$$\hat{H} = -\mu \mathbf{B} \cdot \hat{\mathbf{S}},$$

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

$$|\psi(t)\rangle = \exp\left[-\frac{i}{\hbar}\hat{H}t\right] |\psi(0)\rangle \equiv \hat{U}(t) |\psi(0)\rangle ,$$

$$\mathbf{B} = B_0 \hat{\mathbf{x}}$$

$$\hat{U}(t) = \exp\left[\frac{i\omega_0 t}{2}\hat{\sigma}^x\right],$$

$$\omega_0 \equiv \mu B_0.$$

$$\begin{aligned}
\hat{U}(t) &= \hat{I}\left(1 - \frac{(\omega_0 t/2)^2}{2!} + \frac{(\omega_0 t/2)^4}{4!} + \cdots\right) \\
&\quad + i\hat{\sigma}^x \left(\omega_0 t/2 - \frac{(\omega_0 t/2)^3}{3!} + \frac{(\omega_0 t/2)^5}{5!} + \cdots\right) \\
&= \cos\frac{\omega_0 t}{2}\hat{I} + i \sin\frac{\omega_0 t}{2}\hat{\sigma}^x \\
&\doteq \begin{pmatrix} \cos\frac{\tau}{2} & i\sin\frac{\tau}{2} \\ i\sin\frac{\tau}{2} & \cos\frac{\tau}{2} \end{pmatrix},
\end{aligned}$$

$$\tau \equiv \omega_0 t.$$

$$\hat{U}\,(\theta, \phi, \lambda) \doteq \begin{pmatrix} \cos\frac{\theta}{2} & -e^{i\lambda}\sin\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} & e^{i(\phi+\lambda)}\cos\frac{\theta}{2} \end{pmatrix}$$

`u(theta,phi,lambda)`

$$\hat{U} = \hat{U}\left(\tau, +\frac{\pi}{2}, -\frac{\pi}{2}\right)$$

theoretical predictions of expectation values of the spin operators

$$\langle \hat{S}^\alpha \rangle \equiv \langle \psi | \hat{S}^\alpha | \psi \rangle$$

$$\begin{aligned}
\left\langle \hat{S}^x(t) \right\rangle &= 0 \\
\left\langle \hat{S}^y(t) \right\rangle &= \frac{\hbar}{2} \sin \omega_0 t \\
\left\langle \hat{S}^z(t) \right\rangle &= \frac{\hbar}{2} \cos \omega_0 t .
\end{aligned}$$

Pauli matrices

$$\sigma_1 = \sigma_\mathrm{x} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_2 = \sigma_\mathrm{y} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\sigma_3 = \sigma_\mathrm{z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\sigma_1^2 = \sigma_2^2 = \sigma_3^2 = -i\,\sigma_1\sigma_2\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I$$

Matrix exponentiating

$$e^{ia\left(\hat{n}\cdot\vec{\sigma}\right)} = I\cos a + i(\hat{n}\cdot\vec{\sigma})\sin a$$

$$e^{i\theta\hat{A}} = \cos\theta\ \hat{I} + i\sin\theta\ \hat{A}$$

Baker–Campbell–Hausdorff formula

$$e^X e^Y = e^Z$$

$$Z = X + Y + \frac{1}{2}[X, Y] + \frac{1}{12}[X, [X, Y]] - \frac{1}{12}[Y, [X, Y]] + \cdots ,$$

Zassenhaus formula

$$e^{t(X+Y)} = e^{tX}\ e^{tY}\ e^{-\frac{t^2}{2}[X,Y]}\ e^{\frac{t^3}{6}(2[Y,[X,Y]]+[X,[X,Y]])}\ e^{\frac{-t^4}{24}([[[X,Y],X],X]+3[[[X,Y],X],Y]+3[[[X,Y],Y],Y])} \cdots$$

As a corollary of this, the Suzuki–Trotter decomposition follows.

$$e^{A+B} = \lim_{n\to\infty} (e^{A/n} e^{B/n})^n$$

Lie product formula

A first order formula consists of the approximation stated in the introduction, where the matrix exponential of a sum is approximated by a product of matrix exponentials:

$$e^{A+B} \approx e^{A}e^{B}$$

There exists a second-order formula, called the Suzuki-Trotter decomposition

$$e^{A+B} \approx e^{B/2}e^{A}e^{B/2}$$

$$e^{-it(XX+ZZ)} = e^{-it/2ZZ}e^{-itXX}e^{-it/2ZZ} + \mathcal{O}(t^3).$$

By means of recursions, higher-order approximations can be found

If all Hamiltonian terms commute, the task of simulating this Hamiltonian is reduced to implementing individually.

$$\hat{H} = \hat{A} + \hat{B},$$

$$\left[\hat{A}, \hat{B}\right] \neq 0.$$

$$\mathbf{B} = \frac{B_0}{\sqrt{2}} (\hat{\mathbf{x}} + \hat{\mathbf{y}})$$

$$\hat{H} = \frac{\omega_0}{\sqrt{2}} \left[\hat{\sigma}^x + \hat{\sigma}^y\right].$$

$$\hat{A} = \frac{\omega_0}{\sqrt{2}} \hat{\sigma}^x \text{ and } \hat{B} = \frac{\omega_0}{\sqrt{2}} \hat{\sigma}^y,$$

$$\left[\hat{A}, \hat{B}\right] = \frac{\omega_0^2}{2} \left[\hat{\sigma}^x, \hat{\sigma}^y\right] = i \frac{\omega_0^2}{2} \hat{\sigma}^z \neq 0.$$

$$\hat{U}(t) = \exp\left[-i\hat{H}t/\hbar\right] = \exp\left[-i\hat{A}t/\hbar - i\hat{B}t/\hbar\right].$$

$$\hat{U}_A(t) = \exp\left[-i\hat{A}t/\hbar\right], \qquad \hat{U}_B(t) = \exp\left[-i\hat{B}t/\hbar\right]$$

As $\hat{A}$ and $\hat{B}$ do not commute, $\hat{U}(t) \neq \hat{U}_A(t)\hat{U}_B(t)$.

$$\begin{aligned} &\exp\left[i(\hat{A} + \hat{B})t/\hbar\right] \\ &= \lim_{n\to\infty} \left(\exp\left[-i\hat{A}t/n\hbar\right] \exp\left[-i\hat{B}t/n\hbar\right]\right)^n, \end{aligned}$$

or

$$\hat{U}(t) = \lim_{n\to\infty} \left(\hat{U}_A\left(\frac{t}{n}\right) \hat{U}_B\left(\frac{t}{n}\right)\right)^n.$$

$$\exp\left[i\frac{\omega_0 t}{2\sqrt{2}}\left(\hat{\sigma}^x+\hat{\sigma}^y\right)t\right]=\hat{U}_3\left(\tau,\frac{3\pi}{4},-\frac{3\pi}{4}\right).$$

Theoretical spin expectation values (Time dependant)

$$\left\langle \hat{S}^x(t)\right\rangle = -\frac{\hbar}{2\sqrt{2}}\sin\omega_0 t,$$

$$\left\langle \hat{S}^y(t)\right\rangle = \frac{\hbar}{2\sqrt{2}}\sin\omega_0 t,$$

$$\left\langle \hat{S}^z(t)\right\rangle = \frac{\hbar}{2}\cos\omega_0 t.$$