The effective Hamiltonian of the Pound-Overhauser controlled-NOT gate

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Abstract. In NMR-based quantum computing, it is known that the controlled-NOT gate can be implemented by applying a low-power, monochromatic radio-frequency field to one peak of a doublet in a weakly-coupled two-spin system. This is known in NMR spectroscopy as Pound-Overhauser double resonance. The “transition” Hamiltonian that has been associated with this procedure is however only an approximation, which ignores off-resonance effects and does not correctly predict the associated phase factors. In this paper, the exact effective Hamiltonian for evolution of the spins’ state in a rotating frame is derived, both under irradiation of a single peak (on-transition) as well as between the peaks of the doublet (on-resonance). The accuracy of these effective Hamiltonians is validated by comparing the observable product operator components of the density matrix obtained by simulation to those obtained by fitting the corresponding experiments. It is further shown that an on-resonance field yields a new implementation of the controlled-NOT gate up to phase factors, wherein the field converts the $I_A^z$ state into the antiphase state $2I_A^x I_B^z$, which is then converted into the desired two-spin order $2I_A^z I_B^z$ by a broadband $\pi/2$ pulse selective for the $A$ spin. In the on-transition case, it is explained that while a controlled-NOT gate is approximately obtained whenever the radio-frequency field power is low compared to the spin-spin coupling, at certain specific power levels an exact implementation is obtained up to phase factors. For both these implementations, the phase factors are derived exactly, enabling them to be corrected. In Appendices, the on-resonance Hamiltonian is analytically diagonalized, and proofs are given that, in the weak-coupling approximation, off-resonance effects can be neglected whenever the radio-frequency field power is small compared to the difference in resonance frequencies of the two spins.

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**1. INTRODUCTION**

The c-NOT (controlled-NOT) gate is of central importance in quantum computing (Barenco et al. 1995a, Barenco et al. 1995b). It is well-known (Lloyd 1993) that in quantum computers based on frequency addressing of their q-bits, such as solution-state NMR spectroscopy on spin $\frac{1}{2}$ nuclei (Cory et al. 1997, Gershenfeld and Chuang 1997), the c-NOT gate can be implemented by the application of a two q-bit transition Hamiltonian of the form

$$H_{trn} \equiv \pi I_x^A E_+^B \equiv \frac{\pi}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix},$$

where $E_\pm^B \equiv \frac{1}{2}(1 \pm 2I_z^B)$ is idempotent (cf. (Hatanaka and Yannoni 1981)). Using NMR spectroscopy (Cory et al. 1998), we have previously demonstrated that irradiating exactly one peak of a doublet in a two-spin system with a power $\omega_1$ much less than the coupling between the spins $2\pi J^{AB}$ transforms the equilibrium state in accord with the corresponding propagator, i.e. $\exp(-\i \pi t H_{trn})$

$$= e^{-\i \pi t I_x^A} E_+^B + E_-^B = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\pi t/2) & 0 & -\i \sin(\pi t/2) \\ 0 & 0 & 1 & 0 \\ 0 & -\i \sin(\pi t/2) & 0 & \cos(\pi t/2) \end{pmatrix}. \quad (2)$$

In NMR spectroscopy, this is often called *Pound-Overhauser double resonance* (Slichter 1990). The nonzero phase factors in this matrix can be equalized by a $\pi/2$ evolution $\exp(-\i (\pi/2) I_z^B)$. Nevertheless, the application of this procedure to a (mixture of) superposition states quickly shows that the effective Hamiltonian is not so simple. The transition Hamiltonian is only a nonphysical approximation, which cannot predict all the details of the spins’ evolution under selective irradiation.

In this paper the effective Hamiltonian in a rotating frame (Ernst et al. 1987, Slichter 1990) is derived, which fully describes the evolution of a weakly-coupled, two-spin system under a monochromatic RF (radio-frequency) field, both on-resonance as well as on a single transition. A pictorial representation in terms of effective fields is described, which provides an intuitive description of the spin dynamics under these Hamiltonians. The results of NMR experiments are presented, which demonstrate that the superposition states that evolve under monochromatic RF fields are consistent with those obtained from simulations using these effective Hamiltonians, and with the effective fields picture. Assuming $\omega_1 \ll 2\pi |J^{AB}| \ll |\omega^A - \omega^B|$ and that off-resonance effects can be neglected, it is proven that the transition and effective on-transition
Hamiltonians are equivalent, in the sense that the corresponding propagators are approximately equal up to conditional phases (i.e. a diagonal matrix of phase factors). This implementation of the c-NOT is shown to be exact (up to conditional phases) for \( \omega_1 = 2\pi J_{AB} / \sqrt{4n^2 - 1} \) where \( n > 0 \) is an integer. It is further proven that the application of an on-resonance field with \( \omega_1 = \pi |J_{AB}| \) followed by a broadband \( \pi/2 \) “soft pulse” (covering the entire doublet), both on the \( A \) spin, likewise implements the c-NOT gate up to conditional phases. In both cases, the conditional phases are derived explicitly. In appendices, the on-resonance Hamiltonian is analytically diagonalized, and the assumption that off-resonance effects are negligible whenever \( \omega_1 \ll |\omega^A - \omega^B| \) is rigorously justified under the weak-coupling approximation.

2. THE POUND-OVERHAUSER EFFECTIVE HAMILTONIAN

2.1. Derivation of the effective Hamiltonians

Given a Hamiltonian \( H = H(t) \) and unitary transformation \( U \equiv \exp(-iGt) \) (where \( G = \tilde{G} \) is Hermitian), the evolution of the transformed density matrix \( \rho' = U\rho\tilde{U} \) is given by (Ernst et al. 1987, Slichter 1990)

\[
\dot{\rho'} = \dot{U}\rho\tilde{U} + U\dot{\rho}\tilde{U} + U\rho\dot{\tilde{U}}
\]

\[
= -iG\rho' + i[\rho', H'] + i\rho'G
\]

\[
= i[\rho', H' + G] \equiv i[\rho', H_{\text{eff}}].
\]  

(3)

where \( H' \equiv UHU \) and \( H_{\text{eff}} \equiv H' + G \). The weak-coupling Hamiltonian of a two-spin system is:

\[
H^{AB} = -\omega^A I^A_z - \omega^B I^B_z + 2\pi J^{AB} I^A_z I^B_z,
\]  

(4)

where \( \omega^A, \omega^B \) are the Larmour precession frequencies of the spins, and \( J^{AB} \) the scalar coupling between them. The applied RF field Hamiltonian has the form

\[
H_{\text{RF}} = \omega_1 e^{i\mu G}(I^A_x + I^B_x) e^{-i\mu G}.
\]  

(5)

where the RF power transmitted to the spins is (assuming for convenience that the system is homonuclear) \( \omega_1 > 0, G \equiv \omega_2(I^A_z + I^B_z) \), and \( \omega_2 \) is the frequency of the RF field.

These results show that the time-dependence can be removed from the Hamiltonian \( H = H^{AB} + H_{\text{RF}} \) by transformation to a frame rotating at the frequency \( \omega_2 \). If the frequency \( \omega_2 = \omega_0^A + \pi J^{AB} \) matches the \( |01\rangle \leftrightarrow |11\rangle \) component of the \( A \)-spin doublet, this yields the time-independent “effective Hamiltonian”

\[
H_{\text{eff}} = \pi J^{AB}(I^A_z + 2I^A_x I^B_x) + (\omega_0^A - \omega_0^B + \pi J^{AB})I^B_z + \omega_1(I^A_x + I^B_x).
\]  

(6)

\[\dagger\] In quantum computing, the ground state is generally indexed by “0”, whereas NMR spectroscopists typically put the spin “up” (parallel the field) state before the “down” in their matrices. These two conventions agree only when the gyromagnetic ratio is positive, as will be assumed in this paper.
Figure 1. Effective fields picture of the evolution of the irradiated A-spins in the on-resonance case. There are two subpopulations of molecules: that in which the B-spin is “up”, and that in which the B-spin is “down”. In these two subpopulations, the magnetization due to the A-spins is initially aligned with the applied field (broad banded up arrow). The RF field power is \( \omega_1 = \pi|J_{AB}| \), which in the co-rotating frame yields the effective fields shown with the thin solid arrows inclined at \( \pi/4 \) from the \( z \)-axis. After a time \( t = \pi/((\omega_1)^2 + (\pi J_{AB})^2)^{-1/2} \), these fields have rotated the A-spin in both subpopulations by an angle of \( \pi \) to the \( \pm x \)-axis, which corresponds to the antiphase state \( I^A_z I^B_z \).

In the event that the RF field is placed on-resonance, \( \omega_2 = \omega^A_0 \), and hence

\[
H_{\text{eff}} = 2\pi J_{AB} I^A_z I^B_z + (\omega^A_0 - \omega^B_0) I^B_z + \omega_1 (I^A_x I^B_x + I^A_y I^B_y) .
\] (7)

Note that since \( G \equiv \omega_2(I^A_z + I^B_z) \) commutes with \( I^A_x I^B_x + I^A_y I^B_y \), if we use the full strong coupling Hamiltonian

\[
H^{AB} = -\omega^A_0 I^A_z - \omega^B_0 I^B_z + 2\pi J_{AB} (I^A_x I^B_x + I^A_y I^B_y + I^A_z I^B_z) .
\] (8)

instead of its weak coupling approximation (4), Eqs. (1) and (2) need only be modified by the addition of the term \( 2\pi J_{AB}(I^A_x I^B_x + I^A_y I^B_y) \).
The effective Hamiltonian of the Pound-Overhauser controlled-NOT gate

\[ 2\pi n = t \sqrt{(\omega_1)^2 + (2\pi J)^2} \]

Figure 2. Effective fields picture of the evolution of the irradiated A-spins in the on-transition case. As in Figure 1, the magnetization due to the A-spins in the two subpopulations of molecules is initially aligned with the applied field (broad banded up arrow). The RF field power is \( \omega_1 \ll \pi |J_{AB}| \), which in the co-rotating frame yields the effective fields shown with the thin solid arrows. The one corresponding to the irradiated transition is along the \( x \)-axis, while the other one is displaced towards the \( z \)-axis by an amount \( 2\pi J_{AB} \). After a time \( t = \pi / \omega_1 \), the A-spin in the first subpopulation has been rotated by \( \pi \) to the \(-z\)-axis. If \( \omega_1 \) is set so that at this time the A-spin in the other subpopulation has rotated by a multiple of \( 2\pi \), this yields an exact implementation of the c-NOT up to conditional phases.

2.2. The effective fields picture of the evolution

A physical picture of the spin dynamics may be obtained by breaking the NMR spectrum up into its individual resonance lines, and specifying a distinct effective field for each. This picture assumes we are dealing with an equilibrium density matrix in the high-temperature approximation, so that there are no spin-spin correlations, and neglects relaxation effects. In a frame rotating at the transmitter frequency \( \omega_2 \), the residual static magnetic field at each resonance \( \omega_0 \) is equal to the frequency offset \( \omega_0 - \omega_2 \). Each of these residual fields may be identified with a subpopulation of the molecules present, wherein the other spins are aligned so that their couplings with the spin in question cause it to resonate at the frequency of the residual field. The applied radio-frequency
field contributes a transverse component of strength $\omega_1$ to the net effective field for each resonance. With care, all the results of this paper can be derived by purely geometric means from this “effective fields picture”.

In the on-resonance case with $\omega_1 = \pi J_{AB}$, the effective fields for each resonance line of the A-spin doublet form angles of $\pm \pi/4$ with the z-axis, as shown in Figure 1. Thus the equilibrium magnetization components for each resonance counter-rotate from their initial positions along the z-axis to opposite directions along the x-axis after a time “$t$” given by $\pi = t \sqrt{(\omega_1)^2 + (\pi J_{AB})^2}$. This vector configuration represents the antiphase state $I_A^x I_B^z$, which may be converted to the $I_A^z I_B^z$ state expected after a c-NOT gate by a broadband $\pi/2$ y-pulse selective for the A-spin. In the on-transition case, in contrast, the on-resonance component of the magnetization experiences an effective field in the transverse plane, while the other component experiences a field which is, for $\omega_1 \ll |\omega_0^A - \omega_0^B|$, very nearly along the z-axis. Since it is exactly along the z-axis only in the limit $\omega_1 \rightarrow 0$, however, for any $\omega_1 > 0$ it nutates away from the z-axis, as shown in Figure 2. An exact implementation of the c-NOT gate is nevertheless obtained when $\omega_1$ is chosen so that this component is rotated by an integer multiple of 2$\pi$ back to the z-axis in the time it takes the other component to rotate to the $-z$-axis, namely $t = \pi/\omega_1$.

3. EXPERIMENTAL VALIDATION OF THE EFFECTIVE HAMILTONIAN

In order to demonstrate that these effective Hamiltonians correctly describe the evolution of a weakly-coupled two-spin system under a monochromatic RF field, we used a solution of triply-labeled $^{13}$C alanine ($\text{CO}_2^- - \text{CH}[-\text{NH}_2^+] - \text{CH}_3$) in $\text{D}_2\text{O}$. The carboxyl carbon was treated as the “A” (target) spin, the alpha-carbon as the “B” (control) spin. Since the carboxyl to methyl carbon coupling constant of ca. 1.4 Hz. is less than the peak width, its effects could be ignored, and the effects of the protons eliminated by decoupling. The following three experiments were performed at 16 evenly spaced time points in the interval from $t_{\text{max}}/16$ to $t_{\text{max}}$:

(i) On the $\omega^A$ resonance with $\omega_1 = \pi |J_{AB}|$ ($t_{\text{max}} = \sqrt{2}/|J_{AB}|$).
(ii) On the $\omega^A + \pi J_{AB}$ transition with $\omega_1 = 2\pi |J_{AB}|$ ($t_{\text{max}} = 1/|J_{AB}|$).
(iii) On the $\omega^A + \pi J_{AB}$ transition with $\omega_1 = 4\pi = 2\pi \times 2$ Hz. ($t_{\text{max}} = \pi/\omega_1 = 1/2$ sec.).

Experiments (i) and (iii) validate the correctness of the effective Hamiltonian in the two cases that may be used to implement a c-NOT gate, while (ii) validates the theory for case in which the evolution of coherence is more complicated. All the experiments were performed with the spin system initially at equilibrium in a 9.4 Tesla field.

After the RF field had been applied for each of the 16 time periods used, a 24k point FID (free-induction decay) was collected over 590 msec., zero-filled to 48k, and Fourier transformed to yield the complete spectrum. A 128 point window centered on
Figure 3. Plots of observable product operator components of the density matrix versus 16 equally spaced time points (in percent of $t_{\text{max}}$) for the on-resonance case (i) with $\omega_1 = \pi |J^{AB}|$ and $t_{\text{max}} = \sqrt{2} / |J^{AB}|$. The symbols in this plot (and the corresponding product operator components) are “○” ($I^A_x$), “□” ($I^A_y$), “△” ($I^A_x I^B_z$), and “⋄” ($I^A_y I^B_z$). The solid lines are the simulated results for these components, while the dashed line is the simulated evolution of the diagonal $I^A_z$ component.

The peaks from the A-spin was taken and the absorptive in-phase ($I^A_x$), absorptive anti-phase ($2I^A_x I^B_z$), dispersive anti-phase ($2I^A_y I^B_z$) and dispersive in-phase ($I^A_y$) components of the density matrix extracted from it. This was done by a least-squares fit of a linear combination of model peak shapes for each of these four components to the spectrum window, where the model peak shapes were computed using a coupling constant of 54 Hz. together with a Lorentzian peak shape of half-width 0.85 Hz.

In order to compare these results with the theory, the results predicted from the above effective Hamiltonians were also computed by numerical simulation, using the same coupling constant and resonance frequencies. These results were normalized so that the initial $I^A_z$ state had unit norm, and the experimental fits scaled so that the root-mean-square values of the experimental results were the same as the simulated results. If necessary, the spectrum was adjusted by means of a first-order phase correction so as to obtain the best possible fit, as judged visually. The simulations and final fits to the data for each of these three series of experiments are shown in Figures 3–5. It should be clearly understood that the simulated curves were not fitted to the experiments save by scaling.
Figure 4. Plots of observable product operator components of the density matrix versus 16 equally spaced time points (in percent of $t_{\text{max}}$) for the on-transition case (ii) with $\omega_1 = 2\pi|J^{AB}|$ and $t_{\text{max}} = 1/|J^{AB}|$. The solid lines are the simulated results for these components, while the dashed line depicts the evolution of the diagonal $I^A_z$ (starting from 1) and $I^A_z I^B_z$ (starting from 0) components. The symbols in the plot are the same as in Figure 3.

Given the many sources of systematic error present in NMR spectroscopy (Hoch and Stern 1996), and the fact that the fits were not systematically optimized with respect to the nonlinear parameters (i.e. the coupling constant, resonance frequencies, peak widths/shapes and spectrum phases), the match of the experimental to the simulated results is strong evidence for the validity of the theory. The corresponding simulations using the transition Hamiltonian (not shown) are essentially the same, except that the high-frequency oscillations are not present.

4. DERIVATION OF THE CONDITIONAL PHASE FACTORS

4.1. The on-resonance case

Under the assumption of weak coupling, it is shown in Appendix B that if $\omega_1 \ll |\omega^A - \omega^B|$, the off-resonance effects due to the $I^B_x$ term in $H_{\text{eff}}$ can be ignored. This can be understood intuitively through the effective fields picture for the $B$, since under these fields are essentially along the $z$-axis and hence only induce phase shifts. Thus let
The effective Hamiltonian of the Pound-Overhauser controlled-NOT gate

\[ H^0_{\text{eff}} \equiv H_{\text{eff}} - \omega_1 I^B_x, \]

\[ c_1 \equiv \pi J^{AB}/\omega_1 \quad \text{and} \quad c_2 \equiv (\omega_A^0 - \omega_B^0)/\omega_1, \]

so that

\[ H^0_{\text{eff}}/\omega_1 = c_2 I^B_x + (I^A_x + 2c_1 I^A_x I^B_x) (E_-^B + E_+^B) \]
\[ = c_2 I^B_x + (I^A_x - c_1 I^A_x) E_-^B + (I^A_x + c_1 I^A_x) E_+^B. \]

Since all three terms in this expression commute, it follows that

\[ \exp(-tH^0_{\text{eff}}) = e^{-t\omega_1 I^A_x} E_-^B e^{-t\omega_1 I^A_x} E_+^B e^{-t\omega_1 c_2 I^B_x}, \]

where by the formula for the exponential of an operator multiplied by a commuting idempotent (Somaroo et al. 1998),

\[ \exp(-t\omega_1 I^A_x \pm c_1 I^A_x) E^B_\pm \]
\[ = E^B_\pm + \left( \cos\left(\frac{1}{2}\omega_1 t \sqrt{1+c_2^2}\right) - \frac{2t(I^A_x \pm c_1 I^A_x)}{\sqrt{1+c_2^2}} \sin\left(\frac{1}{2}\omega_1 t \sqrt{1+c_2^2}\right) \right) E^B_\pm. \]
The effective Hamiltonian of the Pound-Overhauser controlled-NOT gate

For $\omega_1 \equiv \pi |J^{AB}|$ and $t \equiv \pi/(\sqrt{2} \omega_1)$, this implies $\exp(-\mathbf{t} \mathbf{H}^0_{\text{eff}})$

\[
\begin{align*}
&= -\mathbf{t} \sqrt{2} \left((\mathbf{I}^A_x - \mathbf{I}^A_z) \mathbf{E}^B + (\mathbf{I}^A_x + \mathbf{I}^A_z) \mathbf{E}^B_+ \right) e^{-\mathbf{t} \pi c_2 \mathbf{I}^B_z / \sqrt{2}} \\
&= -2\mathbf{t} \left((\mathbf{I}^A_x \mathbf{E}^B + \mathbf{I}^A_z \mathbf{E}^B_+) \right) e^{\mathbf{t} \pi c_2 / 2} e^{-\mathbf{t} \pi c_2 \mathbf{I}^B_z / \sqrt{2}} \\
&= e^{-\mathbf{t} \pi / 2} e^{-\mathbf{t} \pi \mathbf{I}^B_x} e^{-\mathbf{t} \pi \mathbf{I}^B_z} e^{-\mathbf{t} \pi c_2 \mathbf{I}^B_z / \sqrt{2}},
\end{align*}
\]

where have we used the fact that $\mathbf{I}^A_y$ anticommutes with $\mathbf{I}^A_x$ and $\mathbf{I}^A_z$ to move its exponential to the far left. Thus the applications of an on-resonance pulse with $\omega_1 = \pi |J^{AB}|$ and $t = \pi/(\sqrt{2} \omega_1)$, followed by an ordinary soft $-\pi/2$ $y$-pulse on spin A, yields the c-NOT gate up to a conditional phase prefactor of $\exp(-\mathbf{t} \mathbf{H}^0_{\text{eff}}(\mathbf{I}^A_z/2 + (c_2 \sqrt{2} - 1) \mathbf{I}^B_z/2 + \mathbf{I}^A_\gamma \mathbf{I}^B_\gamma))$. By moving $\exp(\mathbf{t} \pi \mathbf{I}^A_\gamma/2)$ to the far right instead, one sees that one could just as well precede the on-resonance pulse with a soft $+\pi/2$ $y$-pulse on spin A.

4.2. The on-transition case

We begin again by breaking $\mathbf{H}^0_{\text{eff}} = \mathbf{H}_{\text{eff}} - \omega_1 \mathbf{I}^B_x$ into three commuting parts as above, namely

\[
(\pi/\omega_1) \mathbf{H}^0_{\text{eff}} = \pi \left((c_1 + c_2) \mathbf{I}^B_z + 2c_1 \mathbf{I}^A_z \mathbf{E}^B_+ + \mathbf{I}^A_x (\mathbf{E}^B_+ + \mathbf{E}^B_-) \right)
\]

\[
= \pi \left((c_1 + c_2) \mathbf{I}^B_z + (2c_1 \mathbf{I}^A_z + \mathbf{I}^A_x) \mathbf{E}^B_+ + \mathbf{I}^A_x \mathbf{E}^B_- \right)
\]

\[
= \mathbf{P} + \mathbf{Q}_+ \mathbf{E}^B_+ + \mathbf{Q}_- \mathbf{E}^B_-,
\]

where

\[
\mathbf{P} \equiv \pi(c_1 + c_2) \mathbf{I}^B_z, \quad \mathbf{Q}_+ \equiv \pi(2c_1 \mathbf{I}^A_z + \mathbf{I}^A_x), \quad \text{and} \quad \mathbf{Q}_- \equiv \pi \mathbf{I}^A_x.
\]

Note that $\mathbf{P}$ is diagonal (i.e. along the $z$-axis) and that $\mathbf{H}_{\text{trn}} \equiv \mathbf{Q}_- \mathbf{E}^B_-$, but since $\mathbf{Q}_+ \mathbf{E}^B_+$ is not diagonal, $\exp(-\mathbf{t} \pi/\omega_1) \mathbf{H}^0_{\text{eff}}$ and $\exp(-\mathbf{t} \mathbf{H}_{\text{trn}})$ do not simply differ by conditional phases as in the on-resonance case. Nevertheless, $\mathbf{Q}_+ \mathbf{E}^B_+$ can be readily diagonalized, because

\[
\mathbf{Q}_+ = \pi(e^{-\mathbf{t} \mathbf{I}^A_\gamma} \mathbf{I}^A_\gamma e^{\mathbf{t} \mathbf{I}^A_\gamma}) \sqrt{1 + 4c_1^2},
\]

where $\theta$ is given by $\arctan(1/(2c_1))$.

To show that the effect of this diagonalization upon the propagator $\exp(-\mathbf{t} \mathbf{H}^0_{\text{eff}})$ is small, we evaluate the norm of the difference of the propagator with and without this transformation.\footnote{The norm we use is the square-root of the geometric algebra “scalar part” (denoted by angular brackets $\langle \rangle$) \cite{Somaroo2098} of the product of the quantity with its Hermitian conjugate. For the two spin system considered here the scalar part is four times the trace in the usual product Pauli matrix representation, and hence our norm is just twice the standard Frobenius norm.} Since $\mathbf{I}^A_\gamma$ and $\mathbf{Q}_- = \pi \mathbf{I}^A_x$ don’t commute, we operate with

\[
\mathbf{P} \equiv \pi(c_1 + c_2) \mathbf{I}^B_z, \quad \mathbf{Q}_+ \equiv \pi(2c_1 \mathbf{I}^A_z + \mathbf{I}^A_x), \quad \text{and} \quad \mathbf{Q}_- \equiv \pi \mathbf{I}^A_x.
\]
The effective Hamiltonian of the Pound-Overhauser controlled-NOT gate

\[ \exp(-i \theta I_{\gamma}^A E_{+}^B) \] instead of \( \exp(-i \theta J_{\gamma}^A) \), obtaining

\[
\begin{align*}
&\left\| e^{-i(\pi/\omega_1)H_{\text{eff}}^0} - e^{i\theta I_{\gamma}^A E_{+}^B} e^{-i(\pi/\omega_1)H_{\text{eff}}^0} e^{-i\theta I_{\gamma}^A E_{+}^B} \right\|^2 \\
= &\left\| e^{-iQ_{+} E_{+}^B} - e^{i\theta I_{\gamma}^A} e^{-iQ_{+} E_{+}^B} e^{-i\theta I_{\gamma}^A} \right\|^2 \\
= &2 - 2 \left\langle e^{-i\pi(2I_{\gamma}^A + I_{z}^A)} E_{+}^B e^{i\pi \sqrt{1+4c_{1}^2} I_{z}^A E_{+}^B} \right\rangle \\
= &2 - 2 \left\langle \left( E_{-}^B + E_{+}^B e^{-i\pi(2I_{\gamma}^A + I_{z}^A)} \right) \left( E_{-}^B + E_{+}^B e^{i\pi \sqrt{1+4c_{1}^2} I_{z}^A} \right) \right\rangle \\
= &1 - \left\langle \left( \cos \left( \frac{\pi}{2} \sqrt{1+4c_{1}^2} \right) - i \frac{2c_{1} I_{z}^A + I_{z}^A}{\sqrt{1+4c_{1}^2}} \sin \left( \frac{\pi}{2} \sqrt{1+4c_{1}^2} \right) \right) \left( \cos \left( \frac{\pi}{2} \sqrt{1+4c_{1}^2} \right) + i 2 I_{z}^A \sin \left( \frac{\pi}{2} \sqrt{1+4c_{1}^2} \right) \right) \right\rangle \\
= &1 - \cos^2 \left( \frac{\pi}{2} \sqrt{1+4c_{1}^2} \right) - \sin^2 \left( \frac{\pi}{2} \sqrt{1+4c_{1}^2} \right) \frac{2c_{1}}{\sqrt{1+4c_{1}^2}} \\
= &\sin^2 \left( \frac{\pi}{2} \sqrt{1+4c_{1}^2} \right) \left( 1 - \frac{2c_{1}}{\sqrt{1+4c_{1}^2}} \right)
\end{align*}
\]

The second factor can be converted into the simple bound

\[
\frac{1 + 4c_{1}^2 - 2|c_{1}| \sqrt{1+4c_{1}^2}}{1 + 4c_{1}^2} \leq \frac{1}{4c_{1}^2} = \frac{\omega_{1}^2}{4(\pi J_{AB})^2} \ll 1,
\]

thus showing that \( \exp(iQ_{+} E_{+}^B) \) is essentially a diagonal matrix \( \exp(i\pi \sqrt{1+4c_{1}^2} I_{z}^A E_{+}^B) \) of phase factors as long as \( \omega_{1} \ll \pi |J_{AB}| \). Noting that \( I_{z}^A E_{+}^B \) still commutes with \( H_{\text{trn}} \), it follows that

\[
e^{-i(\pi/\omega_1)H_{\text{eff}}^0} \approx e^{-iH_{\text{trn}}} e^{-i\pi(c_{1} + c_{2}) I_{z}^A} e^{-i\pi \sqrt{1+4c_{1}^2} I_{z}^A E_{+}^B},
\]

where the last two factors are conditional phases.

It is interesting to observe that since \( \sin^2 \left( \frac{\pi}{2} \sqrt{1+4c_{1}^2} \right) = 0 \) if \( \sqrt{1+4c_{1}^2} = 2n \) for an integer \( n > 0 \), an exact implementation of the c-NOT is obtained when \( |c_{1}| \equiv |\pi J_{AB}|/\omega_{1} = \frac{1}{2} \sqrt{4n_{1}^2 - 1} \) or \( \omega_{1} = 2|\pi J_{AB}|/\sqrt{4n_{1}^2 - 1} \), in which case the time required for the c-NOT is \( \pi/\omega_{1} = \sqrt{4n_{1}^2 - 1}/|2J_{AB}| \). For \( n = 1 \), this is \( \sqrt{3}/|2J_{AB}| \), which is longer than the \( 1/|\sqrt{2}J_{AB}| \) required by the on-resonance implementation, although in some circumstances the fact that an additional soft pulse is not needed in the on-transition case might be an advantage.

5. CONCLUSIONS

We have presented a detailed analysis of two Pound-Overhauser implementations of the controlled-NOT gate, one using an on-transition x-pulse with \( \omega_{1} \ll 2\pi |J_{AB}| \), and the other using an on-resonance x-pulse of power \( \omega_{1} = \pi |J_{AB}| \) and duration \( 1/(|\sqrt{2}J_{AB}|) \) followed by a soft \( \pi I_{z}^A \) pulse. The correctness of the effective Hamiltonians for both implementations have been validated by NMR experiments, and the phase corrections derived using geometric algebra. In the course of this analysis, it was shown that the time...
required for the on-transition implementation could be decreased to \( t = \sqrt{3}/(2|J_{AB}|) \) while actually making the implementation exact (up to conditional phases) by increasing the power to \( \omega_1 = 2\pi|J_{AB}|/\sqrt{3} \). Neither the on-resonance nor the on-transition Pound-Overhauser implementation is as efficient as the pulse sequence in (Cory et al. 1998), which takes only \( 1/(2|J_{AB}|) \) plus two soft pulses. Nevertheless, the Pound-Overhauser implementations have the advantage that in systems of more than two spins, it should be easier to find a sequence of \( \pi \) pulses which refocuses the evolution of all the remaining spins while the gate is in progress, because it is not necessary to treat the spins to which the gate is being applied specially. Geometric algebra calculations with sums of transition Hamiltonians (Somaroo et al. 1998) further indicate that the simultaneous irradiation of multiple resonances, which we call \textit{compound pulses}, can be used to directly excite multiple quantum transitions, and thereby accomplish in a single step what might otherwise take considerably more time. Their effective Hamiltonians will be the subject of a future paper.

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Appendix A. DIAGONALIZATION OF THE ON-RESONANCE HAMILTONIAN

In the on-resonance case, the characteristic polynomial \( \det(H_{\text{eff}}/\omega_1 - \lambda) \) of the effective Hamiltonian is a quadratic in \( \lambda^2 \), with eigenvalues

\[
\lambda_{\pm}^2 = \frac{1}{4} \left( 2 + c_1^2 + c_2^2 \pm 2\sqrt{1 + c_2^2(1 + c_1^2)} \right),
\]

where \( c_1 \) and \( c_2 \) are given by Eq. (9). It is therefore reasonable to expect that it will be possible to analytically diagonalize this Hamiltonian, and we now show how this can be done using geometric algebra (Somaroo et al. 1998).

We begin by rewriting the on-resonance Hamiltonian (Eq. (6)) in the form

\[
H_{\text{eff}}/\omega_1 = 2c_1 I_z^A I_z^B + I_x^A + c'_2 I_z^B \exp(\iota \mu 2 I_y^B),
\]

where

\[
c'_2 = \sqrt{1 + c_2^2} \quad \text{and} \quad \tan(\mu) = 1/c_2.
\]

Rotating spin \( \mu \) about \( 2I_y^B \) this yields

\[
H'_{\text{eff}}/\omega_1 = e^{\iota \mu I_y^B} (H_{\text{eff}}/\omega_1)e^{-\iota \mu I_y^B} = 2c_1 I_z^A \exp(-\iota \mu 2 I_y^B) I_z^B + I_x^A + c'_2 I_z^B = 2c_1 I_z^A \left( I_z^B \cos(\mu) + I_x^B \sin(\mu) \right) + I_x^A + c'_2 I_z^B = e^{-\iota \mu 2 I_y^B} \left( 2c'_1 I_z^A I_z^B + 2c_1 I_x^A I_x^B \sin(\mu) + c'_2 I_z^B \right) e^{\iota \mu 2 I_y^B},
\]
The effective Hamiltonian of the Pound-Overhauser controlled-NOT gate

\[ c_1' = \sqrt{1 + c_1^2 \cos^2(\mu)} \quad \text{and} \quad \tan(\nu) = 1/(c_1 \cos(\mu)). \]  

(A.5)

The outer exponentials can be eliminated by applying the opposite rotation, obtaining

\[ H''_{\text{eff}} / \omega_1 \equiv e^{\nu/2I^A_z} (H'_{\text{eff}} / \omega_1)e^{-\nu/2I^A_z} = 2c_1' I^A_z + 2c_1 I^A_z I^B_x \sin(\mu) + c_2' I^B_z. \]  

(A.6)

To complete the diagonalization, this is rewritten as

\[ H''_{\text{eff}} / \omega_1 = \left( \left( c_1' + c_2' \right) I^B_z + c_1 \sin(\mu) I^B_x \right) E^A_+ - \left( \left( c_1' - c_2' \right) I^B_z + c_1 \sin(\mu) I^B_x \right) E^A_- \]  

\[ = 2\lambda_+ I^B_z e^{-\nu/2} E^A_+ - 2\lambda_- I^B_z e^{-\nu/2} E^A_-, \]  

(A.7)

where

\[ \lambda_{\pm} = \frac{1}{2} \sqrt{(c_1' \pm c_2')^2 + (c_1 \sin(\mu))^2} \]  

(A.8)

are the eigenvalues as above, and

\[ \tan(\kappa_{\pm}) = \frac{c_1 \sin(\mu)}{c_1' \pm c_2'}. \]  

(A.9)

Therefore the conditional rotation

\[ K \equiv e^{-\nu/2} I^B_z E^A_+ + e^{-\nu/2} I^B_z E^A_- \]  

\[ = e^{-\nu/2} E^A_+ I^B_z e^{-\nu/2} I^B_z \]  

(A.10)

completes the diagonalization to

\[ K(H''_{\text{eff}} / \omega_1) K = 2\lambda_+ E^A_+ I^B_z - 2\lambda_- E^A_- I^B_z \]  

\[ = \lambda_+ E^A_+ E^B_+ - \lambda_+ E^A_- E^B_- - \lambda_- E^A_- E^B_+ + \lambda_- E^A_+ E^B_. \]  

(A.11)

While it is possible to write down the time-dependent exponential of the diagonalized Hamiltonian, and to transform it back to that of the original Hamiltonian \( H_{\text{eff}} \), the resulting propagator is too complicated to yield much insight into the dynamics. Nevertheless, in the next Appendix the above diagonal form will enable us to give an elementary proof that off-resonance effects can be neglected in the on-resonance case.

**Appendix B. OFF-RESONANCE EFFECTS ON THE PROPAGATORS**

**Appendix B.1. The on-resonance case**

In order to justify the above assumption that the \( I^B_x \) term in the Hamiltonian can be neglected, let us extend our definition of \( H_{\text{eff}} \) (Eq. [4]) to

\[ H^a_{\text{eff}} \equiv 2\pi J^{AB} I^A_z I^B_z + (\omega_0^A - \omega_0^B) I^B_z + \omega_1 (I^A_z + \alpha I^B_z). \]  

(B.1)
Note that \( H_{\text{eff}}^0 |_{\alpha=0} = H_{\text{eff}} \equiv H_{\text{eff}} - \omega_1 \mathbf{I}_x \) as above. Accordingly, Eq. (A.3) is replaced by
\[
\omega_1 = \sqrt{\alpha^2 + c_1^2} \quad \text{and} \quad \tan(\mu) = \alpha/c_1.
\]

The rest of the diagonalization of \( H_{\text{eff}} \) goes through exactly as for \( H_{\text{eff}} = H_{\text{eff}}^0 \). It now follows from Eq. (A.6) that
\[
expon(-tH_{\text{eff}}^0) = \left( e^{-\omega_1 \mathbf{I}_x} e^{-\omega_1 \mathbf{I}_y} e^{-\omega_1 \mathbf{I}_z} e^{-\omega_1 \mathbf{I}_x} e^{-\omega_1 \mathbf{I}_y} e^{-\omega_1 \mathbf{I}_z} e^{-\omega_1 \mathbf{I}_x} e^{-\omega_1 \mathbf{I}_y} e^{-\omega_1 \mathbf{I}_z} \right) \left( e^{\omega_1 \mathbf{I}_x} e^{\omega_1 \mathbf{I}_y} e^{\omega_1 \mathbf{I}_z} e^{\omega_1 \mathbf{I}_x} e^{\omega_1 \mathbf{I}_y} e^{\omega_1 \mathbf{I}_z} e^{\omega_1 \mathbf{I}_x} e^{\omega_1 \mathbf{I}_y} e^{\omega_1 \mathbf{I}_z} \right) \mathbf{I}.
\]

where \( \mu, \nu, \kappa_\pm \) and \( \lambda_\pm \) are all functions of \( \alpha \).

We wish to show that the propagators \( \exp(-tH_{\text{eff}}^0) \) and \( \exp(-tH_{\text{eff}}) \) are approximately equal. Although this is implied by first-order perturbation theory, for any noninfinitesimal perturbation this standard argument falls short of being a rigorous proof. To this end, let us fix \( t \) and define the function
\[
f(\alpha) \equiv \frac{1}{2} \left| \left| e^{-tH_{\text{eff}}^0} - e^{-tH_{\text{eff}}} \right| \right|^2 = 1 - \left\langle e^{-tH_{\text{eff}}^0} e^{tH_{\text{eff}}} \right\rangle.
\]

Using the fact that \( \|U\| = 1 \) for unitary \( U \), the Cauchy-Schwarz and triangle inequalities, and the invariance of the scalar part under cyclic permutations, the magnitude of the derivative may be bounded as follows:
\[
|f'(\alpha)| = \left| \left\langle \partial/\partial \alpha e^{-tH_{\text{eff}}^0} e^{tH_{\text{eff}}} \right\rangle \right| \leq \left| \left| \partial/\partial \alpha e^{-tH_{\text{eff}}^0} \right| \right| \left| e^{tH_{\text{eff}}} \right| = \left| \left| \partial/\partial \alpha e^{-tH_{\text{eff}}^0} \right| \right|
\]
\[
\leq 2 \| t \mathbf{I} y \partial \mu/\partial \alpha \| + 2 \| t \mathbf{I} z \partial \nu/\partial \alpha \| + 2 \| t \mathbf{E} \mathbf{I} y \partial \kappa_+/\partial \alpha \| + 2 \| t \mathbf{E} \mathbf{I} y \partial \kappa_-/\partial \alpha \|
\]
\[
+ \left\langle \omega_1 t \mathbf{E} \mathbf{I} z \partial \lambda_+/\partial \alpha \| + \left\langle \omega_1 t \mathbf{E} \mathbf{I} z \partial \lambda_-/\partial \alpha \| \right\rangle
\]

To bound the first two terms on the right-hand side, the derivatives are evaluated and simplified by means of the assumptions \( 2 \leq 1 + c_1^2 \leq c_2^2 \), i.e.
\[
2 \left\| t \mathbf{I} y \partial \mu/\partial \alpha \| = \left| \partial/\partial \alpha \arctan(\alpha/c_2) \right| \leq \frac{1}{c_2} \left( 1 + (\alpha/c_2)^2 \right) \leq \frac{1}{c_2},
\]

Since multiplying a propagator by a scalar phase factor has no effect on how it transforms the density matrix, the correct way to compare two \( N \times N \) propagators \( U_1, U_2 \) is to compute the expression
\[
1 - \| \text{tr} \left( U_1 \hat{U}_2 \right) \| /N^2 = 1 - \| (U_1 \hat{U}_2)^2 - (iU_1 \hat{U}_2)^2 \| = \frac{1}{4} \| U_1 - iU_2 \| + \frac{1}{4} \| U_1 + iU_2 \|^2 \| U_1 + iU_2 \|^2 - 1.
\]

It is sufficient, however, to show that just one of the above norms vanishes, e.g. \( \| U_1 - U_2 \|^2 \), meaning that the propagators are equal without any overall phase differences, and this turns out to be the case for all the propagators considered in this paper.
The effective Hamiltonian of the Pound-Overhauser controlled-NOT gate

and (using the fact that \(\cos(\mu) = (1 + (\alpha/c_2)^2)^{-1/2}\))

\[
2 \| t2I^A_yI^B_z \partial \nu / \partial \alpha \| = |\partial / \partial \alpha \arctan(1/(c_1 \cos(\mu)))| \\
= |\partial / \partial \alpha \arctan(\sqrt{\alpha^2 + c_2^2}/(c_1c_2))| \\
= \alpha |c_1||c_2|/(\alpha^2 + c_2^2(1 + c_1^2)) \sqrt{\alpha^2 + c_2^2} \\
\leq \frac{|c_1|}{(1 + c_1^2)c_2^2} \leq \frac{1}{|c_1|c_2^2},
\]

where the inequality is obtained by setting \(\alpha = 1\) in the numerator and \(\alpha = 0\) in the denominator.

To bound the terms depending on \(\kappa_\pm\), define \(\xi \equiv \alpha^2 + c_2^2(1 + c_1^2)\), and proceed as follows:

\[
2 \| tE^A_\pm I^B_y \partial \kappa_\pm / \partial \alpha \| = 2^{-1/2} |\partial / \partial \alpha \arctan(c_1 \sin(\mu)/(c_1^2 \pm c_2^2))| \\
= \frac{1}{\sqrt{2}} \left| \frac{\partial}{\partial \alpha} \arctan \left( \frac{\alpha c_1}{\sqrt{\xi \pm (\alpha^2 + c_2^2)}} \right) \right| \\
= \frac{1}{\sqrt{2}} \left| \frac{c_1((\alpha^2 - \alpha^2)\sqrt{\xi} \pm c_2^2(1+c_1^2))}{(\alpha^2 + c_2^2)((1 + \alpha^2 + c_1^2 + c_2^2)\sqrt{\xi} \pm 2\xi)} \right|.
\]

An elementary analysis of the denominator shows that it is nonnegative and reaches its minimum in the interval \([0,1]\) at \(\alpha = 0\) in both the “+” and “−” cases, while the numerator is likewise nonnegative and reaches its maximum at \(\alpha = 0\) in the “+” case and \(\alpha = 1\) in the “−”. This together with further simplifications lead to the bounds

\[
\frac{1}{\sqrt{2}} \left| \frac{\partial \kappa_+}{\partial \alpha} \right| \leq \frac{|c_1|}{\sqrt{2}c_2^2} \quad \text{and} \quad \frac{1}{\sqrt{2}} \left| \frac{\partial \kappa_-}{\partial \alpha} \right| \leq \frac{|c_1|}{\sqrt{2}|c_2|(|c_2| - \sqrt{2}|c_1|)}.
\]

Lastly, the terms depending on \(\lambda_\pm\) are

\[
\| \pm \omega_t^t tE^A_\pm I^B_z \partial \lambda_\pm / \partial \alpha \| = \frac{\omega_t^t}{2\sqrt{2}} \left| \frac{\partial}{\partial \alpha} \frac{1}{2} \sqrt{(c_1^2 \pm c_2^2)^2 + (c_1 \sin(\mu))^2} \right| \\
= \frac{\omega_t^t}{4\sqrt{2}} \left| \frac{\alpha(\sqrt{\xi} \pm 1)}{\sqrt{\xi(1 + \alpha^2 + c_1^2 + c_2^2 \pm 2\sqrt{\xi})}} \right|.
\]

As before, an elementary analysis shows that in both the “+” and “−” cases, the denominator is minimized at \(\alpha = 0\), while the numerator is maximized at \(\alpha = 1\). This together with further simplifications leads to

\[
\frac{\omega_t^t}{2\sqrt{2}} \left| \frac{\partial \lambda_+}{\partial \alpha} \right| \leq \frac{\omega_t^t}{4\sqrt{2}|c_2|} \quad \text{and} \quad \frac{\omega_t^t}{2\sqrt{2}} \left| \frac{\partial \lambda_-}{\partial \alpha} \right| \leq \frac{\omega_t^t}{4(|c_2| - \sqrt{2}|c_1|)}.
\]

Recalling that in the on-resonance case \(\omega_t = \pi|J^{AB}|\), so that \(|c_1| = 1\) and \(\omega_t \leq \omega_{t_{\text{max}}} = \pi/\sqrt{2}\), we finally obtain

\[
|f'(\alpha)| \leq \frac{1}{|c_2|} + \frac{1}{c_2^2} + \frac{1}{\sqrt{2}c_2^2} + \frac{1}{\sqrt{2}|c_2|(|c_2| - \sqrt{2})} + \frac{\pi}{8|c_2|} + \frac{\pi/\sqrt{2}}{4(|c_2| - \sqrt{2})}.
\]
for all $0 \leq \alpha \leq 1$. Letting $g(c_2)$ denote the right-hand side of this inequality, it now follows from our assumption $|c_2| \equiv |\omega_0^A - \omega_0^B|/\omega_1 \gg 1$ that

$$f(1) \equiv \frac{1}{2} \left\| e^{-\iota t H_{\text{eff}}} - e^{-\iota t H_{\text{eff}}^0} \right\|^2 \leq f(0) + \max_{0 \leq \alpha \leq 1} |f'(\alpha)| \quad \text{(B.13)}$$

as desired.

Appendix B.2. The on-transition case

It remains to be shown that $\exp(-\iota(\pi/\omega_1)H_{\text{eff}}) \approx \exp(-\iota(\pi/\omega_1)H_{\text{eff}}^0)$ in the on-transition case. This is again expected from first-order perturbation theory, but a rigorous proof is rendered nontrivial by the fact that $H_{\text{eff}}$ admits no closed-form diagonalization. The proof presented here is based upon the “sinch” commutator series expansion of the directional derivative of the matrix exponential which may be found in (Najfeld and Havel 1995), using however geometric algebra to proceed in a coordinate-free manner (Somaroo et al. 1998).

Thus we define the perturbed Hamiltonian $H_{\text{eff}}^\alpha \equiv H_{\text{eff}}^0 + \alpha \omega_1 I^x$, so that

$$\exp(-\iota t H_{\text{eff}}^\alpha) = e^{-\iota t H_{\text{eff}}^0} - \alpha \omega_1 I^x \cdot \nabla e^{-\iota t H_{\text{eff}}^0} + O(\alpha^2). \quad \text{(B.14)}$$

The “sinch” expansion of the direction derivative is

$$I^x \cdot \nabla e^{-\iota t H_{\text{eff}}^0} \equiv \frac{1}{\omega_1} \frac{d}{d\alpha} e^{-\iota t H_{\text{eff}}^0}$$

$$= e^{-\iota t H_{\text{eff}}^0} \left( \sum_{k=0}^{\infty} \left\{ I^x, \left( \frac{t}{\omega_1} H_{\text{eff}}^\alpha \right)^{2k} \right\} \right) (-1)^k (2k+1)! e^{-\iota t H_{\text{eff}}^0}, \quad \text{(B.15)}$$

where the commutator powers are defined recursively by

$$\{X, Y^0\} \equiv X, \quad \text{and} \quad \{X, Y^k\} \equiv \left[\{X, Y^{k-1}\}, Y\right] \quad (k > 0). \quad \text{(B.16)}$$

The essential thing to note is that $\{I^x, \frac{t}{2} H_{\text{eff}}^\alpha\} = \{I^x, \frac{t}{2} H_{\text{eff}}^0\}$, so that the summation in Eq. (B.15) is independent of $\alpha$.

\* The missing factor of “$t$”, as compared with Eq. (105) in Najfeld and Havel 1995, is due to the fact that we are treating here the time multiplying the Hamiltonian and the time multiplying the perturbation as independent parameters, and dropping the latter.
In order to evaluate the commutator powers explicitly, one proceeds as follows:

\[
\{I_x^B, (\frac{1}{2} H_{\text{eff}}^0)^0\} = I_x^B \quad \text{by definition;}
\]

\[
\{I_x^B, (\frac{1}{2} H_{\text{eff}}^0)^1\} = \omega_1^B \{I_x^B, (c_1 + c_2)I_z^B + 2c_1 I_x^A I_y^B + I_x^A\}
\]

\[
= \omega_1^B ((c_1 + c_2) + 2c_1 I_x^A) [I_x^B, I_z^B]
\]

\[
= \omega_1^B ((c_1 + c_2) + 2c_1 I_x^A) (-\frac{1}{2} I_y^B);
\]

\[
\{I_x^B, (\frac{1}{2} H_{\text{eff}}^0)^2\} = \omega_1^B ((c_1 + c_2) + 2c_1 I_x^A) [-\frac{1}{2} I_y^B, \frac{1}{2} H_{\text{eff}}^0]
\]

\[
= (\omega_1^B ((c_1 + c_2) + 2c_1 I_x^A))^2 I_x^B;
\]

and in general

\[
\{I_x^B, (\frac{1}{2} H_{\text{eff}}^0)^{2k}\} = (\omega_1^B ((c_1 + c_2) + 2c_1 I_x^A))^{2k} I_x^B.
\]

It follows that the commutator series is given by

\[
\sum_{k=0}^\infty \{I_x^B, (\frac{1}{2} H_{\text{eff}}^0)^{2k}\} = \left( \sum_{k=0}^\infty \left(\frac{\omega_1^B ((c_1 + c_2) + 2c_1 I_x^A))^{2k}}{(-1)^k (2k + 1)!}\right) I_x^B \right)
\]

\[
= \text{sinc}(\omega_1^B ((c_1 + c_2) + 2c_1 I_x^A)) I_x^B,
\]

where \(\text{sinc}(X) \equiv \sin(X)/X\) as usual. This can be rewritten in terms of scalar functions as follows:

\[
\text{sinc}(\omega_1^B ((c_1 + c_2) + 2c_1 I_x^A))(E_x^A + E_y^A)
\]

\[
= \text{sinc}(\omega_1^B ((c_1 + c_2) + c_1))E_x^A + \text{sinc}(\omega_1^B ((c_1 + c_2) - c_1))E_y^A.
\]

Finally, on taking norms of both sides of Eq. \((B.15)\), one obtains

\[
\|I_x^B \cdot \nabla e^{-\alpha H_{\text{eff}}^0}\| \leq \|e^{-\frac{\alpha}{2} H_{\text{eff}}^0}\|\text{sinc}(\omega_1^B (c_2 + 2c_1))E_x^A I_x^B
\]

\[
+ \text{sinc}(\omega_1^B c_2)E_x^B I_x^B \|e^{-\frac{\alpha}{2} H_{\text{eff}}^0}\|
\]

\[
\leq |\text{sinc}(\omega_1^B (c_1 + 2c_2))|E_x^A I_x^B
\]

\[
+ |\text{sinc}(\omega_1^B c_2)|E_x^B I_x^B\|
\]

\[
\leq \frac{\sqrt{2}}{\omega_1^B} \left( |c_2 + 2c_1|^{-1} + |c_2|^{-1} \right)
\]

\[
\leq \frac{\sqrt{2}}{t \omega_1} \left( \frac{2(|c_2| + |c_1|)}{|c_2|(|c_2| - 2|c_1|)} \right)
\]

\[
\leq \sqrt{8} (t \omega_1 (|c_2| - 2|c_1|))^{-1}.
\]

Now consider the function

\[
f(\alpha) \equiv \frac{1}{2} \left\| e^{-\alpha H_{\text{eff}}^0} - e^{-\alpha H_{\text{eff}}^0} \right\|^2
\]

\[
= 1 - \left\langle e^{-\alpha H_{\text{eff}}^0} e^{\alpha H_{\text{eff}}^0} \right\rangle,
\]
The effective Hamiltonian of the Pound-Overhauser controlled-NOT gate

the magnitude of whose derivative may be bounded as follows:

\[ |f'(\alpha)| = \left| \left( t \omega_1 I_x^B \cdot \nabla e^{-itH_{\text{eff}}^0} e^{itH_{\text{eff}}^0} \right) \right| \]
\[ \leq t \omega_1 \| I_x^B \cdot \nabla e^{-itH_{\text{eff}}^0} \| \| e^{itH_{\text{eff}}^0} \| \]
\[ \leq \sqrt{8} (|c_2| - 2|c_1|)^{-1} \]  

(B.21)

It follows that

\[ f(1) \equiv \frac{1}{2} \left\| e^{-itH_{\text{eff}}} - e^{-itH_{\text{eff}}^0} \right\|^2 \]
\[ \leq f(0) + \max_{0 \leq \alpha \leq 1} |f'(\alpha)| \]
\[ \leq \frac{\sqrt{8} \omega_1}{|\omega_0^A - \omega_0^B| - 2\pi |J_{AB}|} \ll 1 \]  

(B.22)

for all times \( t \), as desired.

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