Quantum III HW2

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1 Problem 1

We first examine the inner product $\langle\psi_n|W|\psi_i\rangle$, using the ladder operator relation $\hat{X} = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger)$.

$$\langle\psi_n|W|\psi_i\rangle = -qE\sqrt{\frac{\hbar}{2m\omega}}\,\langle\psi_n|(a + a^\dagger)|\psi_n\rangle \tag{1.1}$$

$$\langle\psi_n|W|\psi_i\rangle = -qE\sqrt{\frac{\hbar}{2m\omega}}(\langle\psi_n|\psi_{i-1}\rangle + \langle\psi_n|\psi_{i+1}\rangle) \tag{1.2}$$

$$\langle\psi_n|W|\psi_i\rangle = -qE\sqrt{\frac{\hbar}{2m\omega}}(\delta_{n,n-1} + \delta_{n,n+1}) \tag{1.3}$$

a) We examine the first-order perturbation theory result for C_{10}:

$$C^1_{01} = -\frac{i}{\hbar}\int_0^t dt' e^{i\omega_{10}t'}\,\langle\psi_1|W|\psi_0\rangle \tag{1.4}$$

$$C^1_{01} = qE\sqrt{\frac{\hbar}{2m\omega_0}}\frac{1}{E_1 - E_0}\left(e^{\frac{i}{\hbar}(E_1 - E_0)\tau} - 1\right) \tag{1.5}$$

$$C^1_{01} = qE\sqrt{\frac{1}{2m\hbar\omega_0^3}}\left(e^{i\omega_0\tau} - 1\right) \tag{1.6}$$

$$|C^1_{01}|^2 = \frac{(qE)^2}{2m\hbar\omega_0^3}\left(2 - (e^{i\omega_0\tau} + e^{-i\omega_0\tau}\right) \tag{1.7}$$

$$|C^1_{01}|^2 = \frac{(qE)^2}{m\hbar\omega_0^3}\,(1 - \cos\omega_0\tau) \tag{1.8}$$

The probabiltiy varies at the harmonic ocsillator amgular frequency.

b) We now examine C_{20}. We have seen that $\langle\psi_2|W|\psi_0\rangle = 0$, so the first-order approximation will be 0. For the second-order perturbation results, $\langle\psi_2|W|\psi_1\rangle = \langle\psi_1|W|\psi_0\rangle = -qE\sqrt{\frac{\hbar}{2m\omega}}$. So only the transition through intermediate state $|1\rangle$ will contribute.

$$C_{01}^2 = -\frac{1}{\hbar^2}\int_0^\tau dt' e^{i\omega_{21}t'} W_{21}\int_0^{t\prime} dt' e^{i\omega_{10}t'} W_{10} \tag{1.9}$$

$$C_{01}^2 = \frac{iq^2E^2}{2m\omega_0^2\hbar}\int_0^\tau dt' e^{i2\omega_0 t'} - e^{i\omega_0 t'} \tag{1.10}$$

$$C_{01}^2 = \frac{q^2E^2}{2m\omega_0^3\hbar}\left(\frac{e^{i2\omega_0\tau}-1}{2} - e^{i\omega_0\tau}+1\right) \tag{1.11}$$

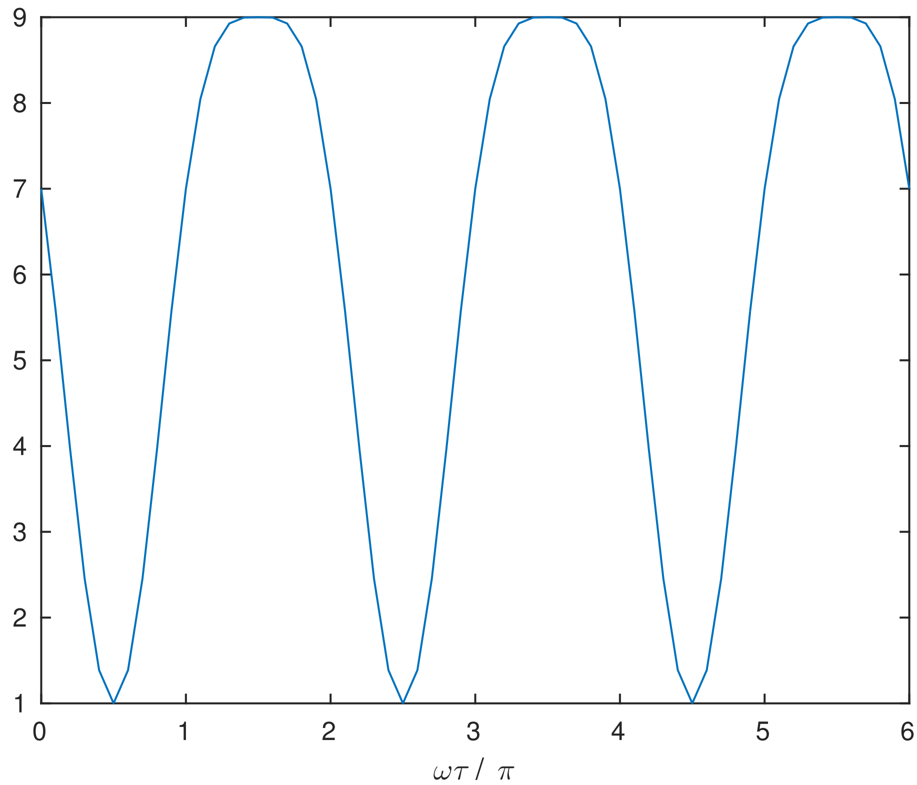
$$C_{01}^2 = \frac{q^2E^2}{4m\omega_0^3\hbar}\left(e^{i\omega_0\tau}-1\right)^2 \tag{1.12}$$

$$|C_{01}^2|^2 = \left(\frac{q^2E^2}{4m\omega_0^3\hbar}\right)^2\left(e^{i\omega_0\tau}-1\right)^2 \tag{1.13}$$

$$|C_{01}^2|^2 = \left(\frac{q^2E^2}{4m\omega_0^3\hbar}\right)^2\left(e^{i2\omega_0\tau}+e^{-i2\omega_0\tau}-4(e^{i\omega_0\tau}+e^{-i\omega_0\tau})+6\right) \tag{1.14}$$

$$|C_{01}^2|^2 = \left(\frac{q^2E^2}{4m\omega_0^3\hbar}\right)^2(2\cos 2\omega_0\tau - 8\cos\omega_0\tau+6) \tag{1.15}$$

A scaled version of this function is plotted below. The probability again oscillates at the harmoic oscillator frequency ω_0.



2 Problem 2

Wigner and Weisskopf analyze a time-dependent perturbation of a stationary system in the interaction picture. They find an energy shift as well as a line broadening using second-order results. Fano found the stationary states of a system with an interaction potential between a discrete state and a continuum of states using the Schrodinger picture. Fano's exact result using the Schordinger picture determines that the discrete state is diluted across a range of continuum states near the discrete-state energy.
If we consider the discrete-continuum interaction terms in the Hamiltonian as a time-dependent perturbation we can view the Wigner-Weisskopf results as an approximation of Fano's results. Wigner-Weisskopf does predict a frequency shift and a broadening of the spectral line. However, the theory does not account for the asymmetric nature of the emission/absorption peaks. Fano's exact approach derives the coefficients of the mixed wavefunction and calculates the general transition probability using the mixed wavefunction. Fano's expression for transition probability explain the asymetric peak shape and predicts an absorption null on one side of the peak.

3 Problem 3

We follow Fano's derivation of the factorization:

$$\begin{aligned}\frac{1}{(\bar{E}-E')(E-E')} =& \frac{1}{\bar{E}-E}\left(\frac{1}{E-E'}-\frac{1}{\bar{E}-E'}\right) \\ &+ \pi^2\delta(\bar{E}-E)\delta(E'-\frac{1}{2}(\bar{E}+E))\end{aligned} \tag{3.1}$$

We begin by determing the Fourier expansion of $\frac{1}{E-E'}$.

$$\frac{1}{E-E'} = \int_{-\infty}^{\infty} \hat{f}(k)e^{i2\pi kE'}dk \tag{3.2}$$

$$\hat{f}(k) = \int_{-\infty}^{\infty} \frac{1}{E-E'}e^{-i2\pi kE'}dE' \tag{3.3}$$

We evaluate 3.3 with its single pole using the residue theorem. When $k > 0$ we will close the contour in the upper half of the complex plane, and we will avoid the pole using a counter-clockwise circle. When $k < 0$ we will close the contour in the lower half of the complex plane, and we will avoid the pole using a clockwise circle. This leads to:

$$P(\int) - i\pi Res = 0 \ (k < 0) \tag{3.4}$$

$$P(\int) + i\pi Res = 0 \ (k > 0) \tag{3.5}$$

The residue at the simple pole can be evaluated using $lim(E' \to E)(E - E')\frac{e^{-i2\pi kE'}}{E-E'} = e^{-i2\pi kE}$. Writing the sign of k as $\frac{k}{|k|}$ we have proved Fano's equation A1:

$$\frac{1}{E - E'} = -i\pi \int_{-\infty}^{\infty} \frac{k}{|k|} e^{i2\pi k(E-E')} dk \tag{3.6}$$

We can now write the double-pole expression as:

$$\frac{1}{(\bar{E} - E')(E - E')} = -\pi^2 \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk' \frac{kk'}{|kk'|} e^{i2\pi[k(\bar{E}-E')+k'(E-E')]} \tag{3.7}$$

Fano now makes the substitution $u = k + k',\ v = \frac{1}{2}(k - k')$ and finds that:

$$u^2 = k^2 + 2kk' + k'^2 \tag{3.8}$$

$$4v^2 = k^2 - 2kk' + k'^2 \tag{3.9}$$

$$\frac{kk'}{|kk'|} = \frac{u^2 - 4v^2}{|u^2 - 4v^2|} \tag{3.10}$$

This expression will be -1 for $u^2 < 4v^2$ and +1 for $u^2 > 4v^2$, so it is equivalent to $2St(u^2 - 4v^2) - 1$ where $St()$ is the step function. This substitution allows us to write equation 7 as:

$$\begin{aligned} \frac{1}{(\bar{E} - E')(E - E')} =& \pi^2 \int_{-\infty}^{\infty} du \ e^{i2\pi u[\frac{1}{2}(\bar{E}+E)-E')]} \\ & \times \left(\int_{-\infty}^{\infty} dv - 2 \int_{-\frac{1}{2}|u|}^{\frac{1}{2}|u|} dv \right) e^{i2\pi v(\bar{E}-E)} \end{aligned} \tag{3.11}$$

For the step function expression we have pulled out a negative sign and recognize the the integral over v is 0 until $v = \frac{1}{2}|u|$. The right integral over v is straightforward:

$$\int_{-\frac{1}{2}|u|}^{\frac{1}{2}|u|} e^{i2\pi v(\bar{E}-E)} \ dv \tag{3.12}$$

$$\frac{1}{2i\pi(\bar{E} - E)} \left(e^{i\pi|u|(\bar{E}-E)} - e^{-i\pi|u|(\bar{E}-E)} \right) \tag{3.13}$$

$$\frac{\sin\left(\pi|u|(\bar{E} - E)\right)}{\pi(\bar{E} - E)} \tag{3.14}$$

Using the Fourier transform definition of the delta function, $\delta(x) = \int e^{i2\pi kx} dk$, we now have:

$$\begin{aligned}\frac{1}{(\bar{E}-E')(E-E')} =& \pi^2 \int_{-\infty}^{\infty} du\ e^{i2\pi u[\frac{1}{2}(\bar{E}+E)-E')]} \\ &\times \left(\delta(\bar{E}-E) - 2\frac{\sin\left(\pi|u|(\bar{E}-E)\right)}{\pi(\bar{E}-E)}\right)\end{aligned} \tag{3.15}$$

Writing $\sin\left(\pi|u|(\bar{E}-E)\right)$ as $\frac{1}{2i}\frac{u}{|u|}\left(e^{i\pi u(\bar{E}-E)} - e^{-i\pi u(\bar{E}-E)}\right)$, we can then collect the exponential terms:

$$\begin{aligned}\frac{1}{(\bar{E}-E')(E-E')} =& \pi^2\delta(\frac{1}{2}(\bar{E}+E)-E')\delta(\bar{E}-E) \\ &+ \frac{i\pi}{\bar{E}-E}\int_{-\infty}^{\infty} du \frac{u}{|u|} e^{i2\pi u(\bar{E}-E')} \\ &- \frac{i\pi}{\bar{E}-E}\int_{-\infty}^{\infty} du \frac{u}{|u|} e^{i2\pi u(E-E')}\end{aligned} \tag{3.16}$$

We have already shown that the second and third integrals are the Fourier representations of $\frac{1}{\bar{E}-E'}$ and $\frac{1}{E-E'}$, so we have finally proved the desired result.

$$\begin{aligned}\frac{1}{(\bar{E}-E')(E-E')} =& \frac{1}{\bar{E}-E}\left(\frac{1}{E-E'} - \frac{1}{\bar{E}-E'}\right) \\ &+ \pi^2\delta(\bar{E}-E)\delta(E' - \frac{1}{2}(\bar{E}+E))\end{aligned} \tag{3.17}$$

4 Problem 4

We start from Fano eq. 10:

$$\begin{aligned}a^*(\bar{E})\{1 + \int dE' V^*_{E'} &\left(\frac{1}{\bar{E}-E'} + z(\bar{E})\delta(\bar{E}-E'\right) \\ &\times \left(\frac{1}{E-E'} + z(E)\delta(E-E')\right) V_{E'}\}a(E) \\ &= \delta(\bar{E}-E)\end{aligned} \tag{4.1}$$

Opening up the expression under the integral we find:

$$\begin{aligned} a^*(\bar{E})a(E)\{1 + &\int |V_{E'}|^2 \frac{1}{(\bar{E}-E')(E-E')} dE' \\ &+ \int |V_{E'}|^2 \frac{z(\bar{E})\delta(\bar{E}-E')}{\bar{E}-E'} dE' \\ &+ \int |V_{E'}|^2 \frac{z(E)\delta(E-E')}{E-E'} dE' \\ &+ \int |V_{E'}|^2 z(\bar{E})z(E)\delta(\bar{E}-E')\delta(E-E') dE' \\ &= \delta(\bar{E}-E) \end{aligned} \tag{4.2}$$

The first expression is expanded using the result of problem 3 and the definition of $F(E) = P\int dE' \frac{|V_{e'}|^2}{E-E'}$.

$$\begin{aligned} \int |V_{E'}|^2 \frac{1}{(\bar{E}-E')(E-E')} dE' = \frac{|V_E|^2}{\bar{E}-E}\left(F(E) - F(\bar{E})\right) \\ + \pi^2 \delta(\bar{E}-E) \end{aligned} \tag{4.3}$$

The second and third expressions in 4.2 can be combined into $\frac{1}{\bar{E}-E}\left(z(E)|V_E^2 - z(\bar{E})|V_{\bar{E}}|^2\right)$. Using $\delta(\bar{E}-E')\delta(E-E') = \delta(\bar{E}-E)\delta(E' - \frac{1}{2}(\bar{E}+E))$ the fourth expression is:

$$\int |V_{E'}|^2 z(\bar{E})z(E)\delta(\bar{E}-E')\delta(E-E') dE' = |V_E|^2 z(E)^2 \delta(\bar{E}-E) \tag{4.4}$$

We can now collect terms:

$$\begin{aligned} &|a(E)|^2 |V_E|^2 (\pi^2 + z(E)^2)\delta(\bar{E}-E) + a^*(\bar{E})a(E) \\ &\quad \times \left\{1 + \frac{1}{\bar{E}-E}\left(F(E) - F(\bar{E}) + z(E)|V_E|^2 - z(\bar{E})|V_{\bar{E}}|^2\right)\right\} \\ &= \delta(\bar{E}-E) \end{aligned} \tag{4.5}$$

Since $F(E) = E - z(E)|V_E|^2 - E_\phi$, the term inside the brackets reduces to $1 + \frac{E-\bar{E}}{\bar{E}-E} = 0$ so the second term vanishes. We then have:

$$|a(E)|^2 = \frac{1}{|V_E|^2(\pi^2 + z(E)^2)} = \frac{|V_E|^2}{(E - E_\phi - F(E))^2 + \pi^2 |V_E|^4} \tag{4.6}$$

5 Problem 5

Following Fano's terminology, the unmixed configurations have wavefunctions ϕ and ψ_E for the discrete and continuum states. The mixed wavefunction is represented by Ψ_E and is a combination of the unmixed wavefunctions with coefficients a and b'_E. The values of a and b'_E are:

$$a = \frac{\sin\Delta}{\pi V_E} \tag{5.1}$$

$$b'_E = \frac{V_{e'}}{\pi V_E^*}\frac{\sin\Delta}{E-E'} - \cos\Delta\delta(E-E') \tag{5.2}$$

$$\Delta = -arctan\left(\frac{\pi|V_E|^2}{E-E_\phi-F(E)}\right) \tag{5.3}$$

With these definitions we can write the transition probability in terms of a general transition operator T:

$$\begin{aligned}\langle\Psi_E|T|i\rangle =& \frac{1}{\pi V_E^*}\langle\phi|T|i\rangle\sin\Delta + \frac{1}{\pi V_E^*}\int dE'\frac{V_{E'}^*\langle\psi_{e'}|T|i\rangle}{E-E'}\sin\Delta \\ &- \int dE'\langle\psi_{E'}|T|i\rangle\cos\Delta\delta(E-E')\end{aligned} \tag{5.4}$$

$$\begin{aligned}\langle\Psi_E|T|i\rangle =& \frac{1}{\pi V_E^*}\langle\phi|T|i\rangle\sin\Delta + \frac{1}{\pi V_E^*}\int dE'\frac{V_{E'}^*\langle\psi_{e'}|T|i\rangle}{E-E'}\sin\Delta \\ &- \langle\psi_E|T|i\rangle\cos\Delta\end{aligned} \tag{5.5}$$

We can define a new wavefunction $\Phi_E = \phi + \int dE'\frac{V_{E'}\psi_{E'}}{E-E'}$ and collect the first two terms:

$$\langle\Phi_E|T|i\rangle = \frac{1}{\pi V_E^*}\langle\phi|T|i\rangle\sin\Delta - \langle\psi_E|T|i\rangle\cos\Delta \tag{5.6}$$

By writing the transition probability in this form we have highlighted the contribution of the Δ term in the coefficients, independent of the particular transition operator T. In particular, examine Δ near the pole at $E = E_\psi - F(E)$. When the denominator approaches 0 from the left then $\Delta = \frac{\pi}{2}$, while $\Delta = -\frac{\pi}{2}$ when the denominator approaches 0 from the right.
The cosine term in Eq. 5.5 will approach zero from either direction, while the sine term will approach ±1 as Δ approaches $\pm\frac{\pi}{2}$. This sudden phase change, combined with the functional form of equation 5.6, creates an asymmetric absorption peak. On the "left" side of the peak there will be a value of E for which the two terms in equation 5.6 cancel and there is a null in the absorption spectra.