1 The secular approximation

1.1 Rotating frame

Define

$$|\psi'(t)\rangle = e^{iH_1 t/\hbar}|\psi(t)\rangle$$

We will seek an equation governing time evolution for $|\psi'(t)\rangle$. First, let's write the ordinary Schrodinger equation in terms of $|\psi'(t)\rangle$:

$$\begin{aligned}
i\hbar\frac{d}{dt}|\psi(t)\rangle =&(H_0+H_1)|\psi(t)\rangle \\
i\hbar\frac{d}{dt}(e^{-iH_1 t/\hbar}|\psi'(t)\rangle) =&(H_0+H_1)e^{-iH_1 t/\hbar}|\psi'(t)\rangle \\
i\hbar(-iH_1/\hbar e^{-iH_1 t/\hbar}|\psi'(t)\rangle + e^{-iH_1 t/\hbar}\frac{d}{dt}|\psi'(t)\rangle) =&(H_0+H_1)e^{-iH_1 t/\hbar}|\psi'(t)\rangle \\
(H_1|\psi'(t)\rangle + i\hbar\frac{d}{dt}|\psi'(t)\rangle) =&e^{iH_1 t/\hbar}(H_0+H_1)e^{-iH_1 t/\hbar}|\psi'(t)\rangle \\
i\hbar\frac{d}{dt}|\psi'(t)\rangle =&(e^{iH_1 t/\hbar}H_0 e^{-iH_1 t/\hbar} + e^{iH_1 t/\hbar}H_1 e^{-iH_1 t/\hbar} - H_1)|\psi'(t)\rangle \\
i\hbar\frac{d}{dt}|\psi'(t)\rangle =&e^{iH_1 t/\hbar}H_0 e^{-iH_1 t/\hbar}|\psi'(t)\rangle
\end{aligned}$$

In the physics literature, this is transformation is often referred to as the "interaction picture", and the last line is the Schrodinger equation in the interaction picture. The $e^{iH_1 t/\hbar}H_0 e^{-iH_1 t/\hbar}$ is the interaction picture Hamiltonian. Several times in the above derivation I have used the fact that H_1 and $e^{-iH_1 t/\hbar}$ commute, and therefore I am free to move the matrix exponentials across the H_1 whenever I would like. This is because the matrix exponential of H_1 is a power series only of H_1, and we expect H_1 to commute with any polynomial function of H_1. This is **not** the case for H_0, and I am not allowed to move $e^{-iH_1 t/\hbar}$ across H_0.

Now let's see if we can do anything with this. matrix product. Remember

$$\begin{aligned}
H_0 =&J(2\sigma_+^e\otimes\sigma_-^p + 2\sigma_-^e\otimes\sigma_+^p + \sigma_z^e\otimes\sigma_z^p) \\
H_1 =&(1/2)g\mu_B B\sigma_z - (1/2)g\mu_N B\sigma_z
\end{aligned}$$

Let's work on the interaction picture Hamiltonian $e^{iH_1 t/\hbar}H_0 e^{-iH_1 t/\hbar}$:

$$e^{iH_1 t/\hbar}H_0 e^{-iH_1 t/\hbar} =e^{(i/2\hbar)gB(\mu_B\sigma_z^e-\mu_N\sigma_z^p)t}J(2\sigma_+\otimes\sigma_- + 2\sigma_-\otimes\sigma_+ + \sigma_z\otimes\sigma_z)e^{(-i/2\hbar)gB(\mu_B\sigma_z^e-\mu_N\sigma_z^p)t}$$

Well that looks complicated. Let's take this piece by piece.

$$\begin{aligned}
e^{(i/2\hbar)gB(\mu_B\sigma_z^e-\mu_N\sigma_z^p)t}\sigma_+\otimes\sigma_- e^{(-i/2\hbar)gB(\mu_B\sigma_z^e-\mu_N\sigma_z^p)t} =& \\
e^{(i/2\hbar)gB\mu_B\sigma_z^e t}\sigma_+^e e^{(-i/2\hbar)gB\mu_B\sigma_z^e t}\otimes e^{(-i/2\hbar)gB\mu_N\sigma_z^e t}\sigma_-^p e^{(i/2\hbar)gB\mu_N\sigma_z^e t} =& \\
e^{i\omega_e t}\sigma_+^e\otimes e^{i\omega_p t}\sigma_-^p =& \\
e^{i(\omega_e+\omega_p)t}\sigma_+^e\otimes\sigma_-^p
\end{aligned}$$

Here, I have made use of the identity $e^{i\alpha\sigma_z}\sigma_+ e^{-i\alpha\sigma_z} = e^{2i\alpha}\sigma_+$, and the analogous equation for σ_-. You should prove this for yourself. It is not difficult, and can be done by direct matrix multiplication. I have also defined here $\omega_e = g\mu_B B/\hbar$ and $\omega_p = g\mu_N B/\hbar$.

The next term is similar, and we find:

$$e^{(i/2\hbar)gB(\mu_B\sigma_z^e-\mu_N\sigma_z^p)t}\sigma_-\otimes\sigma_+ e^{(-i/2\hbar)gB(\mu_B\sigma_z^e-\mu_N\sigma_z^p)t} = \\ e^{-i(\omega_e+\omega_p)t}\sigma_-^e\otimes\sigma_+^p$$

The last part is a bit different, however. We note that $e^{(i/2\hbar)gB(\mu_B\sigma_z^e-\mu_N\sigma_z^p)t}$ commutes with $\sigma_z^e\otimes\sigma_z^p$. Therefore:

$$e^{(i/2\hbar)gB(\mu_B\sigma_z^e-\mu_N\sigma_z^p)t}\sigma_z^e\otimes\sigma_z^p e^{(-i/2\hbar)gB(\mu_B\sigma_z^e-\mu_N\sigma_z^p)t} = \\ \sigma_z^e\otimes\sigma_z^p$$

Putting it all together then, our Schrodinger equation for $|\psi'(t)\rangle$ reads

$$i\hbar\frac{d}{dt}|\psi'(t)\rangle = J(2e^{i(\omega_e+\omega_p)t}\sigma_+^e\otimes\sigma_-^p + 2e^{-i(\omega_e+\omega_p)t}\sigma_-^e\otimes\sigma_+^p + \sigma_z^e\otimes\sigma_z^p)|\psi'(t)\rangle$$

1.2 Neglecting the fast oscillating terms

The frequencies ω_e and ω_p depend linearly on B. For large B, $\omega_e+\omega_p \gg J/\hbar$, and thus the effects of the $\sigma_+\otimes\sigma_-$ terms will very quickly average to zero and can thus be neglected in comparison to the $\sigma_z^e\otimes\sigma_z^p$ term. Of course, this will not be satisfied if B is not large enough. Making this approximation, we have

$$i\hbar\frac{d}{dt}|\psi'(t)\rangle \approx J\sigma_z^e\otimes\sigma_z^p|\psi'(t)\rangle$$

This is known as the rotating wave approximation.

1.3 Going back to the lab frame

The way we go back to the lab frame is to do the inverse thing we did in the first section. We take our evolution equation for $|\psi'(t)\rangle$, and replace it with $|\psi(t)\rangle$, using the definition $|\psi(t)\rangle = e^{-iH_1t/\hbar}|\psi'(t)\rangle$.

$$\begin{aligned} i\hbar\frac{d}{dt}|\psi'(t)\rangle &\approx J\sigma_z^e\otimes\sigma_z^p|\psi'(t)\rangle \\ i\hbar\frac{d}{dt}(e^{iH_1t/\hbar}|\psi(t)\rangle) &= J\sigma_z^e\otimes\sigma_z^p e^{iH_1t/\hbar}|\psi(t)\rangle \\ -H_1e^{iH_1t/\hbar}|\psi(t)\rangle + i\hbar\frac{d}{dt}|\psi(t)\rangle &= J\sigma_z^e\otimes\sigma_z^p e^{iH_1t/\hbar}|\psi(t)\rangle \\ i\hbar\frac{d}{dt}|\psi(t)\rangle &= (H_1 + J\sigma_z^e\otimes\sigma_z^p)|\psi(t)\rangle \end{aligned}$$

In the last line, I made use again of the fact that H_1 commutes with $\sigma_z^e \otimes \sigma_z^p$, by multiplying both sides of the equation with $e^{-iH_1 t/\hbar}$. In any case, the last line is the equation we seek: the term $H1 + J\sigma_z^e \otimes \sigma_z^p = (1/2)g\mu_B B\sigma_z^e - (1/2)g\mu_N B\sigma_z^p + J\sigma_z^e \otimes \sigma_z^p$ is the Hamiltonian in the secular approximation. Thus, in this approximation, the evolution of $|\psi(t)\rangle$ is described by this Hamiltonian.

2 Spin echo

$H = KB\sigma_z$

2.1 What is the state of the qubit after time τ?

We know that $|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle = e^{-iKBt\sigma_z/\hbar}|\psi(0)\rangle$. $|\psi(0)\rangle = |+\rangle$. We also proved a thing in the previous homework about matrix exponentials of this form. We get:

$$\begin{aligned}
|\psi(\tau)\rangle =& \\
e^{-iKB\tau\sigma_z/\hbar}|+\rangle =&(\cos(KB\tau/\hbar)I + i\sin(KB\tau/\hbar)\sigma_z)|+\rangle \\
=&\frac{1}{\sqrt{2}}((\cos(KB\tau/\hbar)I + i\sin(KB\tau/\hbar)\sigma_z)(|0\rangle + |1\rangle) \\
=&\frac{1}{\sqrt{2}}((\cos(KB\tau/\hbar) + i\sin(KB\tau/\hbar))|0\rangle + (\cos(KB\tau/\hbar) - i\sin(KB\tau/\hbar))|1\rangle) \\
=&\frac{1}{\sqrt{2}}(e^{iKB\tau/\hbar}|0\rangle + e^{-iKB\tau/\hbar}|1\rangle)
\end{aligned}$$

where I used the fact that $\sigma_z|0\rangle = |0\rangle$ and $\sigma_z|1\rangle = -|1\rangle$.

2.2 Now apply σ_x at time τ

We can read off from the matrix form of σ_x that $\sigma_x|0\rangle = |1\rangle$ and $\sigma_x|1\rangle = |0\rangle$. Thus,

$$\sigma_x|\psi(\tau)\rangle = \frac{1}{\sqrt{2}}(e^{iKB\tau/\hbar}|1\rangle + e^{-iKB\tau/\hbar}|0\rangle$$

2.3 Now the qubit is allowed to evolve under H for an additional time τ. What is the final qubit state?

We now apply the same evolution to the new state. You could do it again, exactly as above. A faster way to get the same answer is to notice that under this Hamiltonian, $|0\rangle$ acquired a phase $e^{iKB\tau/\hbar}$, and $|1\rangle$ acquired a phase $e^{-iKB\tau/\hbar}$. This is always true because it is the action of the time evolution operator on the basis. Thus, we can just apply these phase factors to our state again, and get

$$
\begin{aligned}
|\psi(2\tau)\rangle =& \frac{1}{\sqrt{2}}(e^{-iKB\tau/\hbar}e^{iKB\tau/\hbar}|1\rangle + e^{iKB\tau/\hbar}e^{-iKB\tau/\hbar}|0\rangle \\
=& \frac{|0\rangle + |1\rangle}{\sqrt{2}} \\
=& |+\rangle
\end{aligned}
$$

Thus. this “echo” returns our state to the original state, regardless of the magnitude of the magnetic field.

3 Circuits

Most of these can shown with just matrix multiplication. I will attach a Mathematica sheet with that algebra. By way of commentary, I only want to point out that, when talking about two qubits, if apply some gate, U to one qubit, and do nothing to the other, the appropriate matrix to write down is either $U \otimes I$ or $I \otimes U$ depending on which qubit is being acted on. The math is worked out in the last page of this document.

4 Single qubit gates

I will use the notation from the Lecture 4 notes on spin resonance for this part.

$$
H_1 = -\frac{1}{2}g\mu_B(B_0\sigma_z + B_1\sin(\omega t)\sigma_x)
$$

4.1 What unitary operator is generated by applying H_1 for a time τ?

From the lecture notes, we have the rotating frame Hamiltonian

$$
H'(t) = \left(\frac{\hbar\omega_L}{2}\sigma_z + e^{i\omega_L\sigma_z t/2}H_1(t)e^{-i\omega_L\sigma_z t/2}\right)
$$

We do the same trick as in the notes, writing

$$
\begin{aligned}
\sin(\omega t)\sigma_x =& \frac{1}{2}((\sin(\omega t)\sigma_x + \cos(\omega t)\sigma_y) + (\sin(\omega t)\sigma_x \cos(\omega t)\sigma_y)) \\
=& \frac{1}{2}(e^{i\omega t - i\pi/2}\sigma_+ + e^{-i\omega t + i\pi/2}\sigma_- + e^{-i\omega t + i\pi/2}\sigma_+ + e^{i\omega t - i\pi/2}\sigma_-)
\end{aligned}
$$

We now have to apply

$$
e^{i\omega_L\sigma_z t/2}(e^{i\omega t - i\pi/2}\sigma_+ + e^{-i\omega t + i\pi/2}\sigma_- + e^{-i\omega t + i\pi/2}\sigma_+ + e^{i\omega t - i\pi/2}\sigma_-)e^{-i\omega_L\sigma_z t/2}
$$

to obtain

$$\begin{aligned} e^{i(\omega_L+\omega)t-i\pi/2}\sigma_+ + e^{-i(\omega_L+i\omega)t+i\pi/2}\sigma_- + e^{i(\omega_L-\omega)t+i\pi/2}\sigma_+ + e^{-i(\omega-\omega_L)t-i\pi/2}\sigma_- \\ \approx e^{i(\omega_L-\omega)t+i\pi/2}\sigma_+ + e^{-i(\omega-\omega_L)t-i\pi/2}\sigma_- \\ = i\sigma_+ - i\sigma_- \\ = -\sigma_y \end{aligned}$$

In the last two lines I assumed resonance, *e.g.* $\omega = \omega_L$, and in the second line I applied the rotating wave approximation.

This is the only part that differs from the lecture notes. Thus, we obtain

$$\begin{aligned} H'(t) &= \left(\frac{\hbar\omega_L}{2}\sigma_z - \frac{\hbar\omega_L}{2}\sigma_z - \frac{\hbar g\mu_B B_1}{2}\sigma_y \right) \\ &= -\frac{\hbar g\mu_B B_1}{2}\sigma_y \end{aligned}$$

The unitary operation this generates (in the rotating frame) is just $e^{-iHt/\hbar} = e^{ig\mu_B B_1 \tau\sigma_y/(2\hbar)}$

4.2 What Hamiltonian can we use to generate $U = \cos\theta\sigma_x + \sin(\theta)\sigma_y$

For this, we can again draw inspiration from our old friend the Euler identity for Pauli operators, noting that, with $\hat{n} = (\cos(\theta), \sin(\theta), 0)$, we have:

$$e^{i\alpha\hat{n}\cdot\vec{\sigma}} = \cos\alpha I + i\sin(\alpha)(\cos\theta\sigma_x + \sin(\theta)\sigma_y)$$

We thus need a Hamiltonian of the form $A(\cos\theta\sigma_x + \sin(\theta)\sigma_y)$. In the context of NMR, we can take $H = \frac{\hbar g\mu_B B}{2}(\cos\theta\sigma_x + \sin(\theta)\sigma_y)$. To generate the unitary, we need to apply this Hamiltonian for a time to make $\alpha = \frac{g\mu_B B\tau}{2} = \pi/2$.

We are supposed to notice here that this problem is simply a generalization of the previous part. Imagine that our field had the phase ϕ, such that

$$H_1 = -\frac{1}{2}g\mu_B(B_0\sigma_z + B_1\sin(\omega t+\phi)\sigma_x)$$

This is what we solved in the last part with $\phi = \pi/2$. If we have a general phase ϕ, the only thing that would change in our above derivation is that, when we our interaction Hamiltonian would now be proportional to

$$\begin{aligned} &e^{i\phi}\sigma_+ + e^{-i\phi}\sigma_- \\ &= \cos\phi\sigma_x - \sin\phi\sigma_y \end{aligned}$$

Thus, by changing the phase of the driving field, we change the axis about which we rotate our qubit.

In[27]:=

Problem 3

First, let's build the matrices. For the controlled gates, we need to think about what happens to the basis vectors. For instance, CPHASE takes each vector to itself whenever the first qubit is 0, and applies Z if the first qubit is one. So |00> -> |00>, |01> -> |01>, |10> -> |10> and |11> -> -|11>.

In[59]:=

```
H = (1 / (Sqrt[2])) * (1   1
                       1  -1); (* Hadamard *)
H2 = KroneckerProduct[IdentityMatrix[2], H];
```

$$\text{CPHASE} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix};$$

$$\text{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix};$$

```
(* CNOT with control on 2nd qubit *)
```

$$\text{rCNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix};$$

$$\text{SWAP} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix};$$

$$U = \begin{pmatrix} a & b \\ c & d \end{pmatrix};$$

(a)

In[44]:=

```
H2.CPHASE.H2 // MatrixForm
CNOT // MatrixForm
```

Out[44]//MatrixForm=

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

Out[45]//MatrixForm=

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

(b)

In[46]:=
```
H2.CNOT.H2 // MatrixForm
CPHASE // MatrixForm
```

Out[46]//MatrixForm=

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

Out[47]//MatrixForm=

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

(c)

In[57]:=
```
CNOT.rCNOT.CNOT // MatrixForm
SWAP // MatrixForm
```

Out[57]//MatrixForm=

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Out[58]//MatrixForm=

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

(d)

(i)

In[65]:=
```
KroneckerProduct[IdentityMatrix[2], U] // MatrixForm
```

Out[65]//MatrixForm=

$$\begin{pmatrix} a & b & 0 & 0 \\ c & d & 0 & 0 \\ 0 & 0 & a & b \\ 0 & 0 & c & d \end{pmatrix}$$

(ii)

In[66]:=
```
KroneckerProduct[U, IdentityMatrix[2]] // MatrixForm
```

Out[66]//MatrixForm=

$$\begin{pmatrix} a & 0 & b & 0 \\ 0 & a & 0 & b \\ c & 0 & d & 0 \\ 0 & c & 0 & d \end{pmatrix}$$

(iii) For the controlled U, we apply U to the basis elements whenever the first qubit is in |1>

In[67]:=
```
CU = {{1, 0, 0, 0}, {0, 1, 0, 0}, {0, 0, a, c}, {0, 0, b, d}} // MatrixForm
```

Out[67]//MatrixForm=

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & a & c \\ 0 & 0 & b & d \end{pmatrix}$$

(iv) Now for the control on the second qubit

In[68]:=
```
rCU = {{1, 0, 0, 0}, {0, a, 0, b}, {0, 0, 1, 0}, {0, c, 0, d}} // MatrixForm
```

Out[68]//MatrixForm=

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & a & 0 & b \\ 0 & 0 & 1 & 0 \\ 0 & c & 0 & d \end{pmatrix}$$