3 The Harmonic Oscillator

I now want to use Dirac's formalism to study a simple system – the one-dimensional harmonic oscillator – with which you should already be familiar. Our aim here is not to learn new things about harmonic oscillators; indeed, we'll mostly just recover results you've known about since you first heard of simple harmonic motion. Rather, our aim is to get accustomed to this more abstract approach to QM, seeing how it's a very powerful way to think about the subject.

The steps we follow in our treatment of the harmonic oscillator will form a good prototype for the way we'll approach many other problems in QM. We'll see these same steps repeated in various contexts throughout thef course.

3.1 Raising and Lowering Operators

The Hamiltonian of a harmonic oscillator of mass m and classical frequency ω is

$$H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2 . \tag{3.1}$$

where X and P are the position and momentum operators, respectively. To analyse this, we begin by defining the dimensionless combination

$$A = \frac{1}{\sqrt{2m\hbar\omega}}\left(m\omega X + \mathrm{i}P\right) . \tag{3.2}$$

A is not a Hermitian operator, but since X and P are both Hermitian, we see that the adjoint of A is

$$A^\dagger = \frac{1}{\sqrt{2m\hbar\omega}}\left(m\omega X - \mathrm{i}P\right) . \tag{3.3}$$

Roughly, the motivation for introducing these operators is that they allow us to 'factorize' the Hamiltonian. More precisely, we have

$$\begin{aligned} A^\dagger A &= \frac{1}{2m\hbar\omega}\left(m\omega X - \mathrm{i}P\right)\left(m\omega X + \mathrm{i}P\right) \\ &= \frac{1}{2m\hbar\omega}\left(P^2 + m^2\omega^2 X^2 + \mathrm{i}m\omega[X,P]\right) \\ &= \frac{H}{\hbar\omega} - \frac{1}{2} \end{aligned} \tag{3.4}$$

so we can write our Hamiltonian as

$$H = \hbar\omega\left(A^\dagger A + \frac{1}{2}\right) = \hbar\omega\left(N + \frac{1}{2}\right) , \tag{3.5}$$

where

$$N = A^\dagger A . \tag{3.6}$$

A and $A^\dagger$ are often called *lowering* and *raising* operators, respectively, whilst N is often called the *number* operator. (The reason for these names will become apparent soon.) Notice that computing the spectrum of H is obviously equivalent to computing the spectrum of N.

Whenever we're presented with some new operators, the first thing to do is to work out their commutation relations. In this case, the fundamental commutation relations $[X, P] = \mathrm{i}\hbar$ show that

$$\begin{aligned}\left[A, A^\dagger\right] &= \frac{1}{2m\hbar\omega}\left(m^2\omega^2[X,X] - \mathrm{i}m\omega[X,P] + \mathrm{i}m\omega[P,X] + [P,P]\right)\\ &= -\frac{\mathrm{i}m\omega}{2m\hbar\omega}\left([X,P] - [P,X]\right)\\ &= 1\,,\end{aligned} \tag{3.7}$$

whilst $[A, A] = 0 = [A^\dagger, A^\dagger]$ trivially. It will also be useful to compute commutators involving N. We have

$$[N, A^\dagger] = [A^\dagger A, A^\dagger] = \left(A^\dagger[A, A^\dagger] + [A^\dagger, A^\dagger]A\right) = A^\dagger\,, \tag{3.8}$$

where the final step uses (3.7). We learn that, similarly, $[N, A] = -A$ by taking the adjoint of (3.8).

Let's see what these commutators teach us about the possible energy levels. Suppose that $|n\rangle$ is a correctly normalised eigenstate of N, so that $N|n\rangle = n|n\rangle$ and $\langle n|n\rangle = 1$. We have

$$NA^\dagger|n\rangle = (A^\dagger N + [N, A^\dagger])|n\rangle = A^\dagger(N+1)|n\rangle = (n+1)A^\dagger|n\rangle \tag{3.9}$$

so $A^\dagger|n\rangle$ is an eigenstate of N with eigenvalue $n+1$. Similarly,

$$NA|n\rangle = (AN + [N, A])|n\rangle = (n-1)A|n\rangle \tag{3.10}$$

so $A|n\rangle$ is an eigenstate of N with eigenvalue $n-1$. Acting with $A^\dagger$ thus raises the eigenvalue of N by one unit, whilst acting with A lowers it by one, giving these operators their names. The above algebra shows that if we can find just one energy eigenstate $|n\rangle$, then we can construct a whole family of them by repeatedly applying either $A^\dagger$ or A. The energies of these new states will be $(n+k+\frac{1}{2})\hbar\omega$ for some $k \in \mathbb{Z}$. However, we can't yet conclude that the energy levels are quantized, because we don't yet know that there isn't a continuum of possible starting-points $|n\rangle$ (or indeed any!).

This brings us to the second key step: we must now investigate the norm of our states. Since N is Hermitian all its eigenvalues must certainly be real, but in fact they're also non-negative, because

$$n = n\langle n|n\rangle = \langle n|N|n\rangle = \langle n|A^\dagger A|n\rangle = \|A|n\rangle\|^2 \geq 0 \tag{3.11}$$

with $n = 0$ iff $A|n\rangle = 0$, by properties of the norm. If $A|n\rangle \neq 0$ then it is an eigenstate of N with eigenvalue $n-1$, but we've just shown that there are no states in $\mathcal{H}$ with negative eigenvalue for N, so this lowering process must terminate. That will be the case iff n is a non-negative *integer*.

Putting all this together, we have a ground state $|0\rangle$ of energy $\frac{1}{2}\hbar\omega$ and an infinite tower of excited states $|n\rangle$ of energy

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega\,, \qquad \text{where } n \in \mathbb{N}_0\,. \tag{3.12}$$

These energy levels should be familiar from IB QM.

Acting on an energy eigenstate with the raising operator does not necessarily give us an excited state that is correctly normalised. In $d = 1$, energy eigenstates of the harmonic oscillator are non-degenerate[16], so we must have $A^\dagger|n\rangle = c_n|n+1\rangle$ for some constant c_n (which may depend on n). Taking the norm of both sides shows that

$$|c_n|^2 = \|A^\dagger|n\rangle\|^2 = \langle n|AA^\dagger|n\rangle = \langle n|N+1|n\rangle = n+1\,. \tag{3.13}$$

Therefore, the correctly normalised state is

$$|n+1\rangle = \frac{1}{\sqrt{n+1}}A^\dagger|n\rangle = \frac{1}{\sqrt{(n+1)!}}(A^\dagger)^{n+1}|0\rangle\,. \tag{3.14}$$

Likewise, you can check that $|n-1\rangle = \frac{1}{\sqrt{n}}A|n\rangle$ for $n \geq 1$, whilst again $A|0\rangle = 0$.

We've seen that everything about the energy levels of the harmonic oscillator follows from *i*) the algebra (*i.e.* the commutation relations) of raising and lowering operators, together with *ii*) considering the norm. Again, we'll follow these same two steps in analysing the eigenvalues and eigenstates of various operators throughout this course. This also parallels what you did in IB QM: there, by looking for series solutions of Schrödinger's equation, you could find an energy eigenstate for all $E \in \mathbb{R}$. However, these eigenstates were only normalizable if the series you found terminated. It was requiring this termination (*i.e.* normalizability) that lead to quantization of the energies.

I hope I've persuaded you that the algebraic approach above is somewhat cleaner and more efficient than looking for series solutions to Schrödinger's equation. Nothing has been lost, and we can easily use Dirac's formalism to recover the explicit wavefunctions of our eigenstates. For example, in the position representation, the defining equation $A|0\rangle = 0$ of the ground state becomes

$$0 = \sqrt{2m\hbar\omega}\,\langle x|A|0\rangle = \langle x|m\omega X + \mathrm{i}P|0\rangle = \left(m\omega x + \hbar\frac{d}{dx}\right)\psi_0(x)\,, \tag{3.15}$$

---

[16] Here is a proof, which holds for any potential $V(x)$ and energy E for which $\exists\, x_0 > 0$ s.t. $V(x) - E > 0$ $\forall\,|x| > x_0$. In one dimension, the TISE $-\hbar^2\psi''/2m + V(x)\psi = E\psi$ is a 2^{nd}-order ode. Thus, for any fixed value of E, it has exactly two linearly independent solutions. Let $\psi_1(x)$ and $\psi_2(x)$ be the two solutions defined by the conditions

$$\begin{aligned} \psi_1(x_0) &= 1 \qquad \text{and} \qquad \psi_1'(x_0) = 0\,, \\ \psi_2(x_0) &= 0 \qquad \text{and} \qquad \psi_2'(x_0) = 1\,, \end{aligned}$$

where x_0 is chosen so that $V(x) - E \geq M^2 > 0$ for all $|x| > x_0$ and some $M > 0$. Any solution of Schrödinger's equation for this $V(x)$ and E is a linear combination of these two; our aim is to prove that (up to overall scale) there is only one combination that is normalizable.

Since they each solve the TISE, the Wronskian

$$W(\psi_1, \psi_2) = \psi_1\psi_2' - \psi_2\psi_1'$$

is constant $\forall\, x$, and evaluating at $x = x_0$ gives $W(\psi_1, \psi_2) = 1$. Also, our condition on $V(x) - E$ implies that $\psi_{1,2}(x)$ remain positive over the entire range $x \in (x_0, \infty)$ and grow at least as fast as e^{Mx} as $x \to \infty$.

Since they are normalizable, $\psi_{1,2}(x) \to 0$ as $|x| \to \infty$. By itself, this does not quite allow us to conclude that $W = 0$, since we need to know that ψ' are bounded. For this we'll need a condition on the potential, and it turns out that a sufficient criterion is that To see this, suppose where $\psi_0(x) = \langle x|0\rangle$ is the position space wavefunction of our ground state. This is a first order o.d.e. whose solution is

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar}x^2\right) , \tag{3.16}$$

where the overall constant is fixed (up to phase) by the normalization requirement $\langle 0|0\rangle = \int_{\mathbb{R}} |\psi_0(x)|^2 = 1$. This is the same Gaussian wavefunction for the ground state of the harmonic oscillator familiar from IB QM. If needed, the wavefunctions of the excited states may be found by acting with $A^\dagger = (m\omega X - \mathrm{i}P)/\sqrt{2m\hbar\omega}$, which in the position representation is the differential operator $\frac{1}{\sqrt{2}}\left(-\alpha\frac{d}{dx} + x/\alpha\right)$, where $\alpha = \sqrt{\hbar/m\omega}$. You can check (or just Google) that these operators generate the usual Hermite polynomials.

3.2 Dynamics of Oscillators

At this stage, we've learned everything about the set $\{|n\rangle\}$ of energy eigenstates of the quantum harmonic oscillator and their corresponding energies $E_n = (n + \frac{1}{2})\hbar\omega$. However, we still haven't said anything about the physics of how quantum oscillators actually *behave*. Classically, we know that a harmonic oscillator would undergo periodic motion with a period $T = 2\pi/\omega$. Furthermore, the energy of the classical oscillator is independent of the period, but is proportional to the square of the amplitude of oscillation. To what extent is the same true of our quantum oscillator?

To say anything about the *motion* of a quantum system, we need to examine the TDSE. To get started, first suppose our system is prepared at time $t = 0$ to be in some energy eigenstate $|n\rangle$. Then by the TDSE, at a later time t it will have evolved to

$$|n, t\rangle = \mathrm{e}^{-\mathrm{i}(n+1/2)\omega t}|n\rangle\,. \tag{3.17}$$

Consequently, no eigenstate has a time dependence which oscillates at the classical frequency ω. Even worse, no matter which energy eigenstate our oscillator is in, the expected position of the oscillator at any given time t is

$$\langle n, t|X|n, t\rangle = \mathrm{e}^{+\mathrm{i}(n+1/2)\omega t}\,\langle n|X|n\rangle\,e^{-\mathrm{i}(n+1/2)\omega t} = \langle n|X|n\rangle\,, \tag{3.18}$$

where we've used the linearity / antilinearity properties of the inner product. The *rhs* is independent of time, so none of these states *move* – our oscillator does not appear to be oscillating!

To find some interesting dynamics, we must consider not a single energy eigenstate, but rather a *superposition.* This is a much more realistic assumption: there's no practical way we could prepare a macroscopic system to be in just one energy eigenstate. Let's now suppose our oscillator is prepared at $t = 0$ to be in some generic state $|\psi, 0\rangle = \sum_n c_n|n\rangle$. The c_n should be chosen so that $\langle\psi|\psi\rangle = 1$, but are otherwise arbitrary. Then at time t this state will have evolved to

$$|\psi, t\rangle = \sum_{n=0}^{\infty} c_n\,\mathrm{e}^{-\mathrm{i}E_n t/\hbar}\,|n\rangle \tag{3.19}$$

by the TDSE.

Now let's examine where we expect to find such a generic state. We have

$$\begin{aligned}\langle\psi,t|X|\psi,t\rangle &= \left(\sum_m \bar{c}_m\,\mathrm{e}^{\mathrm{i}E_m t/\hbar}\langle m|\right) X \left(\sum_n c_n\,\mathrm{e}^{-\mathrm{i}E_n t/\hbar}\,|n\rangle\right)\\ &= \sum_{n,m} \bar{c}_m\,c_n\,\mathrm{e}^{\mathrm{i}(m-n)\omega t}\,\langle m|X|n\rangle\,.\end{aligned} \tag{3.20}$$

To evaluate the inner product $\langle m|X|n\rangle$, we write[17]

$$X = \sqrt{\frac{\hbar}{2m\omega}}\left(A + A^\dagger\right) \tag{3.21}$$

in terms of the raising and lowering operators. Recalling that $A^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$ and $A|n\rangle = \sqrt{n}\,|n-1\rangle$, we have

$$\langle m|X|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}\,\langle m|n-1\rangle + \sqrt{n+1}\,\langle m|n+1\rangle\right)\,, \tag{3.22}$$

showing that $\langle m|X|n\rangle$ is non-zero only when $m = n \pm 1$. The double sum in (3.20) thus reduces to

$$\begin{aligned}\langle\psi,t|X|\psi,t\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\left(\sum_{n=1}^{\infty} \sqrt{n}\,\bar{c}_{n-1}c_n\,\mathrm{e}^{-\mathrm{i}\omega t} + \sqrt{n}\,\bar{c}_n c_{n-1}\,\mathrm{e}^{+\mathrm{i}\omega t}\right)\\ &= \sum_n x_n\cos(\omega t + \phi_n)\,,\end{aligned} \tag{3.23}$$

where the real numbers x_n and ϕ_n are defined by

$$\sqrt{\frac{2n\hbar}{m\omega}}\,\bar{c}_n c_{n-1} = x_n\,\mathrm{e}^{\mathrm{i}\phi_n}\,. \tag{3.24}$$

Equation (3.23) shows that $\langle X\rangle$ oscillates sinusoidally at exactly the classical frequency ω whenever our oscillator is prepared in any generic[18] superposition of energy eigenstates. Furthermore, as for the classical oscillator, *the frequency of oscillation is independent of the energy.* In the calculation above, this occurs because the separation between every adjacent pair of energy levels is always $\hbar\omega$.

For a macroscopic oscillator, the only non-negligible amplitudes will be those where $n \approx n_{\mathrm{cl}}$ for some $n_{\mathrm{cl}} \gg 1$. Consequently, a measurement of the energy is certain to yield some value close to $E_{n_{\mathrm{cl}}} = (n_{\mathrm{cl}} + \frac{1}{2})\hbar\omega \approx n_{\mathrm{cl}}\hbar\omega$. For each eigenstate, we have

$$\langle n|X^2|n\rangle = \frac{\hbar}{2m\omega}\,\langle n|AA^\dagger + A^\dagger A|n\rangle = \frac{E_n}{m\omega^2} \tag{3.25}$$

---

[17] To do this calculation using the techniques of IB QM, you would have worked in the position representation and said

$$\langle m|X|n\rangle = \int_{-\infty}^{\infty}\left(H_m(x)\,\mathrm{e}^{-x^2/2\alpha}\right)^*\,x\,H_n(x)\,\mathrm{e}^{-x^2/2\alpha}\,dx$$

where $H_n(x)$ are Hermite polynomials of degree n and $\alpha = \hbar/m\omega$. This is correct, but the integral looks rather unpleasant to evaluate. Fortunately, our operator formalism means we never even have to try!

[18] Here, 'generic' simply means we must have non-zero amplitudes $c_n = \langle n|\psi\rangle$ for at least one pair of adjacent energy levels.

so the mean value $\overline{\langle X^2 \rangle} = E_{n_{\rm cl}}/(m\omega^2)$. Classically, the time average of x^2 is proportional to the average potential energy, which for a harmonic oscillator is just half the total energy. Thus, classically we have $\overline{x^2} = E/(m\omega^2)$ in agreement with the quantum result. The correspondence principle requires that the quantum and classical results agree for large values of E. That they agree even for low energies is a coincidence due to special symmetries of the harmonic oscillator.

3.2.1 Anharmonic Oscillations

Suppose that, instead of the pure harmonic oscillator, we have a potential that has a minimum at $x = 0$ around which it grows approximately quadratically while $|x| \ll a$, but then asymptotes to a constant value at large $|x|$. Particles of low energy will have position space wavefunctions that are supported near the minimum of $V(x)$, so we'd expect the low-lying energy levels to be roughly equal to those of a corresponding harmonic oscillator. Particles of higher energy would start to see the fact that the potential is not purely harmonic. In fact, for any such asymptotically constant potential with a single extremum, the separation between energy levels gets smaller and smaller as we approach the asymptotic value $\lim_{x\to\infty} V(x)$ of the potential (beyond which we have a continuum of non-bound states)[19].

Let's prepare a state to be in two adjacent energy levels, say

$$|\psi\rangle = c_n|n\rangle + c_{n+1}|n+1\rangle\,,$$

where $|n\rangle$ is the $n^{\rm th}$ energy eigenstate of our anharmonic potential, whatever it may be. Since the potential is symmetric around $x = 0$, its eigenstates have definite parity and so $\langle n|X|n\rangle = 0$ for all $|n\rangle$. Therefore, at time t,

$$\langle \psi, t|X|\psi, t\rangle = \bar{c}_n c_{n+1}\, \mathrm{e}^{\mathrm{i}(E_n - E_{n+1})t/\hbar}\, \langle n|X|n+1\rangle + \text{c.c.}\,. \tag{3.26}$$

This is again a sinusoidally oscillating function of time, but now the period $T = 2\pi\hbar/(E_{n+1} - E_n)$ depends on n since we no longer expect the energy levels to be equally spaced. In fact, since the energy levels get closer together as n increases, if we give our particle a larger amplitude of oscillation – and hence more energy – it will take longer to execute a complete an oscillation. This is just what we'd expect classically.

For example, consider the *Pöschl-Teller* potential

$$V(X) = -V_0 \operatorname{sech}^2(\kappa X) \tag{3.27}$$

for some constant $V_0 > 0$ and length scale $a = 1/\kappa$ (see figure 3). This has bound state energy levels[20]

$$E_n = -\frac{\hbar^2\kappa^2}{2m}(\nu - n)^2 \qquad \text{for } 0 \le n < \nu\,, \tag{3.28}$$

where ν is the positive root of $\nu(\nu+1) = 2mV_0/\hbar^2\kappa^2$. The separation between adjacent bound state energy levels is thus

$$E_{n+1} - E_n = (2(\nu - n) - 1)\hbar^2\kappa^2/2m \tag{3.29}$$

---

[19] For a proof, see *e.g.* chapter 6 of S. Gustafson & I.M. Singer, *Mathematical Concepts of Quantum Mechanics*, Springer (2010). (Both this result and its proof are non-examinable in this course.)

[20] Exercise: Try to prove this. It's similar to one of the questions on Problem Sheet 1.

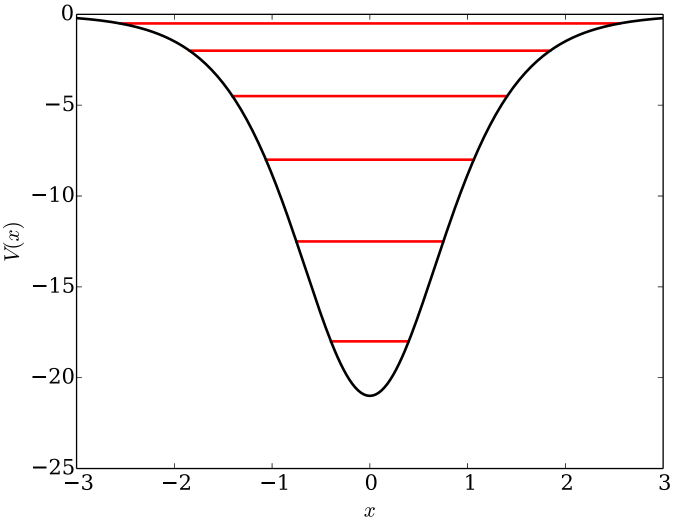

Figure 3: *The Pöschl-Teller potential* $V(x) = -V_0 \operatorname{sech}^2(\kappa X)$ *and its energy levels. Figure by Nicoguaro, taken from this Wikipedia page.*

and deceases as n increases towards ν. (These formulæbreak down when $n \geq \nu$, where we enter the continuum of non-normalizable states.)

If $V_0 \gg \hbar^2\kappa^2/2m$ then the potential is very deep and contains many bound states. In this regime, we have $\nu \approx \sqrt{2mV_0/\hbar^2\kappa^2} \gg 1$ and so from (3.29) we find that a superposition of low-lying states will oscillate with a frequency

$$\omega \approx \frac{\hbar\kappa^2}{m}\nu \approx \kappa\sqrt{\frac{2V_0}{m}}\,. \tag{3.30}$$

For $x \ll 1/\kappa$, we may approximate $-V_0 \operatorname{sech}^2(\kappa x) \approx -V_0 + V_0\kappa^2 x^2$, so this frequency is indeed just what we'd expect for the corresponding harmonic oscillator. On the other hand, a superposition of states clustered around $n = \nu/2$ will oscillate at around half this frequency as neighbouring energy levels in this region are only separated by about half as much.

If we include a wider range of states in our initial superposition, then we'll instead find a sequence of terms[21]

$$\begin{aligned}\langle\psi,t|X|\psi,t\rangle = \cdots + \ \bar{c}_{n-1}c_n\, \mathrm{e}^{\mathrm{i}(E_{n-1}-E_n)t/\hbar}\,\langle n-1|X|n\rangle + \bar{c}_{n+1}c_n\, \mathrm{e}^{\mathrm{i}(E_{n+1}-E_n)t/\hbar}\,\langle n+1|X|n\rangle \\ + \bar{c}_{n+3}c_n\, \mathrm{e}^{\mathrm{i}(E_{n+3}-E_n)t/\hbar}\,\langle n+3|X|n\rangle + \cdots\,.\end{aligned} \tag{3.31}$$

Since this is no longer a harmonic oscillator, we do not generically expect $\langle n+3|X|n\rangle = 0$. Let's define a frequency $\Omega = (E_{n_{\mathrm{cl}}+1} - E_{n_{\mathrm{cl}}})/\hbar$ where $n_{\mathrm{cl}} \gg 1$. Provided the c_n's are clustered around this large central value $n = n_{\mathrm{cl}}$ sufficiently tightly that the difference between adjacent energy levels is roughly constant over the range of n for which the c_n are

---

[21] Note that for a symmetric potential, we again have $\langle n+2k|X|n\rangle = 0$ by parity.

appreciable, then, to reasonable accuracy, all the terms that contribute to (3.31) oscillate with frequencies that are integer multiples of $\Omega_{n_{\rm cl}}$. Thus the motion will be periodic, but anharmonic, just as we expect classically.

If we release the anharmonic oscillator from some large extension x_0, then initially the wavefunction will be a superposition of many energy levels, with coefficients that ensure $\langle x|\psi\rangle = \sum_n c_n \langle x|n\rangle$ is sharply peaked around x_0. At time t, this state will evolve to

$$|\psi, t\rangle = \mathrm{e}^{-\mathrm{i}E_{n_{\rm cl}}t/\hbar} \sum_n c_n \, \mathrm{e}^{\mathrm{i}(E_{n_{\rm cl}} - E_n)t/\hbar} \, |n\rangle \, .$$

Since the separation between energy levels varies, the frequencies appearing in this sum are not all integer multiples of any Ω_N. Consequently, after a time of order $2\pi/\Omega_N$, most terms in the sum will have not quite returned to their original values, so the wavefunction at $t = 2\pi/\Omega$ will be less sharply peaked around X. With each subsequent passing of time $2\pi/\Omega_N$, the wavefunction will become more and more diffusely spread. Classically, if we release an oscillator with a rather uncertain value for it's energy, then for a pure harmonic oscillator we always know where to find the oscillator at later times, since it's period is independent of the energy. However, for an anharmonic oscillator, the period depends on the energy, so after a long time our oscillator is equally likely to be located anywhere.