

## Chapter 26

### Why Are Big Things Classical?

*Why does decoherence happen very rapidly for objects with large numbers of degrees of freedom?*

Last Update: 7/1/12

#### 1. What is the Problem?

Decoherence, via interaction with the environment, causes the density matrix of a system to become diagonal in a particular basis called the pointer basis. The simple example in [Chapter 24](#) has illustrated that the pointer states of a system approximate to its energy eigenstates if its energy level spacings are large compared with the energies characterising the interaction with the environment. Decoherence naturally einselects the energy eigenstates in this situation. The energy eigenstates are usually spatially delocalised and hence delocalisation is the natural condition in such a case. An example is the state of an atomic, or molecular, electron.

On the other hand, macroscopic objects tend not to be in delocalised states. They tend to be in classical states in which energy is localised. Why is it that being “big” causes this? To be consistent with the decoherence programme, “big” things must tend to have very closely spaced energy levels – so that even an extremely weak interaction with the environment will decohere them away from their pure energy eigenstates. Accordingly, this Chapter provides some simple illustrations of how very close spacing of energy levels often arises naturally when the system’s number of degrees of freedom is large.

Although this helps to explain why classical behaviour is typical for ‘big’ things, the exceptions to this general tendency are extremely important. In fact the most interesting things are exceptions to the rule, and are interesting for that very reason, see §5.

#### 2. The Continuum Field Limit

Consider a lattice consisting of a large number of bonded atoms – sufficiently many that we may treat it approximately as an elastic continuum. Phonons with wave-vector  $\vec{k}$  are associated with an energy  $\hbar\omega$  and in the long wavelength limit we can consider the almost-continuum to have a constant velocity of sound,  $v_s$ , such that  $\omega = v_s |\vec{k}|$ .

Hence  $\hbar\omega$  can be regarded as the approximate eigen-energies where the eigenstates are given by,

$$|\vec{k}| = \frac{\pi}{L} \sqrt{n_x^2 + n_y^2 + n_z^2} \quad (1)$$

where we have assumed a cube of material of side  $L$  and  $N_1$  atoms per side, hence with lattice spacing  $a = L / N_1$ . In (1), the quantum numbers  $(n_x, n_y, n_z)$  take the values 1, 2, 3... to a maximum of  $N_1$ . In a true continuum the quantum numbers could be arbitrarily large, but for a discrete lattice the number of classical natural frequencies is limited to the number of degrees of freedom.

Considering a 1D line of atoms the energy spacing is thus,

$$\Delta E \approx \frac{\pi\hbar v_s}{aN_1} \quad (2)$$

The energy level spacing decreases asymptotically to zero for large numbers of atoms in inverse proportion to the number of atoms in the line,  $\propto 1/N_1$ .

If we consider a 2D square array of atoms, the minimum energy spacing is obtained as the difference of (1), evaluated at  $n_x = 1, n_y = N_1$  and  $n_x = 2, n_y = N_1$ , giving, for large  $N_1$ ,

$$\sqrt{2^2 + N_1^2} - \sqrt{1^2 + N_1^2} \approx \frac{3}{2N_1} \quad (3)$$

Hence,

$$\Delta E_{\min} \approx \frac{3\pi\hbar v_s}{LN_1} = \frac{3\pi\hbar v_s}{aN_1^2} = \frac{3\pi\hbar v_s}{aN_2} \quad (4)$$

where  $N_2 = N_1^2$  is the number of atoms in the square array. Hence the result is the same as for the 1D case: the minimum energy level spacing reduces asymptotically to zero in inverse proportion to the total number of atoms.

For the 3D case we get, using  $n_x = 1, n_y = N_1$  and  $n_z = N_1$ , and  $\Delta n_x = 1$ ,

$$\Delta E_{\min} \approx \frac{3\pi\hbar v_s}{2\sqrt{2}LN_1} = \frac{3\pi\hbar v_s}{2\sqrt{2}aN_1^2} = \frac{3\pi\hbar v_s}{2\sqrt{2}a(N_3)^{2/3}} \quad (5)$$

The minimum energy spacing still tends asymptotically to zero as the total number of atoms,  $N_3 = N_1^3$ , becomes large, but now only as the 2/3 power of the total number of atoms. Because the minimum energy spacing is vanishingly small for large  $N$ , even the weakest environmental interaction will decohere the system away from its energy eigenstates, generally resulting in localisation for large objects (but not invariably!).

### 3. An Exciton Example

The illustration of §2 has considered only the vibrational (phonon) modes. There may be other degrees of freedom which result in smaller energy level spacings. This might happen, for example, if the atoms/molecules have an accessible excited state, and these excited states can mutually interact. In such cases the interaction can break the initial  $N$ -fold degeneracy resulting from the possibility that an excitation could be located on any of the  $N$  atoms. The weaker the interaction, the closer are the resulting split levels. Consequently very close energy levels must be regarded as a generically common. Moreover, as we shall now show, even if the interaction is strong, the minimum eigen-energy spacing tends to zero rapidly as  $N$  becomes large.

Consider a system comprising  $N$  particles in a line. Each particle is assumed to have just two energy states, energy 0 or  $E$ . The Hilbert space of this system is of dimension  $2^N$ . However, we suppose there is insufficient energy available to excite two or more particles to their higher energy state, but sufficient to excite a single particle. In this  $N$  dimensional sub-space the Hamiltonian in the energy basis is simply the  $N \times N$  diagonal matrix with diagonal elements all equal to  $E$ . Any  $N$  dimensional vector is an eigenvector because this is an  $N$ -fold degenerate energy level. However we will take the basis to be defined by which particle is excited. We now introduce an

interaction between nearest neighbours only consisting of a potential energy  $\Delta$ . The Hamiltonian therefore becomes,

$$(H) = \begin{pmatrix} E & \Delta & 0 & 0 & 0 & 0 & 0 \\ \Delta & E & \Delta & 0 & 0 & 0 & 0 \\ 0 & \Delta & E & \Delta & 0 & 0 & 0 \\ 0 & 0 & \Delta & E & \Delta & 0 & 0 \\ 0 & 0 & 0 & \Delta & E & \Delta & 0 \\ 0 & 0 & 0 & 0 & \Delta & E & \Delta \\ 0 & 0 & 0 & 0 & 0 & \Delta & E \end{pmatrix} \quad (6)$$

(illustrated here for  $N = 7$ ). The interaction between the particles breaks the degeneracy, the perturbed energy levels being given by the solutions to the secular equation,

$$\|H - \lambda\| = \begin{vmatrix} E - \lambda & \Delta & 0 & 0 & 0 & 0 & 0 \\ \Delta & E - \lambda & \Delta & 0 & 0 & 0 & 0 \\ 0 & \Delta & E - \lambda & \Delta & 0 & 0 & 0 \\ 0 & 0 & \Delta & E - \lambda & \Delta & 0 & 0 \\ 0 & 0 & 0 & \Delta & E - \lambda & \Delta & 0 \\ 0 & 0 & 0 & 0 & \Delta & E - \lambda & \Delta \\ 0 & 0 & 0 & 0 & 0 & \Delta & E - \lambda \end{vmatrix} = 0 \quad (7)$$

(again illustrated here for  $N = 7$ ). The easiest means of solving (7) is numerically using the proprietary matrix manipulation software of your choice. However, it is fun to do these things analytically as far as possible. Using the substitution,

$$x = (E - \lambda)^2 \quad (8)$$

and denoting the secular determinant as  $\|N\|$ , it is readily seen that,

$$\|N\| = \sqrt{x}\|N - 1\| - \Delta^2\|N - 2\| \quad (9)$$

Hence the secular equations are found to reduce to,

$N$	Secular Equation for the Energy Levels
2	$x - \Delta^2 = 0$
3	$x = 0$ or $x - 2\Delta^2 = 0$
4	$x^2 - 3\Delta^2x + \Delta^4 = 0$
5	$x = 0$ or $x^2 - 4\Delta^2x + 3\Delta^4 = 0$
6	$x^3 - 5\Delta^2x^2 + 6\Delta^4x - \Delta^6 = 0$
7	$x = 0$ or $x^3 - 6\Delta^2x^2 + 10\Delta^4x - 4\Delta^6 = 0$
8	$x^4 - 7\Delta^2x^3 + 15\Delta^4x^2 - 10\Delta^6x + \Delta^8 = 0$
9	$x = 0$ or $x^4 - 8\Delta^2x^3 + 21\Delta^4x^2 - 20\Delta^6x + 5\Delta^8 = 0$
10	$x^5 - 9\Delta^2x^4 + 28\Delta^4x^3 - 35\Delta^6x^2 + 15\Delta^8x - \Delta^{10} = 0$

The  $x = 0$  solutions give  $\lambda = E$  whereas the  $n^{\text{th}}$  order polynomials in  $x$  have  $n$  positive roots  $x_r$  which provide  $2n$  energy levels  $\lambda = E \pm \sqrt{x_r}$ . Relative to the mean energy  $E$ , and in units of the interaction strength  $\Delta$ , the energy levels are,

<b>N</b>	$(\lambda - E) / \Delta$	<b>Minimum Spacing / <math>\Delta</math></b>
2	$\pm 1$	2
3	$-\sqrt{2}, 0, +\sqrt{2}$	$\sqrt{2}$
4	$-\sqrt{\frac{(3+\sqrt{5})}{2}}, -\sqrt{\frac{(3-\sqrt{5})}{2}}, +\sqrt{\frac{(3-\sqrt{5})}{2}}, +\sqrt{\frac{(3+\sqrt{5})}{2}}$	1
5	$-\sqrt{3}, -1, 0, +1, +\sqrt{3}$	$\sqrt{3} - 1$
6	-1.802, -1.247, -0.445, 0.445, 1.247, 1.802	0.5549
7	-1.8478, -1.4142, -0.7654, 0, 0.7654, 1.4142, 1.8478	0.4336
8	-1.8794, -1.5321, -1, 0, 1, 1.5321, 1.8794	0.3473
9	$\pm 1.90211, \pm 1.61803, \pm 1.17557, \pm 0.61804, 0$	0.28408
10	$\pm 1.91899, \pm 1.68250, \pm 1.30972, \pm 0.83083, \pm 0.28464$	0.23649

The last column gives the smallest spacing between adjacent energy levels, which in every case is between the lowest excited state and the second lowest:

$$E_2 - E_1 = \lambda_2 - \lambda_1.$$

Numerical evaluation of the eigenvalues is the simplest means of continuing, and this gives the reducing minimum energy spacing to be,

<b>N</b>	<b>Minimum Spacing / <math>\Delta</math></b>
11	0.19980
12	0.17097
13	0.14792
14	0.12920
15	0.11381
16	0.10100
17	0.09023
18	0.08109
19	0.073263
20	0.066516
25	0.043534
30	0.030679
35	0.022774
40	0.017571
50	0.011366
75	0.0051225
100	0.0029014

The minimum energy spacing is plotted against  $N$  in Figure 1 (up to  $N = 10$ ) and in Figure 2 (up to  $N = 100$ ) and finally in Figure 3 (up to  $N = 100$  but on log-log scales).

The energy spacing is clearly asymptotic to zero as  $N$  increases. The slope of the log-log plot of Figure 3 suggests that the asymptotic behaviour is that the minimum spacing decreases  $\propto \frac{1}{N^2}$ . *How can this be proved analytically?*

The presence of this sort of “exciton” behaviour therefore promotes very small minimum energy spacing, being smaller for weaker internal coupling within the system. But, regardless of the internal coupling strength, the minimum energy spacing becomes vanishingly small for large  $N$ , so that even the weakest environmental interaction will decohere the system away from its energy eigenstates. The common, but not invariable, result is the localisation of large objects.

#### 4. The 1D Line of Atoms Revisited

We return briefly to the 1D problem addressed in §2: a line of atoms interacting through a quadratic potential between nearest neighbours (whose limit is the elastic continuum). Denoting the displacement of the  $i^{\text{th}}$  atom of mass  $m$  as  $x_i$ , the classical equations of motion, assuming a spring constant  $\kappa$  between each pair of atoms, are,

$$m\ddot{x}_1 = -\kappa x_1 - \kappa(x_1 - x_2) \quad (10a)$$

$$m\ddot{x}_2 = -\kappa(x_2 - x_1) - \kappa(x_2 - x_3) \quad (10b)$$

$$m\ddot{x}_3 = -\kappa(x_3 - x_2) - \kappa(x_3 - x_4), \text{ etc.} \quad (10c)$$

The classical natural frequencies are therefore given by  $\omega_n = \sqrt{\lambda_n} \cdot \omega_0$ , where  $\omega_0 = \sqrt{\kappa/m}$  and  $\lambda_n$  are the roots of,

$$\begin{vmatrix} 2-\lambda & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 2-\lambda & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 2-\lambda & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2-\lambda & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2-\lambda & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 2-\lambda & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 2-\lambda \end{vmatrix} = 0 \quad (11)$$

(illustrated for the case  $N = 7$ ). But (11) is of the same form as (7). So we know already that the asymptotic behaviour of the  $\lambda_n$  is that the minimum spacing obeys,

$$\text{LIM } N \rightarrow \infty \quad \Delta\lambda_{\min} = \lambda_2 - \lambda_1 \propto \frac{1}{N^2} \quad (12)$$

So we have,

$$\begin{aligned} \Delta E_{\min} &= E_2 - E_1 = (\sqrt{\lambda_2} - \sqrt{\lambda_1})\omega_0 = \omega_0\sqrt{\lambda_1} \left\{ \sqrt{\frac{\lambda_2}{\lambda_1}} - 1 \right\} = \omega_0\sqrt{\lambda_1} \left\{ \sqrt{1 + \frac{A}{N^2\lambda_1}} - 1 \right\} \\ &= \omega_0\sqrt{\lambda_1} \left\{ \left[ 1 + \frac{1}{2} \frac{A}{N^2\lambda_1} \right] - 1 \right\} = \frac{\omega_0}{2} \frac{A}{N^2\sqrt{\lambda_1}} \propto \frac{1}{N^2 E_1} \propto \frac{1}{N} \end{aligned} \quad (13)$$

The last step follows because the energy levels in 1D are proportional to  $\frac{n_x}{L} \propto \frac{n_x}{N}$  (this follows from Equ.(1) and also from the numerical solution in §3). Consequently,

the lowest energy eigenstate,  $n_x = 1$ , is proportional to  $1/N$ . Hence (13) reproduces the continuum result of §2, i.e., that the elastic line of atoms has a minimum energy spacing which reduces in inverse proportion to  $N$ .

## 5. The Exceptions are of Greater Interest

Obviously one cannot conclude anything rigorous or universal from a few very simple illustrations. The purpose of these examples has been only to make plausible the claim that ‘big’ objects will most often tend to have some very closely spaced eigen-energies, and hence will most often decohere away from their energy eigenstates and towards localised states. In this context ‘big’ means only that the system has a large number of degrees of freedom,  $N \gg 1$ . A few tens of degrees of freedom might be ‘big’, so biggish molecules may be large enough. This is why molecules can often be regarded as having a definite shape. Much of chemistry, especially biochemistry, is concerned with the geometrical interlocking of pairs of molecules. A successful chemical reaction may depend upon correct geometrical compatibility. This “lego brick” view of molecular interactions would hardly be possible if atoms were delocalised, resulting in molecules of indeterminate shape. **Hmm...such a quantum superposition of shapes might actually facilitate a greater range of possible reactions?? Not sure I've got this right. Research and/or drop.**

**However, it would be a mistake to think that macroscopic quantum phenomena were impossible. Superfluidity, superconductivity and Bose-Einstein condensation are all examples of essentially quantum phenomena, involving sustained coherence, which are observable on the macroscopic scale. One of the key features which permit these phenomena to arise is the existence of energy gaps in their spectra. Is this true????**

**Include brief review of superconductivity and Superfluidity and Bose-Einstein condensates – and the entangling of macroscopic diamonds? – to illustrate that some Big Things are rather interestingly quantum mechanical – so the generalities of the Chapters are just that – but there are interesting exceptions.**

Figure 1

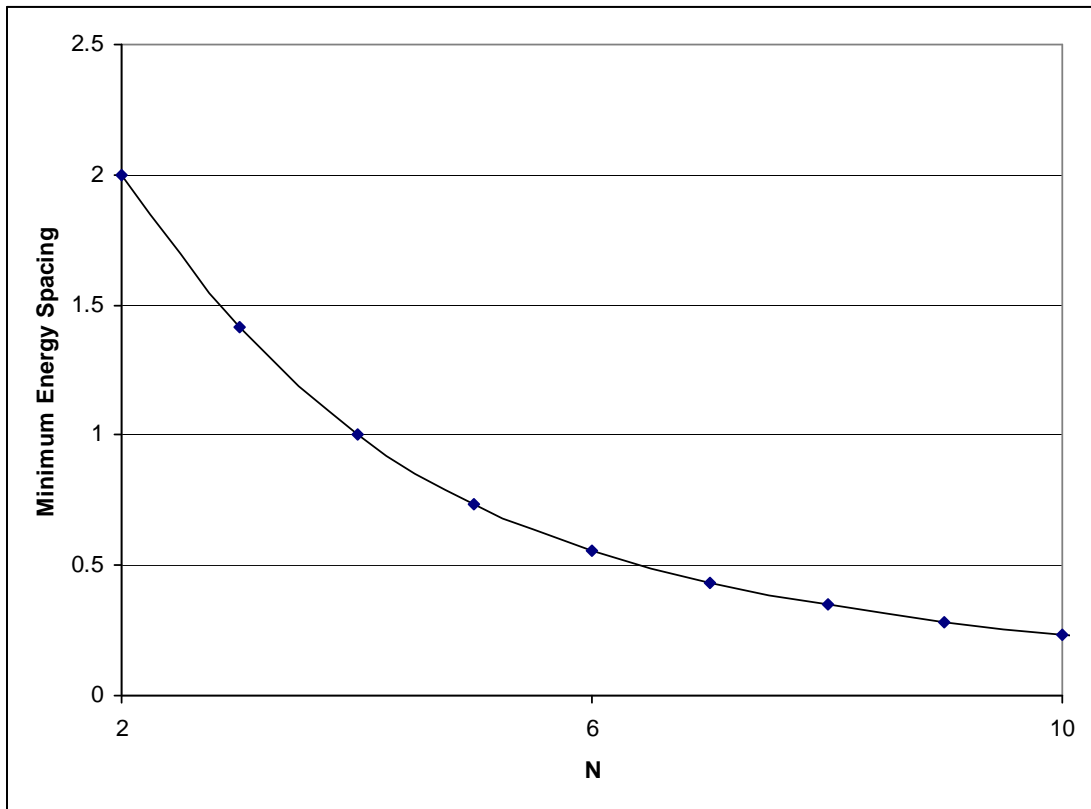


Figure 2

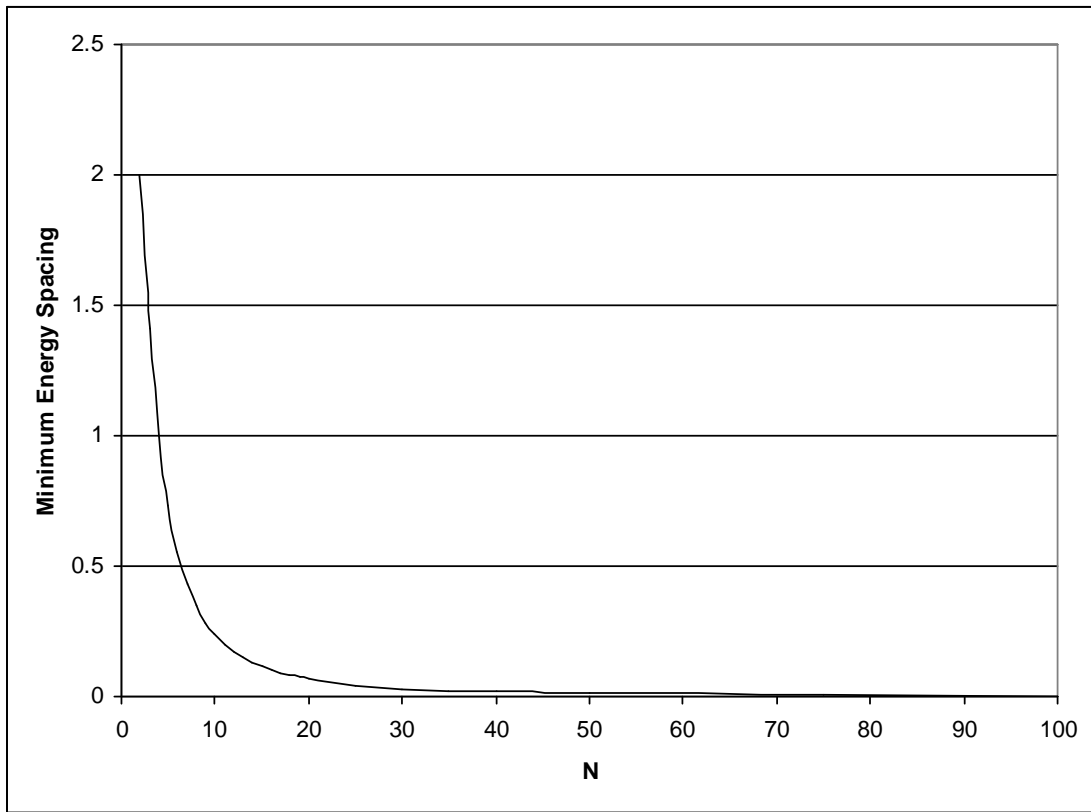
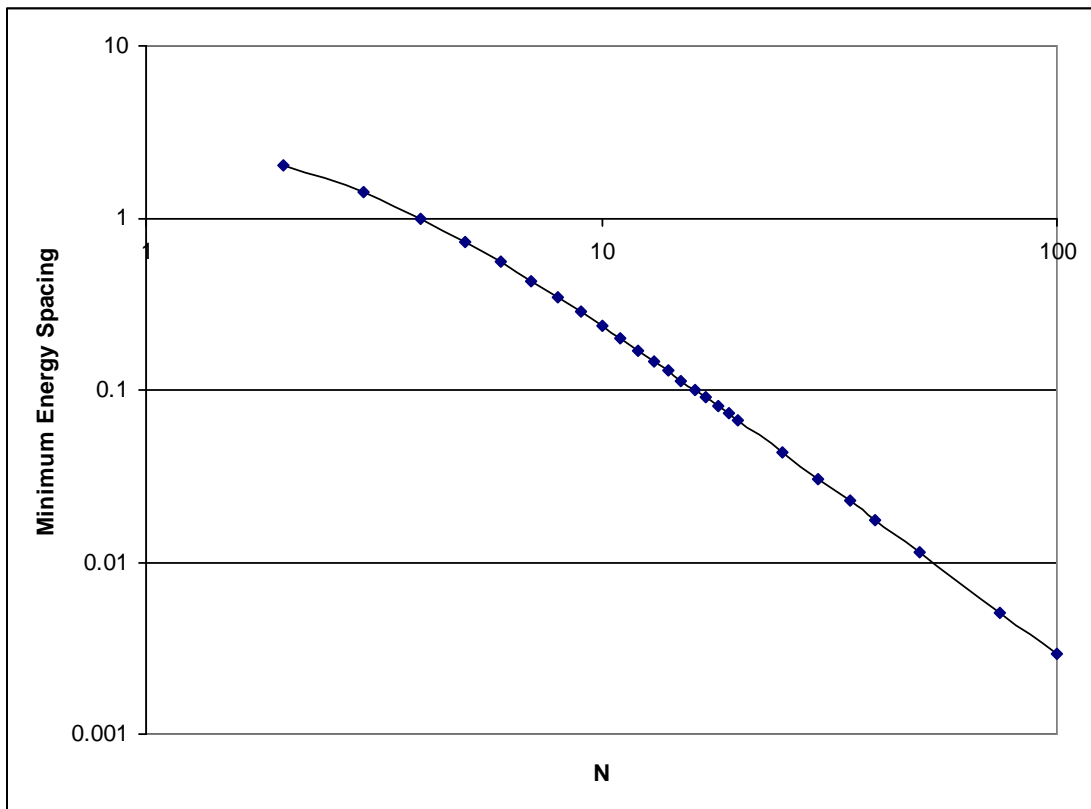


Figure 3





This document was created with Win2PDF available at <http://www.win2pdf.com>.  
The unregistered version of Win2PDF is for evaluation or non-commercial use only.  
This page will not be added after purchasing Win2PDF.