Factor of π identified PhL 3.28.08

Look at Saxon's Golden Rule derivation on page 210. If you start a system in pure state k, then (63) tells you the probability for system to have leaked into state m after time t. The function of t is the sinc function, it is not proportional to t. This is for two discrete states k and m. It is completely general for any H'. So I want k and m to be my two basic stupid spin states? In Saxon page 208, we assume $a_n(t) = c_n(t)\ e^{-iEnt/\hbar}$ so we factor out the time dependence that this state would have if H'=0. Completely general again.

So I guess the real problem is this:

state k = initial	= spin in state β + photon energy ω	$E_k = \varepsilon\beta + \hbar\omega = E$
state m = final	= spin in α state	$E_m = \varepsilon\alpha$

where we are absorbing a photon. Imagine a spectrum S(ω) of photons. Then E_k is a continuous spectrum. If we follow this through, we end up with (67) which is the Golden Rule with the 2π. For sure, the function ρ(E) is the energy density. We can always related this to ρ'(ω) with a factor of $\hbar$ but no π's will be involved.

So here is our Golden Rule

$W = 2\pi/\hbar\ \rho(E)\ |H'_{mk}|^2$ ρ(E) = density of states

Now according to Levitt page (16.5), we have

$J(\omega) = \tau_c/(1 + \tau_c^2\omega^2)$ // a bell curve as shown page 520 (not a gaussian/normal however)

Notice these facts:

$$\int_0^\infty d\omega\ J(\omega) = \text{dimensionless} = \tau \int_0^\infty d\omega\ 1/[\ 1 + \omega^2\tau^2] = \int_0^\infty dx\ /[\ 1+x^2] = \pi/2$$ Schaum page 95 a=1.

Therefore,

$$\int_{-\infty}^{\infty} d\omega\ J(\omega) = \pi$$

So this "spectral density" is not normalized to 1 as it should be.

Aside on Negative ω: what do we *say* about the negative frequency side of this spectrum? We certainly show it in our plots as on Levitt page 520, and it certainly is part of the usual Fourier Theory. I comment on this on page 20 of my book Spectral Theory. Since the autocorrelation function Levitt page 517 is a real function of time τ, its FT is going to have the property that $J(-\omega) = J(\omega)^*$. But G(t) is not only real

but symmetric in its argument, and this means J(ω) is real, so we have J(-ω) = J(ω). Since J has value for ω < 0 as just shown, you certainly cannot just "throw it away".

Aside on Normalization: If we start with the autocorrelation function G'(t) = 1*exp(-|t|/τ_c), we find J'(ω) = 2τ_c/(1 + [$\tau_c\omega$]^2) which is easy to show using Schaum page 98 top integral. The area under this thing is going to be:

$$\int_{-\infty}^{\infty} d\omega\ J'(\omega) = 2\pi$$

It just happens that this autocorrelation function yields a spectral density which is not properly normalized to unity, when we start with autocorrelation as a simple exponential with unit value at τ=0. Fine.

If we are going to do Golden Rule calculations, we must use a properly normalized spectral density and that would be

$J_n(\omega) = J(\omega)/\pi$ if we define $J(\omega) \equiv \tau_c/(1 + \tau_c^2\omega^2)$

and then

$$\int_{-\infty}^{\infty} d\omega\ J_n(\omega) = 1$$

Now, our Golden Rule is this:

$W = 2\pi/\hbar\ \rho(E)\ |H'_{mk}|^2$

we have $\rho(E)dE = J_n(\omega)d\omega$ = number of states in the indicated band dE or dω, and $dE = \hbar d\omega$

$\rho(E) = J_n(\omega) * d\omega/dE = J_n(\omega)/\hbar$

Our Golden Rule is now

$W = 2\pi/\hbar^2\ J_n(\omega)\ |H'_{mk}|^2$

and in our spin world, the $\hbar^2$ denominator will be cancelled by stuff inside H', example to follow.

Now, if you want to use J(n) as in Levitt, you use $J_n(\omega) = J(\omega)/\pi$ to get

$W = (2/\hbar^2)\ J(\omega)|H'_{mk}|^2$

Now, Levitt does not use H, but instead uses $H = \hbar\ \mathcal{H}$ where the units of $\mathcal{H}$ are ω instead of E. If we put this in we get:

Golden Rule :

$$W = 2\,J(\omega)|\mathcal{H}'_{mk}|^2 \qquad J(\omega) = \tau_c/(1+\tau_c^2\omega^2) \qquad \int_{-\infty}^{\infty} d\omega\, J(\omega) = \pi$$

This then is our final result and this is why there is no π in the Golden Rule as used in Levitt, and also why there are no $\hbar$ factors.

Sample calculation:

The dipole-dipole says $\mathcal{H}' = b\,[\,3e_j e_j - \delta_{ij}]\,I_{1i}I_{2j}$ where $b = -(\mu_0/4\pi)\,\gamma_1\gamma_2\hbar/r^3$.

We find for example that

$$\langle\alpha\alpha|\,\mathcal{H}'\,|\alpha\beta\rangle = (3/4)\,e_z(e_x - i\,e_y)\,b$$

$$|\langle\alpha\alpha|\,\mathcal{H}'\,|\alpha\beta\rangle|^2 = (3/4)^2\,e_z(1-e_z^2)\,b^2$$

If we average this over 4π we get

$$(\,|\langle\alpha\alpha|\,\mathcal{H}'\,|\alpha\beta\rangle|^2)_{av} = 3/40\;b^2$$

If we then insert this into our Golden Rule, we get

$$W = 2\,J(\omega)(|\mathcal{H}'_{mk}|^2)_{av} = 2\,J(\omega_0)\,[\,3b^2/40] = (3/20)\,J(\omega_0)\,b^2$$

This agrees with Levitt page 529.