Jonathan Bergknoff
August, 2005

My project was a math REU at Rutgers University during summer 2005. My advisor was Joel Lebowitz. The research topic was **Ionization of a Two-Level System**

Outline: We are interested in the ionization of a simple quantum system. To begin, we choose a system with two bound states and a continuum of scattering states. One such system is given by the Hamiltonian

$$H_0 = -\frac{\partial^2}{\partial x^2} - q\left[\delta(x-1) + \delta(x+1)\right]; \qquad q > 1. \tag{1}$$

The condition $q > 1$ is necessary for our purposes; for $|q| < 1$ only one bound state exists. In this model, ionization refers to occupation of the scattering states. We want to add a perturbative forcing term to the Hamiltonian and see how the system behaves.

Eigenfunctions of H_0: In position space, the eigenfunctions of H_0 are symmetric or anti-symmetric functions of x. Specifically, the ground state $u_s(x)$ is symmetric and its eigenvalue is $E_s = -\omega_s = -\gamma^2 < 0$, with γ determined by a transcendental equation. The excited state $u_a(x)$ is anti-symmetric and its eigenvalue is $E_a = -\omega_a = -\lambda^2 < 0$, with λ determined by a transcendental equation. Symmetric and anti-symmetric scattering states, $\varphi_s(k,x)$ and $\varphi_a(k,x)$ respectively, exist for each real k and have eigenvalues k^2. In summary,

$$H_0 u_s(x) = -\gamma^2 u_s(x) \tag{2}$$
$$H_0 u_a(x) = -\lambda^2 u_a(x) \tag{3}$$
$$H_0 \varphi_s(k,x) = k^2 \varphi_s(k,x) \tag{4}$$
$$H_0 \varphi_a(k,x) = k^2 \varphi_a(k,x) \tag{5}$$

The explicit nature of the eigenfunctions is unnecessary for this discussion, so it's omitted. It is available in the cited paper.

Perturbative Forcing: The forcing that we choose is of the form

$$H_1 = qr[\delta(x-1) - \delta(x+1)]\sin\omega t \tag{6}$$

with $r > 0$ a small parameter, the strength of the perturbation, and ω the frequency of the forcing. This can be imagined as shaking the attractive δ functions at ± 1.

Goal: The complete (perturbed) system is now described by a Hamiltonian

$$H = H_0 + H_1. \tag{7}$$

and the quantity of interest is a wave function Ψ solving the Schrödinger equation:

$$H\Psi = i\frac{\partial}{\partial t}\Psi. \tag{8}$$

Approach: We go about solving the Schrödinger equation by expanding Ψ in terms of the eigenfunctions of H_0. Writing

$$\Psi(x,t) = \theta_s(t)u_s(x)e^{i\omega_s t} + \theta_a(t)u_a(x)e^{i\omega_a t} + \int_0^\infty dk\; e^{-ik^2 t}\left[\zeta_s(k,t)\varphi_s(k,x) + \zeta_a(k,t)\varphi_a(k,x)\right], \tag{9}$$

the problem becomes determination of the time-dependent coefficients $\theta_{s/a}$. The probability of the particle being bound at time t is $B(t) = |\theta_a|^2 + |\theta_s|^2$ so the probability of finding the particle ionized at time t is $I(t) = 1 - B(t)$.

Under the condition of the Schrödinger equation, we get equations determining the time evolution of the time-dependent coefficients. In particular,

$$\theta_s(t) = \theta_s(0) - 2ia \int_0^t dt'\ e^{-i\gamma^2 t'} Y^+(t') \tag{10}$$

$$\theta_a(t) = \theta_a(0) - 2ib \int_0^t dt'\ e^{-i\lambda^2 t'} Y^-(t') \tag{11}$$

with a, b determined constants (named α, β in the cited paper) and $Y^\pm(t)$ defined as

$$Y^\pm(t) = \frac{r}{2}\sqrt{q}\,[\Psi(1,t) \mp \Psi(-1,t)] \sin \omega t. \tag{12}$$

Define the Laplace transform $\tilde{F}(p)$ of $F(t)$ by $\tilde{F}(p) = \int_0^\infty dt\ e^{-pt} F(t)$. The inverse Laplace transform $F(t)$ of $\tilde{F}(p)$ is given by $F(t) = \frac{1}{2\pi}\int_{c-i\infty}^{c+i\infty} dp\ e^{pt}\tilde{F}(p)$ for real $c > 0$. Under a change of variables, equations 10 and 11 become

$$\theta_s(t) = \theta_s(0) - \frac{\alpha}{\pi}\int_{c-i\infty}^{c+i\infty} dp\ \frac{e^{pt}}{p}\tilde{Y}^+(p + i\gamma^2) \tag{13}$$

$$\theta_a(t) = \theta_a(0) - \frac{\beta}{\pi}\int_{c-i\infty}^{c+i\infty} dp\ \frac{e^{pt}}{p}\tilde{Y}^-(p + i\lambda^2) \tag{14}$$

A recurrence relation emerges (details are in the cited paper) if we define $\tilde{Y}_n^\pm = \tilde{Y}^\pm(p + in\omega)$. Then

$$\tilde{Y}_n^- - \alpha_{n+2}\tilde{Y}_{n+2}^- - \beta_{n-2}\tilde{Y}_{n-2}^- = I_n^- \tag{15}$$

$$\tilde{Y}_n^+ - \gamma_{n+2}\tilde{Y}_{n+2}^+ - \delta_{n-2}\tilde{Y}_{n-2}^+ = I_n^+ \tag{16}$$

with $\alpha_n, \beta_n, \gamma_n, \delta_n, I_n^\pm$ all completely determined functions of p and ω. The index n runs over all integers $\{\ldots, -1, 0, 1, \ldots\}$. Initial conditions are included in the $I_n^\pm$ and make no appearances elsewhere.

Further Solutions: At this point, one can employ an approximation and truncate the recurrence relations 15, 16. This was done in the cited paper for 2 (or less) photon processes, i.e. when the energy gap from the continuum (at energy zero) to the ground state $-\omega_s$ is less than twice the forcing frequency ω.

Another approach that I proposed follows: First assume a solution

$$\tilde{Y}_k^- = \sum_{k'=-\infty}^{\infty} G_{k,k'} I_{k'} \tag{17}$$

with some matrix G to be determined. Then rewriting equation 15 in terms of G yields the condition

$$G_{k,k'} - \alpha_{k+2}G_{k+2,k'} - \beta_{k-2}G_{k-2,k'} = \delta_{k,k'} \tag{18}$$

which can be summarized as a matrix equation $AG = 1$ where A is the matrix

$$A_{k,k'} = \begin{cases} 1; & k = k' \\ -\beta_{k-2}; & k = k' + 2 \\ -\alpha_{k+2}; & k = k' - 2 \\ 0; & \text{otherwise} \end{cases}. \tag{19}$$

Then inverting A gives $\tilde{Y}^- = \tilde{Y}_0^-$ in principle. To actually compute the integral in 13, one is likely to look for poles of the integrand and then add residues. These poles correspond to values of p for which A is not invertible.

Either task (inversion of A or solving $\det A = 0$) is likely impossible symbolically in even the simplest cases. It is necessary to make an approximation and then employ numerical methods. When I attempted to numerically find zeroes of $\det A$ for a specific case, I met with limited success. This process may not be very helpful for obtaining concrete results.

Acknowledgements: The paper cited throughout is "Excitation and ionization of a simple two level system by a harmonic force" by A. Rokhlenko and J. L. Lebowitz of Rutgers University. I want to thank Joel Lebowitz, Alex Rokhlenko, Ovidiu Costin and Chris Stucchio for all of their guidance and help throughout the summer.