1 Perturbation Theory

Sometimes we are faced with solving a problem of the form

$$E\psi = H\psi + H_c\psi \tag{1}$$

where the Hamiltonian is split into two parts, H and H_c. H is large but simple and H_c is small but complicated. An approximate solution can be obtained by first solving $E\psi = H\psi$ and then using these solutions to obtain successively better approximations to the full solution. To understand how this works it is best to rewrite the above equation as

$$E\psi = H\psi + \epsilon J\psi \tag{2}$$

where J is now the roughly the same size as H and $|\epsilon| \ll 1$. We then do something that apparently makes the problem more complex, but in fact results in a simplification — namely, we assume that ϵ is a variable that can take on a range of values from zero up to some maximum value $\epsilon_0 \ll 1$. Setting $\epsilon = 0$ results in the simple problem $E\psi = H\psi$, which we assume we can solve exactly.

1.1 Time Independent Perturbation Theory

We now explore the case where J has no explicit time dependence.

1.1.1 Derivation

Since $H_c = \epsilon J$ is small, we assume that the solutions to the full problem don't differ fractionally by more than ϵ from the small problem. We therefore write the eigenvalues and eigenvectors E_n and ψ_n of the full problem as the eigenvalues and eigenvectors that solve the simple problem plus successive corrections of order ϵ, ϵ^2, etc.:

$$E_n = E_n^{(0)} + \epsilon E_n^{(1)} + \epsilon^2 E_n^{(2)} + \ldots \tag{3}$$

and

$$\psi_n = \psi_n^{(0)} + \epsilon \psi_n^{(1)} + \epsilon^2 \psi_n^{(2)} + \ldots \tag{4}$$

We substitute equations (3) and (4) into equation (2). Coefficients of each power of ϵ have to satisfy equation (2) independently since ϵ is assumed to be variable. The zeroth and first order components of equation (2) with $E = E_n$ and $\psi = \psi_n$ are

$$E_n^{(0)}\psi_n^{(0)} = H\psi_n^{(0)} \tag{5}$$

and

$$E_n^{(1)}\psi_n^{(0)} + E_n^{(0)}\psi_n^{(1)} = H\psi_n^{(1)} + J\psi_n^{(0)}. \tag{6}$$

Equation (5) is just the easy problem, which we know how to solve.

In order to make further progress, we need to realize that the first order correction to the full eigenvector, $\psi_n^{(1)}$, can be represented in terms of the eigenvectors of the simple problem, $\psi_n^{(0)}$:

$$\psi_n^{(1)} = \sum_m a_{nm}\psi_m^{(0)}. \tag{7}$$

This follows because because of the *completeness* property of the eigenvectors of a Hermitian operator; since these vectors are the orthogonal unit vectors of a Cartesian coordinate system in the vector space, *any* vector in the space can be represented as the sum of the product of these unit vectors with the components of the arbitrary vector. As an example, suppose that H is the free particle Hamiltonian, in which case the $\psi_m^{(0)} \propto \exp(ik_m x)$. In this case equation (7) becomes a Fourier series.

Complete freedom in the choice of a_{nm} is not allowed, because the first order corrected eigenvectors, $\psi_n^{(0)} + \epsilon\psi_n^{(1)}$, must be orthonormal, at least to first order in ϵ. Since

$$\psi_l'\psi_n = (\psi_l^{(0)'} + \epsilon\psi_l^{(1)'})(\psi_n^{(0)} + \epsilon\psi_n^{(1)}) \approx \delta_{ln} + \epsilon(a_{ln}^* + a_{nl}), \tag{8}$$

where terms containing ϵ^2 have been dropped, we must have

$$a_{ln}^* + a_{nl} = 0. \tag{9}$$

For $l = n$, this means that a_{nn} must be purely imaginary. Constructing the first order correct eigenvector thus yields

$$\psi_n = \psi_n^{(0)}(1 + \epsilon a_{nn}) + \epsilon \sum_{m \neq n} a_{nm}\psi_m^{(0)}. \tag{10}$$

Finally, to first order in ϵ this can be written

$$\psi_n = [\psi_n^{(0)} + \epsilon \sum_{m \neq n} a_{nm}\psi_m^{(0)}](1 + \epsilon a_{nn}). \tag{11}$$

Since a_{nn} is imaginary, $|1 + \epsilon a_{nn}| = 1$ to first order in ϵ, and all this factor does is add a small change in phase to ψ_n. However, this has no physical consequences, since taking the absolute value squared of ψ_n to get a probability eliminates the phase factor. Thus, for simplicity we set $a_{nn} = 0$ with no loss of generality.

Substituting equation (7) into equation (6) and rearranging results in

$$E_n^{(1)}\psi_n^{(0)} = \sum_m a_{nm}(E_m^{(0)} - E_n^{(0)})\psi_m^{(0)} + J\psi_n^{(0)}, \tag{12}$$

where advantage has been taken of the fact that $H\psi_m^{(0)} = E_m^{(0)}\psi_m^{(0)}$. This equation may now be used to determine the first order corrections to the eigenvalue, $E_n^{(1)}$. Multiplying equation (12) on the left by $\psi_n^{(0)\prime}$ and recalling that $\psi_m^{(0)\prime}\psi_n^{(0)} = \delta_{mn}$, we find that

$$E_n^{(1)} = \psi_n^{(0)\prime} J \psi_n^{(0)}. \tag{13}$$

Similarly multiplying equation (12) on the left by $\psi_l^{(0)\prime}$, where $l \neq n$, results in

$$a_{nl} = \frac{\psi_l^{(0)\prime} J \psi_n^{(0)}}{E_n^{(0)} - E_l^{(0)}} \qquad l \neq n, \tag{14}$$

which may be substituted into equation (7):

$$\psi_n^{(1)} = \sum_{m \neq n} \frac{\psi_m^{(0)\prime} J \psi_n^{(0)}}{E_n^{(0)} - E_m^{(0)}} \psi_m^{(0)}. \tag{15}$$

Substituting equations (13) and (15) into equations (3) and (4) yields first order estimates of the eigenvalues and eigenvectors of the full problem. Note by the way that equation (14) satisfies equation (9).

Often first order estimates produce an approximation of sufficient accuracy and it is not necessary to proceed further. However, higher order approximations may be obtained by similar means. On a cautionary note, there is no guarantee that this series of approximations actually converges. This possibility needs to be taken seriously especially when ϵ_0 approaches unity.

state	$\epsilon = 0$	$\epsilon = 0.2$		$\epsilon = 1.0$		$\epsilon = 5.0$	
number	exact	approx	exact	approx	exact	approx	exact
1	0.500	0.641	0.640	1.207	1.166	4.036	2.617
2	1.499	1.570	1.569	1.853	1.825	3.269	2.659
3	2.498	2.551	2.551	2.764	2.777	3.826	4.289
4	3.496	3.540	3.541	3.718	3.720	4.604	4.573
5	4.494	4.532	4.533	4.688	4.692	5.463	5.735
6	5.490	5.525	5.526	5.665	5.668	6.364	6.420
7	6.487	6.519	6.519	6.647	6.650	7.288	7.402
8	7.482	7.512	7.512	7.631	7.633	8.227	8.283
9	8.477	8.505	8.505	8.617	8.619	9.176	9.239
10	9.472	9.498	9.498	9.604	9.605	10.13	10.18

Table 1: Energy eigenvalues for scaled anharmonic oscillator with various values of ϵ. The columns labelled "approx" were calculated using first order perturbation theory with the harmonic oscillator solutions computed using *ho_demo.r* with 200 points. Those labelled "exact" were computed using *anho_demo.r*.

1.1.2 Anharmonic Oscillator

In this section we explore the use of perturbation theory in obtaining approximate solutions to the harmonic oscillator potential slightly modified by a bump in the center. More precisely, we look for eigenvalues of the Hamiltonian

$$H = (p^2 + x^2)/2 + \epsilon \exp(-x^2) \tag{16}$$

where p is the momentum operator, x is the position operator, and where the last term is the perturbation part. The first 10 eigenvalues of the harmonic oscillator, as computed using *ho_demo.r* using 200 points, are shown in the first column of table 1. The next three pairs of columns show the corresponding perturbation energies calculated using equation (13) with $J = \exp(-x^2)$ and $\psi_n^{(0)}$ obtained from *ho_demo.r*. This calculation is implimented in the demonstration *perturb1_demo.r*.

Notice how the approximate and exact values differ very little for $\epsilon = 0.2$. For $\epsilon = 1.0$ there is still fair agreement, while for $\epsilon = 5.0$ there is significant disagreement, especially for the lower energy states. These states are affected more by the perturbation potential energy, as it is confined to the region of small $|x|$. The perturbation thus exists for only a small part of the effective domain of the higher energy states.

1.2 Time Dependent Perturbation Theory

Sometimes the perturbation part of the Hamiltonian is time dependent. For instance, the Hamiltonian

$$H_{total} = H + \epsilon J(t) = (p^2 + x^2)/2 + \epsilon x \cos(\omega t) \tag{17}$$

represents a mass-spring system with natural angular frequency $\omega_0 = 1$ and an additional force $-\epsilon \cos(\omega t)$ applied to the mass. In other words, this is the Hamiltonian for a forced harmonic oscillator with forcing frequency ω.

If the Hamiltonian depends explicitly on time then the energy of the system is not conserved, and the time independent treatment cannot be used as in the previous section. The time dependent Schrödinger equation is

$$i\frac{\partial \psi}{\partial t} = H\psi + \epsilon x \cos(\omega t)\psi. \tag{18}$$

We write the state vector ψ in terms of the eigenvectors of the simple part of the Hamiltonian, H,

$$\psi = \sum_m a_m(t)\psi_m, \tag{19}$$

substitute this into equation (18), and multiply from the right by ψ_n'. Recalling that $\psi_n'\psi_m = \delta_{nm}$, this yields

$$i\frac{\partial a_n}{\partial t} = E_n a_n + \epsilon \cos(\omega t)\sum_m (\psi_n' x \psi_m) a_m, \tag{20}$$

where E_n is the nth eigenvalue of the simple part of the Hamiltonian. Setting $X_{nm} = \psi_n' x \psi_m$ and $A_n = a_n \exp(iE_n t)$ and expanding the cosine in terms of complex exponentials, this can be written

$$i\frac{\partial A_n}{\partial t} = \sum_m \frac{\epsilon X_{nm}}{2}\{\exp[i(\omega + E_n - E_m)t] + \exp[i(-\omega + E_n - E_m)t]\}A_m. \tag{21}$$

The matrix X_{nm} is simply the components of the x operator resolved in energy space. The components of X_{nm} are often called the *dipole moments* for transitions between the states denoted by the subscripted numbers. As equation (21) shows, the amplitude for going directly from state m to state n is zero if the dipole moment for that transition is zero.

For the harmonic oscillator it turns out that the only nonzero values of X_{nm} occur when $n = m \pm 1$. See the RLaB demonstration *dipole_demo.r* for a way to calculate X_{nm} for various potentials. This is an example of a *selection rule*, i. e., a rule that specifies when certain transitions are forbidden.

This problem splits naturally into two subcases, resonant and nonresonant forcing. Forcing is said to be resonant when $\omega = E_n - E_m$ for some pair of states m and n. For the harmonic oscillator this corresponds to the case where the forcing frequency is equal to the classical resonant frequency or some integer multiple of it. In addition, when the forcing is weak, i. e., when $|\epsilon| \ll 1$, nonresonant forcing is particularly easy to handle.

1.2.1 Weak Nonresonant Forcing

If the forcing is weak and nonresonant, and in addition if we assume that the system is initially in state k, then it turns out that the amplitudes to be in a state other than k will always remain small. Let us make this assumption and justify it after the fact by assuming that the dominant term in the sum on the right side of equation (21) is the one with $m = k$. We further assume that $A_k \approx 1$, which makes equation (21) reduce to

$$i\frac{\partial A_n}{\partial t} = \frac{\epsilon X_{nk}}{2}\{\exp[i(\omega + E_n - E_k)t] + \exp[i(-\omega + E_n - E_k)t]\}. \qquad (22)$$

This may be solved by direct integration:

$$A_n = \frac{\epsilon X_{nk}}{2}\left\{\frac{\exp(i\omega t)}{E_k - E_n - \omega} + \frac{\exp(-i\omega t)}{E_k - E_n + \omega}\right\}\exp[-i(E_k - E_n)t]. \qquad (23)$$

The initial assumption that $|A_n| \ll 1$ for $n \neq l$ is justified if $|\epsilon X_{nk}/\Delta E| \ll 1$, where ΔE is the smaller of the two energy denominators in the above equation.

Note that A_n becomes larger as the absolute value of the difference between the energies of states k and n approaches the frequency of the forcing.

Figure 1 shows an example of nonresonant forcing, as computed by the RLaB demonstration *forcing_demo.r*. A harmonic oscillator starts out in

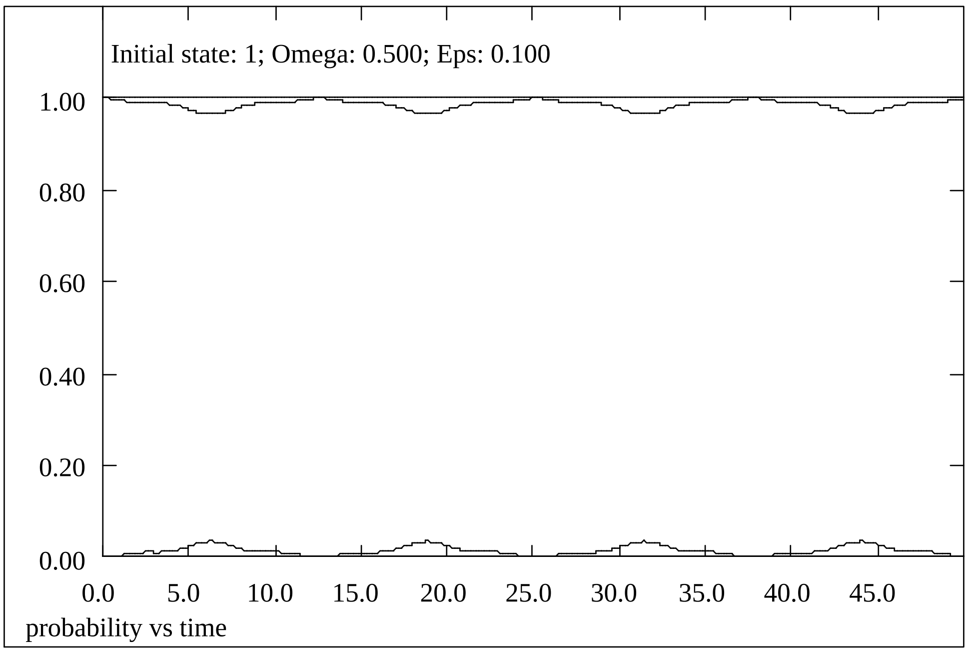

Figure 1: Example of nonresonant forcing of the harmonic oscillator, computed using *forcing_demo.r*. The nondimensional forcing frequency is $\omega = 0.5$ and the forcing strength is $\epsilon = 0.1$. The solid line is the sum of all the probabilities. This remains at unity as expected. The dashed oscillating line just under it represents the probability of finding the system in the ground state. Probabilities to be in all other states remain small.

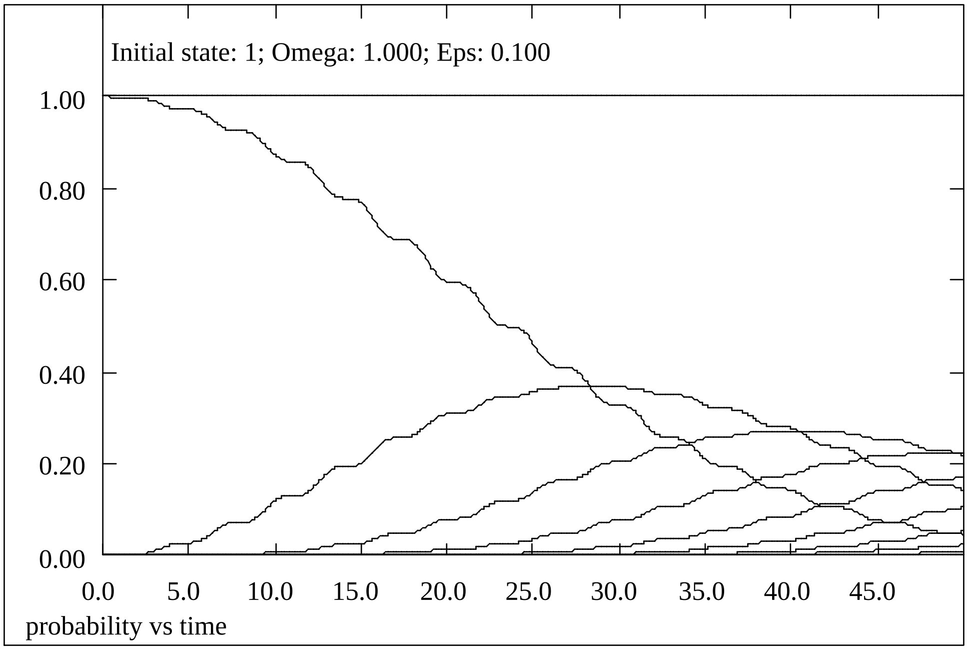

Figure 2: As in figure 1 except $\omega = 1$. The curves labelled c3, c4, c5, etc., give the probabilities to be in the ground state, the first excited state, the second excited state, etc.

the ground state and is subjected to forcing with nondimensional frequency $\omega = 0.5$, which is half the frequency (or energy) difference between harmonic oscillator states. The forcing strength is $\epsilon = 0.1$. Notice that the amplitudes to be in other than the ground state remain very small.

1.2.2 Resonant Forcing

Figure 2 shows another *forcing_demo.r* simulation with $\omega = 1$, i. e., it represents a case of resonant forcing. Notice how the probability to be in the ground state decreases with time. The probability to be in the first, second, third, etc., excited state first increases from zero and then begins to decrease. In other words, resonant forcing of the oscillator gradually raises it to a higher and higher level of excitation, as it does in classical mechanics.