmatrix} \omega'_x\omega_x[\sin(\omega_0[2t-\tau]) - \sin(\omega_0\tau)] \\ -\omega'_y\omega_y[\sin(\omega_0[2t-\tau]) + \sin(\omega_0\tau)] \\ +\omega'_y\omega_x[\cos(\omega_0[2t-\tau]) + \cos(\omega_0\tau)] \\ +\omega'_x\omega_y[\cos(\omega_0[2t-\tau]) - \cos(\omega_0\tau)] \end{bmatrix}$$

$$\dot{\varphi} = \int_0^t \frac{d\tau}{2} \begin{bmatrix} \cos(\omega_0\tau)[\omega'_y\omega_x - \omega'_x\omega_y] \\ -\sin(\omega_0\tau)[\omega'_x\omega_x + \omega'_y\omega_y] \\ +\sin(\omega_0[2t-\tau])[\omega'_x\omega_x - \omega'_y\omega_y] \\ +\cos(\omega_0[2t-\tau])[\omega'_y\omega_x + \omega'_x\omega_y] \end{bmatrix}$$

# Third skipped algebra

$$\dot{\varphi} = \alpha^2 \cos((\omega_0 - \omega_r)t)[\frac{1 - \cos((\omega_0 - \omega_r)t)}{\omega_0 - \omega_r}]$$
$$= \frac{\alpha^2}{\omega_0 - \omega_r}\left[\cos((\omega_0 - \omega_r)t) - \tfrac{1}{2}\cos(2t(\omega_0 - \omega_r)) - \tfrac{1}{2}\right]$$

Cosine terms vanish after taking time average

# Connection to Berry’s phase

"In fact, in a classical system does not have a phase but we can understand how the effect is manifested in a classical system by noting that in a spin 1/2 system the difference in phase between the two eigenstate vectors corresponds to the azimuthal angle of the expectation value of the spin vector. Thus, Berry's phase (of opposite signs for the two eigenstates) can be expected to appear as a precession of the classical angular momentum in a system exposed to adiabatic cycling of the magnetic field."

# Math, connections to Berry's phase

Adiabatically traversing parameter space in a closed loop

Give final results here, the "familiar" solid angle with (hopefully) a figure. Could we relate it to Pendlebury with the correct relations for a and b to alpha? alpha is constant, assumes circular motion b/c same amplitude for x and y

Berry's phase is adiabatic limit of Bloch-Siegert shift

Note to self: Look at pg 22 of JINST

JINST basically takes $\dot{\varphi} = -\frac{1}{2}\frac{\alpha^2}{\omega_0 - \omega_r}$ and says α = γa * γb

# Useful (?) figures/equations to put in

$$\omega_x = \alpha\cos(\omega_r t) \text{ and } \omega_y = -\alpha\sin(\omega_r t)$$

$$\omega_x = ax + bv_y \qquad b = \gamma\frac{E}{c}.$$

$$\omega_y = ay + bv_x \qquad a = \frac{\gamma}{2}\frac{\partial B_z}{\partial z}$$

$$\phi_B = \dot{\varphi}_B\frac{2\pi}{\omega_r}$$

$$= -\frac{\pi\alpha^2}{\omega_0^2 - \omega_r^2}$$

$$-\Omega = -\frac{\pi\alpha^2}{\omega_0^2}$$