Time dependent spin-spin coupling

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Derivation of Thomas-Reiche-Kuhn sum rules for position operator.

blog: https://tetraquark.vercel.app/posts/time_dependent_spin_spin_coupling/?src=pdf

email: quarktetra@gmail.com

Problem Statement

Consider two spin-1/2 particles in the state with $S_{1z} = 1/2$ and $S_{2z} = -1/2$ at time $t = -\infty$. They are then subject to an interaction of the form

$$H_1 = a_0 e^{-t^2/\tau^2} \mathbf{S_1} \cdot \mathbf{S_2}, \tag{1}$$

where a_0 and $\tau > 0$ are constant parameters. We want to calculate the probability of finding the system in the state with $S_{1z} = -1/2$ and $S_{2z} = 1/2$ at $t = \infty$.

The exact solution

We first note that the Schrödinger equation can formally be solved as

$$\psi(t) = e^{-i\int_{t_0}^{t} d\tilde{t} H(\tilde{t})} \psi(t_0). \tag{2}$$

However, it is important to mention that if the Hamiltonian does not commute with itself at different times, $[H(t_1), H(t_2)] \neq 0$, then we cannot exponentiate H to get the solution above. In that case we would have to solve the differential equation honestly. Since the Hamiltonian in Eq. 1 commutes with itself at any different times, Eq. 2 will work. Now we need to handle exponential of an operator, H. It could be dealt with an infinite Taylor expansion, but that would be painful. A better method is to consider the problem in the eigenbasis of H. We expand the initial state in terms of the eigenstates of H so that H in the exponent can be replaced by its eigenvalues. The initial state is $|\uparrow\downarrow\rangle$. We will need the Clebsch-Gordan coefficients for 2-spin 1/2 particles.

Let us remember what the Clebsch-Gordan are: First of all $|1, \pm 1\rangle$ is trivial, the states have to be both $\uparrow$ ($\downarrow$) so that spin along z is $+1$ (-1). The hard ones are $|0,0\rangle$ and $|1,0\rangle$. They are superposition of $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ so that spin along z is zero. We can first figure out the coefficients for $|0,0\rangle$, which is the state to be annihilated by $S_- = S_{1-} + S_{1-}$. Applying this onto this state will immediately reveal that $|0,0\rangle = \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}$. And $|1,0\rangle$ has to be orthogonal to $|0,0\rangle$ which means $|1,0\rangle = \frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}}$ up to a phase, which is irrelevant. From here we can get inverse Clebsch-Gordan coefficients to expand $|\uparrow\downarrow\rangle$, which gives

$$|| \uparrow\downarrow\rangle = \frac{|0,0\rangle + |1,0\rangle}{\sqrt{2}}. \tag{3}$$

H can be written as

$$\begin{aligned} H_1(t) &= a_0 e^{-\frac{t^2}{\tau^2}} \mathbf{S_1} \cdot S_2 = a_0 e^{-\frac{t^2}{\tau^2}} \frac{\mathbf{J^2} - \mathbf{S_1^2} - \mathbf{S_2^2}}{2} \\ &= \frac{a_0}{2} e^{-\frac{t^2}{\tau^2}} (\mathbf{J^2} - \mathbf{S_1^2} - \mathbf{S_2^2}). \end{aligned} \tag{4}$$

We know that $S_1^2 = S_2^2 = 3/4$. Then,

$$\begin{aligned} |\psi(t)\rangle &= exp\left[-i \int_{t_0}^{t} d\tilde{t} \frac{a_0}{2} e^{-\frac{\tilde{t}^2}{\tau^2}} (\mathbf{J^2} - \mathbf{S_1^2} - \mathbf{S_2^2})\right] \frac{|0,0\rangle + |1,0\rangle}{\sqrt{2}} \\ &= exp\left[-if(t)(2 - 3/4 - 3/4)\right] \frac{|1,0\rangle}{\sqrt{2}} + exp\left[-if(t)(0 - 3/4 - 3/4)\right] \frac{|0,0\rangle}{\sqrt{2}} \\ &= e^{-\frac{if(t)}{2}} \frac{|1,0\rangle}{\sqrt{2}} + e^{\frac{3if(t)}{2}} \frac{|0,0\rangle}{\sqrt{2}}, \end{aligned} \tag{5}$$

where $f(t) \equiv \int_{t_0}^{t} d\tilde{t} \frac{a_0}{2} e^{-\frac{\tilde{t}^2}{\tau^2}}$. We can get the probabilities of measurements in this basis, or we can go back to the original one which is more transparent. We expand $|0,0\rangle$ and $|1,0\rangle$ in spin up-down basis to get

$$\begin{aligned} |\psi(t)\rangle &= \left[e^{-\frac{if(t)}{2}} + e^{\frac{3if(t)}{2}}\right] \frac{|\uparrow,\downarrow\rangle}{2} + \left[-e^{\frac{3f(t)}{2}} + e^{-\frac{if(t)}{2}}\right] \frac{|\downarrow,\uparrow\rangle}{2} \\ &= e^{i/2f(t)} \left(\cos[f(t)]|\uparrow,\downarrow\rangle - i\sin[f(t)]|\downarrow,\uparrow\rangle\right). \end{aligned} \tag{6}$$

The probabilities become

$$\text{Prob}\left(|\uparrow,\downarrow\rangle \to |\uparrow,\downarrow\rangle\right) = \cos^2[f(t)], \quad \text{Prob}(|\uparrow,\downarrow\rangle \to |\downarrow,\uparrow\rangle) = \sin^2[f(t)]. \tag{7}$$

The solution with perturbation theory

We can approach the from the perspective of time dependent perturbation theory. The fundamental object we have to compute is

$$d_{fi}(t) = -i \int_{t_0}^{t} d\tilde{t} e^{iE_{fi}^{(0)}} \langle f|H_1(\tilde{t})|i\rangle + \delta_{fi}. \tag{8}$$

For this problem we are not calculating a function of an operator, operator appears by itself, and it is easy to get the answer in this basis using

$$2\,\mathbf{S_1}\cdot\mathbf{S_2} = S_{1-}S_{2+} + S_{1+}S_{2-} + 2\,S_{1z}S_{2z}. \tag{9}$$

For $f = i$ only $S_{1z}S_{2z}$ contributes to give

$$d_{f=i}(t) = -i\int_{t_0}^{t} d\tilde{t}e^{iE^{(0)}_{fi}\tilde{t}}\langle\uparrow,\downarrow|H_1(\tilde{t})|\uparrow,\downarrow\rangle + 1 = 1 + \frac{if(t)}{2}. \tag{10}$$

For $f = |\downarrow,\uparrow\rangle$ only $S_{1+}S_{2-}$ contributes to give

$$d_{f\neq i}(t) = -i\int_{t_0}^{t} d\tilde{t}e^{iE^{(0)}_{fi}\tilde{t}}\langle\downarrow,\uparrow|H_1(\tilde{t})|\uparrow,\downarrow\rangle = -if(t). \tag{11}$$

There are two important points here. First one is $E^{(0)}_{fi}$. Remember that superscript (0) reminds us that it comes from the differences of background energy originating from H_0, and for this case $E^{(0)}_{fi} = 0$. Second point is rather technical, but still important. If you calculate probabilities from $d_{f=i}(t)$ and $d_{f\neq i}(t)$, you see that the sum is not equal to 1. This is because the coefficients are not normalized yet. The normalized amplitudes would be the ones above divided by the normalization. The corresponding probabilities are

$$\frac{f^2(t)}{1+5f^2(t)/4},\ \frac{1+f^2(t)/4}{1+5/4f^2(t)}. \tag{12}$$

Note that this normalization is too precise, it is like giving a result of a division with 2 decimal points although the numbers you started with have 1 decimal point. In other words the procedure we follow is correct only in the f^2 order, and we need to expand the result and drop terms higher than f^2 to get

$$\frac{1}{1+5f^2(t)/4} \simeq 1 - 5f^2(t)/4. \tag{13}$$

Therefore, the probabilities with the correct accuracy are given by

$$\text{Prob}\,(|\uparrow,\downarrow\rangle \to |\uparrow,\downarrow\rangle) = 1 - f^2(t), \text{and }\ \text{Prob}(|\uparrow,\downarrow\rangle \to |\downarrow,\uparrow\rangle) = f^2(t). \tag{14}$$

Note that the normalization procedure did not change $\text{Prob}\,(|\uparrow,\downarrow\rangle \to \downarrow,\uparrow\rangle)$ since it was already of f^2 order, it just changed the other one so that total probability is 1. In all the other transitions are ruled out, we could use this idea to get

$$\text{Prob}\,(|\uparrow,\downarrow\rangle \to |\uparrow,\downarrow\rangle) = 1 - \text{Prob}\,(|\uparrow,\downarrow\rangle \to |\downarrow,\uparrow\rangle)\,. \tag{15}$$

However, if there are more than two possible transitions, we will have to normalize the coefficients first. Note that perturbative result is in agreement with the exact one in Eq. 7 at f^2 order if $f \ll 1$. This is also the requirement from the perturbation side since we approximated the solution to the integral equation with the first trial function $f(t)$. If $f \ll 1$, cutting the trial at the first order is a good approximation to the exact solution.