

SOLUTION MANUAL
Quantum Mechanics for Engineers

Leon van Dommelen

August 25, 2018

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Chapter 1

Special Relativity [Draft]

1.1 Overview of Relativity

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1.1.3 The universal speed of light

1.1.4 Disagreements about space and time

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1.3 Relativistic Mechanics

1.3.1 Intro to relativistic mechanics

1.3.2 Lagrangian mechanics

Chapter 2

Mathematical Prerequisites

2.1 Complex Numbers

2.1.1 Solution mathcplx-a

Question:

Multiply out $(2 + 3i)^2$ and then find its real and imaginary part.

Answer:

Multiplying out the square gives $2^2 + 12i + (3i)^2$. Since $i^2 = -1$, you get $-5 + 12i$. This means that the real part is -5 and the imaginary part 12 .

2.1.2 Solution mathcplx-b

Question:

Show more directly that $1/i = -i$.

Answer:

The probably most straightforward way is to take i to the other side, $1 = -i^2$, and then note that $i^2 = -1$.

2.1.3 Solution mathcplx-c

Question:

Multiply out $(2 + 3i)(2 - 3i)$ and then find its real and imaginary part.

Answer:

You get $2^2 - (3i)^2$, which is $4 + 9 = 13$ so the real part is 13 and the imaginary part is zero.

2.1.4 Solution mathcplx-d

Question:

Find the magnitude or absolute value of $2 + 3i$.

Answer:

The magnitude $|2 + 3i|$ of $2 + 3i$ is the square root of $2 + 3i$ times its complex conjugate $2 - 3i$:

$$|2 + 3i| = \sqrt{(2 + 3i)(2 - 3i)} = \sqrt{2^2 - (3i)^2}.$$

Since $i^2 = -1$, $|2 + 3i| = \sqrt{13}$.

2.1.5 Solution mathcplx-e

Question:

Verify that $(2 - 3i)^2$ is still the complex conjugate of $(2 + 3i)^2$ if both are multiplied out.

Answer:

$$(2 - 3i)^2 = -5 - 12i \text{ and } (2 + 3i)^2 = -5 + 12i.$$

2.1.6 Solution mathcplx-f

Question:

Verify that e^{-2i} is still the complex conjugate of e^{2i} after both are rewritten using the Euler formula.

Answer:

$$e^{-2i} = \cos(2) - i \sin(2) \text{ and } e^{2i} = \cos(2) + i \sin(2).$$

2.1.7 Solution mathcplx-g

Question:

Verify that $(e^{i\alpha} + e^{-i\alpha})/2 = \cos \alpha$.

Answer:

Apply the Euler formula for both exponentials and note that $\sin(-\alpha) = -\sin \alpha$.

2.1.8 Solution mathcplx-h

Question:

Verify that $(e^{i\alpha} - e^{-i\alpha})/2i = \sin \alpha$.

Answer:

Apply the Euler formula for both exponentials and note that $\sin(-\alpha) = -\sin \alpha$.

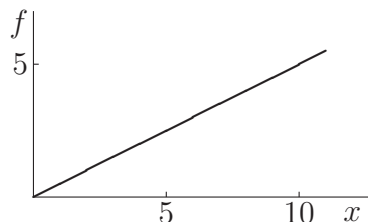
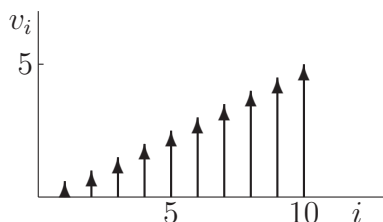
2.2 Functions as Vectors

2.2.1 Solution funcvec-a

Question:

Graphically compare the spike diagram of the 10-dimensional vector \vec{v} with components $(0.5, 1, 1.5, 2, 2.5, 3, 3.5, 4, 4.5, 5)$ with the plot of the function $f(x) = 0.5x$.

Answer:

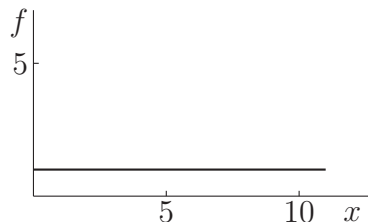
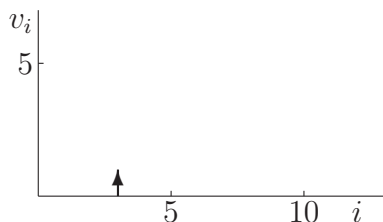


2.2.2 Solution funcvec-b

Question:

Graphically compare the spike diagram of the 10-dimensional unit vector \hat{i}_3 , with components $(0, 0, 1, 0, 0, 0, 0, 0, 0, 0)$, with the plot of the function $f(x) = 1$. (No, they do not look alike.)

Answer:



The equivalent of a unit vector for functions is not the function 1, it is the Dirac delta function. This function will be discussed in detail later, but simply put, it is a single, infinitely high spike.

2.3 The Dot, oops, INNER Product

2.3.1 Solution dot-a

Question:

Find the following inner product of the two vectors:

$$\left\langle \begin{pmatrix} 1+i \\ 2-i \end{pmatrix} \middle| \begin{pmatrix} 2i \\ 3 \end{pmatrix} \right\rangle$$

Answer:

Take complex conjugates at the left and sum products of corresponding components as in

$$(1-i) \times (2i) + (2+i) \times 3 = 2i + 2 + 6 + 3i = 8 + 5i$$

2.3.2 Solution dot-b

Question:

Find the length of the vector

$$\begin{pmatrix} 1+i \\ 3 \end{pmatrix}$$

Answer:

Take the square root of the inner product of the vector with itself:

$$\sqrt{\left\langle \begin{pmatrix} 1+i \\ 3 \end{pmatrix} \middle| \begin{pmatrix} 1+i \\ 3 \end{pmatrix} \right\rangle}$$

which works out like

$$\sqrt{(1-i)(1+i) + (3)(3)} = \sqrt{1-i^2+9} = \sqrt{11}$$

2.3.3 Solution dot-c

Question:

Find the inner product of the functions $\sin(x)$ and $\cos(x)$ on the interval $0 \leq x \leq 1$.

Answer:

$$\langle \sin(x) | \cos(x) \rangle = \int_0^1 \sin(x) \cos(x) dx = -\frac{1}{4} \cos(2x) \Big|_0^1 = \frac{1}{4} (1 - \cos(2))$$

2.3.4 Solution dot-d

Question:

Show that the functions $\sin(x)$ and $\cos(x)$ are orthogonal on the interval $0 \leq x \leq 2\pi$.

Answer:

They are by definition orthogonal if the inner product is zero. Check that:

$$\langle \sin(x) | \cos(x) \rangle = \int_0^{2\pi} \sin(x) \cos(x) dx = -\frac{1}{4} \cos(2x) \Big|_0^{2\pi} = \frac{1}{4} (1 - \cos(4\pi)) = 0$$

2.3.5 Solution dot-e

Question:

Verify that $\sin(x)$ is not a normalized function on the interval $0 \leq x \leq 2\pi$, and normalize it by dividing by its norm.

Answer:

$$\|\sin(x)\| = \sqrt{\langle \sin(x) | \sin(x) \rangle} = \sqrt{\int_0^{2\pi} \sin^2(x) dx} = \sqrt{\pi}$$

Since $\|\sin(x)\|$ is not one, $\sin(x)$ is not a normalized function on $0 \leq x \leq 2\pi$. If you divide by its norm, i.e. by $\sqrt{\pi}$, however,

$$\|\sin(x)/\sqrt{\pi}\| = \sqrt{\int_0^{2\pi} (\sin(x)/\sqrt{\pi})(\sin(x)/\sqrt{\pi}) dx} = \sqrt{\pi/\pi} = 1$$

2.3.6 Solution dot-f

Question:

Verify that the most general multiple of $\sin(x)$ that is normalized on the interval $0 \leq x \leq 2\pi$ is $e^{i\alpha} \sin(x)/\sqrt{\pi}$ where α is any arbitrary real number. So, using the Euler formula, the following multiples of $\sin(x)$ are all normalized: $\sin(x)/\sqrt{\pi}$, (for $\alpha = 0$), $-\sin(x)/\sqrt{\pi}$, (for $\alpha = \pi$), and $i \sin(x)/\sqrt{\pi}$, (for $\alpha = \pi/2$).

Answer:

A multiple of $\sin(x)$ means $c \sin(x)$, where c is some complex constant, so the magnitude is

$$\|c \sin(x)\| = \sqrt{\langle c \sin(x) | c \sin(x) \rangle} = \sqrt{\int_0^{2\pi} (c \sin(x))^* (c \sin(x)) dx}$$

You can always write c as $|c|e^{i\alpha}$ where α is some real angle, and then you get for the norm:

$$\|c \sin(x)\| = \sqrt{\int_0^{2\pi} (|c|e^{-i\alpha} \sin(x)) (|c|e^{i\alpha} \sin(x)) dx} = \sqrt{\int_0^{2\pi} |c|^2 \sin^2(x) dx} = |c|\sqrt{\pi}$$

So for the multiple to be normalized, the magnitude of c must be $|c| = 1/\sqrt{\pi}$, but the angle α can be arbitrary.

2.3.7 Solution dot-g

Question:

Show that the functions $e^{4i\pi x}$ and $e^{6i\pi x}$ are an orthonormal set on the interval $0 \leq x \leq 1$.

Answer:

You need to show that both functions are normalized, $\|e^{4i\pi x}\| = 1$ and $\|e^{6i\pi x}\| = 1$, and that they are mutually orthogonal, $\langle e^{4i\pi x} | e^{6i\pi x} \rangle = 0$. Work each out in turn (don't forget to take complex conjugate of the first function in the inner products):

$$\|e^{4i\pi x}\| = \sqrt{\langle e^{4i\pi x} | e^{4i\pi x} \rangle} = \sqrt{\int_0^1 e^{-4i\pi x} e^{4i\pi x} dx} = \sqrt{\int_0^1 1 dx} = 1$$

$$\|e^{6i\pi x}\| = \sqrt{\langle e^{6i\pi x} | e^{6i\pi x} \rangle} = \sqrt{\int_0^1 e^{-6i\pi x} e^{6i\pi x} dx} = \sqrt{\int_0^1 1 dx} = 1$$

$$\langle e^{4i\pi x} | e^{6i\pi x} \rangle = \int_0^1 e^{-4i\pi x} e^{6i\pi x} dx = \int_0^1 e^{2i\pi x} dx = \frac{1}{2i\pi} e^{2i\pi x} \Big|_0^1 = 0$$

(Since the Euler formula shows that $e^{i2\pi} = 1$.)

2.4 Operators

2.4.1 Solution mathops-a

Question:

So what is the result if the operator d/dx is applied to the function $\sin(x)$?

Answer:

Its derivative, the function $\cos(x)$, [1, p. 60].

2.4.2 Solution mathops-b

Question:

If, say, $\widehat{x^2} \sin(x)$ is simply the function $x^2 \sin(x)$, then what *is* the difference between $\widehat{x^2}$ and x^2 ?

Answer:

Nothing that affects the price of eggs. Just the way you *think* about them. You think of $\widehat{x^2}$ as the operator that turns a function like $\sin(x)$ into the function $x^2 \sin(x)$. But you think of x^2 as a recipe that turns a value like 3 into $3^2 = 9$.

2.4.3 Solution mathops-c

Question:

A less self-evident operator than the above examples is a translation operator like $\mathcal{T}_{\pi/2}$ that translates the graph of a function towards the left by an amount $\pi/2$: $\mathcal{T}_{\pi/2}f(x) = f(x + \frac{1}{2}\pi)$. (Curiously enough, translation operators turn out to be responsible for the law of conservation of momentum.) Show that $\mathcal{T}_{\pi/2}$ turns $\sin(x)$ into $\cos(x)$.

Answer:

Using various standard trig manipulations, [1, pp. 43-44]:

$$\mathcal{T}_{\pi/2} \sin(x) = \sin\left(x + \frac{1}{2}\pi\right) = \cos(-x) = \cos(x).$$

Or just compare the graphs visually, [1, p. 43].

2.4.4 Solution mathops-d

Question:

The inversion, or parity, operator Π turns $f(x)$ into $f(-x)$. (It plays a part in the question to what extent physics looks the same when seen in the mirror.) Show that Π leaves $\cos(x)$ unchanged, but turns $\sin(x)$ into $-\sin(x)$.

Answer:

According to [1, p. 43], $\cos(-x) = \cos(x)$, but $\sin(-x) = -\sin(x)$. Compare also the graphs of the functions on the same page; Π flips the graph of a function over around the y -axis.

2.5 Eigenvalue Problems

2.5.1 Solution eigvals-a

Question:

Show that e^{ikx} , above, is also an eigenfunction of d^2/dx^2 , but with eigenvalue $-k^2$. In fact, it is easy to see that the square of any operator has the same eigenfunctions, but with the square eigenvalues.

Answer:

Differentiate the exponential twice, [1, p. 60]:

$$\frac{d}{dx} e^{ikx} = ik e^{ikx} \quad \frac{d}{dx} \left(\frac{d}{dx} e^{ikx} \right) = \frac{d}{dx} (ik e^{ikx}) = (ik)^2 e^{ikx}$$

So d^2/dx^2 turns e^{ikx} into $(ik)^2 e^{ikx}$; the eigenvalue is therefore $(ik)^2$ which equals $-k^2$.

2.5.2 Solution eigvals-b

Question:

Show that any function of the form $\sin(kx)$ and any function of the form $\cos(kx)$, where k is a constant called the wave number, is an eigenfunction of the operator d^2/dx^2 , though they are not eigenfunctions of d/dx .

Answer:

The first derivatives are, [1, p. 60]:

$$\frac{d}{dx} \sin(kx) = k \cos(kx) \quad \frac{d}{dx} \cos(kx) = -k \sin(kx)$$

so they are not eigenfunctions of d/dx . But a second differentiation gives:

$$\begin{aligned} \frac{d}{dx} \left(\frac{d}{dx} \sin(kx) \right) &= \frac{d}{dx} (k \cos(kx)) = -k^2 \sin(kx) \\ \frac{d}{dx} \left(\frac{d}{dx} \cos(kx) \right) &= \frac{d}{dx} (-k \sin(kx)) = -k^2 \cos(kx) \end{aligned}$$

2.5.3 Solution eigvals-c

Question:

Show that $\sin(kx)$ and $\cos(kx)$, with k a constant, are eigenfunctions of the inversion operator Π , which turns any function $f(x)$ into $f(-x)$, and find the eigenvalues.

Answer:

By definition of Π , and then using [1, p. 43]:

$$\Pi \sin(kx) = \sin(-kx) = -\sin(kx) \quad \Pi \cos(kx) = \cos(-kx) = \cos(kx)$$

So by definition, both are eigenfunctions, and with eigenvalues -1 and 1 , respectively.

2.6 Hermitian Operators

2.6.1 Solution herm-a

Question:

A matrix A is defined to convert any vector $\vec{r} = x\hat{i} + y\hat{j}$ into $\vec{r}_2 = 2x\hat{i} + 4y\hat{j}$. Verify that \hat{i} and \hat{j} are orthonormal eigenvectors of this matrix, with eigenvalues 2, respectively 4.

Answer:

Take $x = 1, y = 0$ to get that $\vec{r} = \hat{i}$ transforms into $\vec{r}_2 = 2\hat{i}$. Therefore \hat{i} is an eigenvector, and the eigenvalue is 2. The same way, take $x = 0, y = 1$ to get that \hat{j} transforms into $4\hat{j}$, so \hat{j} is an eigenvector with eigenvalue 4. The vectors \hat{i} and \hat{j} are also orthogonal and of length 1, so they are orthonormal.

In linear algebra, you would write the relationship $\vec{r}_2 = A\vec{r}$ out as:

$$\begin{pmatrix} x_2 \\ y_2 \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 0 & 4 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 2x \\ 4y \end{pmatrix}$$

In short, vectors are represented by columns of numbers and matrices by square tables of numbers.

2.6.2 Solution herm-b

Question:

A matrix A is defined to convert any vector $\vec{r} = (x, y)$ into the vector $\vec{r}_2 = (x+y, x+y)$. Verify that $(\cos 45^\circ, \sin 45^\circ)$ and $(\cos 45^\circ, -\sin 45^\circ)$ are orthonormal eigenvectors of this matrix, with eigenvalues 2 respectively 0. Note: $\cos 45^\circ = \sin 45^\circ = \frac{1}{2}\sqrt{2}$.

Answer:

For $\vec{r} = (\cos 45^\circ, \sin 45^\circ) = (\frac{1}{2}\sqrt{2}, \frac{1}{2}\sqrt{2})$, $x = y = \frac{1}{2}\sqrt{2}$ so $\vec{r}_2 = (\sqrt{2}, \sqrt{2})$, and that is twice \vec{r} . For $\vec{r} = (\cos 45^\circ, -\sin 45^\circ) = (\frac{1}{2}\sqrt{2}, -\frac{1}{2}\sqrt{2})$, $x = -y = \frac{1}{2}\sqrt{2}$ so $\vec{r}_2 = (0, 0)$, and that is zero times \vec{r} .

The square length of $\vec{r} = (\cos 45^\circ, \sin 45^\circ)$ is $\vec{r} \cdot \vec{r}$, which is given by the sum of the square components: $\cos^2 45^\circ + \sin^2 45^\circ$. That is one, so the vector is of length one. The same for $\vec{r} = (\cos 45^\circ, -\sin 45^\circ)$. The dot product of $(\cos 45^\circ, \sin 45^\circ)$ and $(\cos 45^\circ, -\sin 45^\circ)$ is $\cos^2 45^\circ - \sin^2 45^\circ$. That is zero, because $\cos 45^\circ = \sin 45^\circ$, so the two eigenvectors are orthogonal.

In linear algebra, you would write the relationship $\vec{r}_2 = A\vec{r}$ out as:

$$\begin{pmatrix} x_2 \\ y_2 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x + y \\ x + y \end{pmatrix}$$

2.6.3 Solution herm-c

Question:

Show that the operator $\widehat{2}$ is a Hermitian operator, but \widehat{i} is not.

Answer:

By definition, $\widehat{2}$ corresponds to multiplying by 2, so $\widehat{2}g$ is simply the function $2g$. Now write the inner product $\langle f|\widehat{2}g\rangle$ and see whether it is the same as $\langle 2f|g\rangle$ for any f and g :

$$\langle f|\widehat{2}g\rangle = \int_{\text{all } x} f^* 2g \, dx = \int_{\text{all } x} (2f)^* g \, dx = \langle \widehat{2}f|g\rangle$$

since the complex conjugate does not affect a real number like 2. So $\widehat{2}$ is indeed Hermitian.

On the other hand,

$$\langle f|\widehat{i}g\rangle = \int_{\text{all } x} f^* i g \, dx = \int_{\text{all } x} -(if)^* g \, dx = -\langle \widehat{i}f|g\rangle$$

so \widehat{i} is not Hermitian. An operator like \widehat{i} that flips over the sign of an inner product if it is moved to the other side is called “skew-Hermitian”. An operator like $\widehat{2} + \widehat{i}$ is neither Hermitian nor skew-Hermitian.

2.6.4 Solution herm-d

Question:

Generalize the previous question, by showing that any complex constant c comes out of the right hand side of an inner product unchanged, but out of the left hand side as its complex conjugate;

$$\langle f|cg\rangle = c\langle f|g\rangle \quad \langle cf|g\rangle = c^*\langle f|g\rangle.$$

As a result, a number c is only a Hermitian operator if it is real: if c is complex, the two expressions above are not the same.

Answer:

Since constants can be taken out of an integral:

$$\begin{aligned}\langle f|cg\rangle &= \int_{\text{all } x} f^*cg \, dx = c \int_{\text{all } x} f^*g \, dx = c\langle f|g\rangle \\ \langle cf|g\rangle &= \int_{\text{all } x} (cf)^*g \, dx = c^* \int_{\text{all } x} f^*g \, dx = c^*\langle f|g\rangle.\end{aligned}$$

2.6.5 Solution herm-e

Question:

Show that an operator such as \hat{x}^2 , corresponding to multiplying by a real function, is an Hermitian operator.

Answer:

If the operator corresponds to multiplying by a real function of x , call it $r(x)$, then

$$\langle f|\hat{r}g\rangle = \int_{\text{all } i} f^*rg \, dx = \int_{\text{all } i} (rf)^*g \, dx = \langle \hat{r}f|g\rangle$$

since the complex conjugate does not affect a real function.

2.6.6 Solution herm-f

Question:

Show that the operator d/dx is *not* a Hermitian operator, but id/dx is, assuming that the functions on which they act vanish at the ends of the interval $a \leq x \leq b$ on which they are defined. (Less restrictively, it is only required that the functions are “periodic”; they must return to the same value at $x = b$ that they had at $x = a$.)

Answer:

You first need to show that

$$\left\langle f \left| \frac{d}{dx} g \right. \right\rangle$$

is not the same as

$$\left\langle \frac{d}{dx} f \left| g \right. \right\rangle$$

in order for d/dx not to be a Hermitian operator.

By definition,

$$\left\langle f \left| \frac{d}{dx} g \right. \right\rangle = \int_a^b f^* \frac{dg}{dx} dx.$$

You can use “integration by parts,” [1, p. 64], to move the derivative from g to f :

$$\left\langle f \left| \frac{d}{dx} g \right. \right\rangle = f^* g \Big|_a^b - \int_a^b \frac{df^*}{dx} g dx = f^*(b)g(b) - f^*(a)g(a) - \int_a^b \left(\frac{df}{dx} \right)^* g dx$$

(the differentiation can be moved inside the complex conjugate since it is a real operation.) Since the functions f and g are the same at the end points a and b you have

$$\left\langle f \left| \frac{d}{dx} g \right. \right\rangle = - \int_a^b \left(\frac{df}{dx} \right)^* g dx = - \left\langle \frac{d}{dx} f \left| g \right. \right\rangle$$

This makes d/dx a skew-Hermitian operator, rather than a Hermitian one: flipping over the operator to the other side changes the sign of the inner product.

To get rid of the change of sign, you can add a factor i to the operator, since the i adds a compensating minus sign when you bring it inside the complex conjugate:

$$\left\langle f \left| i \frac{d}{dx} g \right. \right\rangle = - \int_a^b \left(-i \frac{df}{dx} \right)^* g dx = \left\langle i \frac{d}{dx} f \left| g \right. \right\rangle$$

This makes id/dx a Hermitian operator.

2.6.7 Solution herm-g

Question:

Show that if A is a Hermitian operator, then so is A^2 . As a result, under the conditions of the previous question, $-d^2/dx^2$ is a Hermitian operator too. (And so is just d^2/dx^2 , of course, but $-d^2/dx^2$ is the one with the positive eigenvalues, the squares of the eigenvalues of id/dx .)

Answer:

To show that A^2 is Hermitian, just move the two operators A to the other side of the inner product one by one. As far as the eigenvalues are concerned, each application of A to one of its eigenfunctions multiplies by the eigenvalue, so two applications of A multiplies by the square eigenvalue.

2.6.8 Solution herm-h

Question:

A complete set of orthonormal eigenfunctions of $-d^2/dx^2$ on the interval $0 \leq x \leq \pi$ that are zero at the end points is the infinite set of functions

$$\frac{\sin(x)}{\sqrt{\pi/2}}, \frac{\sin(2x)}{\sqrt{\pi/2}}, \frac{\sin(3x)}{\sqrt{\pi/2}}, \frac{\sin(4x)}{\sqrt{\pi/2}}, \dots$$

Check that these functions are indeed zero at $x = 0$ and $x = \pi$, that they are indeed orthonormal, and that they are eigenfunctions of $-d^2/dx^2$ with the positive real eigenvalues

$$1, 4, 9, 16, \dots$$

Completeness is a much more difficult thing to prove, but they are. The completeness proof in the notes covers this case.

Answer:

Any eigenfunction of the above list can be written in the generic form $\sin(kx)/\sqrt{\pi/2}$ where k is a positive whole number, in other words where k is a “natural” number (one of 1, 2, 3, 4, ...) If you show that the stated properties are true for this generic form, it means that they are true for every eigenfunction.

First check the end points. The graph of the sine function, [1, item 12.22], shows that a sine is zero whenever its argument is a whole multiple of π . That makes both $\sin(k0) = \sin(0)$ and $\sin(k\pi)$ zero. So $\sin(kx)/\sqrt{\pi/2}$ must be zero at $x = 0$ and $x = \pi$ too.

Now check that the norm of the eigenfunctions is one. First find the norm of $\sin(kx)$ by itself:

$$\|\sin(kx)\| = \sqrt{\langle \sin(kx) | \sin(kx) \rangle} = \sqrt{\int_0^\pi \sin(kx)^* \sin(kx) dx}.$$

Since the sine is real, the complex conjugate does not do anything, and you get

$$\|\sin(kx)\| = \sqrt{\int_0^\pi \sin^2(kx) dx} = \sqrt{\pi/2}$$

using [1, item 18.26]. Dividing this by $\sqrt{\pi/2}$, the norm $\left\| \sin(kx)/\sqrt{\pi/2} \right\|$ becomes one; every eigenfunction is normalized.

To verify that $\sin(kx)/\sqrt{\pi/2}$ is orthogonal to every other eigenfunction, take the generic other eigenfunction to be $\sin(lx)/\sqrt{\pi/2}$ with l a natural number different from k . You must

then show that the inner product of these two eigenfunctions is zero. Since the normalization constants do not make any difference here, you can just show that $\langle \sin(kx) | \sin(lx) \rangle$ is zero. You get

$$\langle \sin(kx) | \sin(lx) \rangle = \int_0^\pi \sin(kx) \sin(lx) dx = 0$$

using again [1, item 18.26].

Ahem. Completeness. Well, just don't worry about it. There are a heck of a lot of functions here. Infinitely many of them, to be precise. Surely, with infinitely many functions, you should be able to approximate any given function to good accuracy?

(This statement is, of course, deliberately ludicrous. In fact, if you leave out a single eigenfunction, say the $\sin(x)$ function, the remaining infinitely many functions $\sin(2x)$, $\sin(3x)$, ... can simply not reproduce it by themselves. The *best* they can do is being zero and not try to approximate $\sin(x)$ at all. Still, if you do include $\sin(x)$ in the sequence, *any* (reasonable) function can be described accurately by a combination of the sines. It was hard to prove initially; in fact, Fourier in his thesis did *not*. The first proof is due to Dirichlet.)

2.6.9 Solution herm-i

Question:

A complete set of orthonormal eigenfunctions of the operator id/dx that are periodic on the interval $0 \leq x \leq 2\pi$ are the infinite set of functions

$$\dots, \frac{e^{-3ix}}{\sqrt{2\pi}}, \frac{e^{-2ix}}{\sqrt{2\pi}}, \frac{e^{-ix}}{\sqrt{2\pi}}, \frac{1}{\sqrt{2\pi}}, \frac{e^{ix}}{\sqrt{2\pi}}, \frac{e^{2ix}}{\sqrt{2\pi}}, \frac{e^{3ix}}{\sqrt{2\pi}}, \dots$$

Check that these functions are indeed periodic, orthonormal, and that they are eigenfunctions of id/dx with the real eigenvalues

$$\dots, 3, 2, 1, 0, -1, -2, -3, \dots$$

Completeness is a much more difficult thing to prove, but they are. The completeness proof in the notes covers this case.

Answer:

Any eigenfunction of the above list can be written in the generic form $e^{kix}/\sqrt{2\pi}$ where k is a whole number, in other words where k is an integer, one of $\dots, -3, -2, -1, 0, 1, 2, 3, \dots$. If you show that the stated properties are true for this generic form, it means that they are true for every eigenfunction.

Now periodicity requires that $e^{ki2\pi}/\sqrt{2\pi} = e^0/\sqrt{2\pi}$, and the Euler formula verifies this: sines and cosines are the same if the angle changes by a whole multiple of 2π . (For example, 2π , 4π , -2π , etcetera are physically all equivalent to a zero angle.)

The derivative of $e^{kix}/\sqrt{2\pi}$ with respect to x is $kie^{kix}/\sqrt{2\pi}$, and multiplying by i you get $-ke^{kix}/\sqrt{2\pi}$, so $e^{kix}/\sqrt{2\pi}$ is an eigenfunction of id/dx with eigenvalue $-k$.

To see that $e^{kix}/\sqrt{2\pi}$ is normalized, check that its norm is unity:

$$\left\| \frac{e^{kix}}{\sqrt{2\pi}} \right\| = \sqrt{\int_0^{2\pi} \frac{1}{\sqrt{2\pi}} e^{-kix} \frac{1}{\sqrt{2\pi}} e^{kix} dx} = \sqrt{\int_0^{2\pi} \frac{1}{2\pi} dx} = 1.$$

To verify that $e^{kix}/\sqrt{2\pi}$ is orthogonal to every other eigenfunction, take the generic other eigenfunction to be $e^{lix}/\sqrt{2\pi}$ with l an integer different from k . You must then show that the inner product of these two eigenfunctions is zero. Since the normalization constants do not make any difference here, you can just show that $\langle e^{kix} | e^{lix} \rangle$ is zero. You get

$$\langle e^{kix} | e^{lix} \rangle = \int_0^{2\pi} e^{-kix} e^{lix} dx = \int_0^{2\pi} e^{(l-k)ix} dx = \frac{1}{(l-k)i} e^{(l-k)ix} \Big|_0^{2\pi} = 0$$

since $e^{(l-k)i2\pi} = e^0 = 1$. So different eigenfunctions are orthogonal, their inner product is zero.

2.7 Additional Points

2.7.1 Dirac notation

2.7.2 Additional independent variables

Chapter 3

Basic Ideas of Quantum Mechanics

3.1 The Revised Picture of Nature

3.2 The Heisenberg Uncertainty Principle

3.3 The Operators of Quantum Mechanics

3.4 The Orthodox Statistical Interpretation

3.4.1 Only eigenvalues

3.4.2 Statistical selection

3.5 A Particle Confined Inside a Pipe

3.5.1 The physical system

3.5.2 Mathematical notations

3.5.3 The Hamiltonian

3.5.4 The Hamiltonian eigenvalue problem

3.5.5 All solutions of the eigenvalue problem

3.5.5.1 Solution piped-a

Question:

Write down eigenfunction number 6.

Answer:

Substituting $n = 6$ in the generic expression for the eigenfunctions,

$$\psi_n = \sqrt{\frac{2}{\ell_x}} \sin\left(\frac{n\pi}{\ell_x}x\right)$$

you get

$$\psi_6 = \sqrt{\frac{2}{\ell_x}} \sin\left(\frac{6\pi}{\ell_x}x\right)$$

3.5.5.2 Solution piped-b

Question:

Write down eigenvalue number 6.

Answer:

Substituting $n = 6$ in the generic expression for the eigenvalues,

$$E_n = \frac{n^2 \hbar^2 \pi^2}{2m\ell_x^2}$$

you get

$$E_6 = \frac{36\hbar^2 \pi^2}{2m\ell_x^2}$$

3.5.6 Discussion of the energy values

3.5.6.1 Solution pipee-a

Question:

Plug the mass of an electron, $m = 9.109\,38\,10^{-31}$ kg, and the rough size of an hydrogen atom, call it $\ell_x = 2\,10^{-10}$ m, into the expression for the ground state kinetic energy and see how big it is. Note that $\hbar = 1.054\,57\,10^{-34}$ J s. Express in units of eV, where one eV equals $1.602\,18\,10^{-19}$ J.

Answer:

$$E_1 = \frac{\hbar^2 \pi^2}{2m\ell_x^2} = \frac{(1.054\,57\,10^{-34}\text{ J s})^2 \pi^2}{2 \cdot 9.109\,38\,10^{-31}\text{ kg} (2\,10^{-10}\text{ m})^2} = 1.506\,10^{-18}\text{ J}$$

or 9.4 eV. The true value is about 4.5 eV. That is in the ball park.

3.5.6.2 Solution pipee-b

Question:

Just for fun, plug macroscopic values, $m = 1$ kg and $\ell_x = 1$ m, into the expression for the ground state energy and see how big it is. Note that $\hbar = 1.054\,57\,10^{-34}$ J s.

Answer:

$$E_1 = \frac{\hbar^2 \pi^2}{2m\ell_x^2} = \frac{(1.054\,57\,10^{-34}\text{ J s})^2 \pi^2}{2 \cdot 1\text{ kg} \cdot 1\text{ m}^2} = 5.488\,10^{-68}\text{ J}$$

or $3.4\,10^{-49}$ eV. That energy is much less than you could ever hope to observe physically. A single photon of light would dwarf it by 50 orders of magnitude.

3.5.6.3 Solution pipee-c

Question:

What is the eigenfunction number, or quantum number, n that produces a macroscopic amount of energy, 1 J, for macroscopic values $m = 1$ kg and $\ell_x = 1$ m? With that many energy levels involved, would you see the difference between successive ones?

Answer:

Putting the generic expression for the eigenvalues,

$$E_n = \frac{n^2 \hbar^2 \pi^2}{2m\ell_x^2}$$

equal to 1 J and plugging in the given numbers:

$$\frac{n^2 (1.05457 \cdot 10^{-34} \text{ J s})^2 \pi^2}{2 \cdot 1 \text{ kg} \cdot 1 \text{ m}^2} = 1 \text{ J}.$$

Solving for n , you get $n = 4.26864 \cdot 10^{33}$. Obviously, there is no way to distinguish that many energy levels. A calculator cannot even display all 34 digits of this number, even if you knew \hbar to enough digits accuracy to compute 34 digits.

3.5.7 Discussion of the eigenfunctions

3.5.7.1 Solution pipef-a

Question:

So how does, say, the one-dimensional eigenstate ψ_6 look?

Answer:

As the graph below shows, it has six blobs where the particle is likely to be found, separated by bands where there is vanishing likelihood of finding the particle.

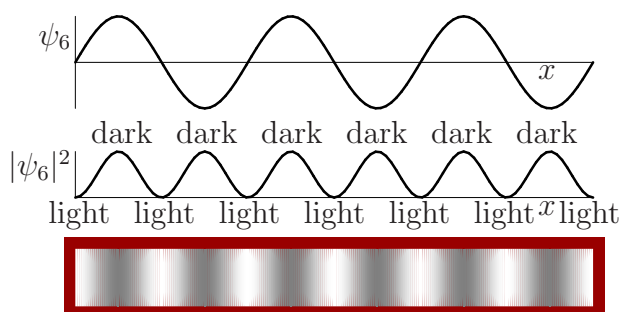


Figure 3.1: One-dimensional eigenstate ψ_6 .

3.5.7.2 Solution pipef-b

Question:

Generalizing the results above, for eigenfunction ψ_n , any n , how many distinct regions are there where the particle may be found?

Answer:

There are n of them.

3.5.7.3 Solution pipef-c

Question:

If you are up to a trick question, consider the following. There are no forces inside the pipe, so the particle has to keep moving until it hits an end of the pipe, then reflect backward until it hits the other side and so on. So, it has to cross the center of the pipe regularly. But in the energy eigenstate ψ_2 , the particle has *zero* chance of ever being found at the center of the pipe. What gives?

Answer:

Almost every word in the above story is a gross misstatement of what nature really is like when examined on quantum scales. A particle *does not have* a position, so phrases like “hits an end”, “reflect backward”, and “keep moving” are truly meaningless. On macroscopic scales a particle may have an relatively precisely defined position, but that is only because there is uncertainty in energy. If you could bring a macroscopic particle truly into a single energy eigenstate, it too would have no position. And the smallest thing you might do to figure out where it is would kick it out of that single energy state.

3.5.8 Three-dimensional solution

3.5.8.1 Solution pipeg-a

Question:

If the cross section dimensions ℓ_y and ℓ_z are one tenth the size of the pipe length, how much bigger are the energies E_{y1} and E_{z1} compared to E_{x1} ? So, by what percentage is the one-dimensional ground state energy E_{x1} as an approximation to the three-dimensional one, E_{111} , then in error?

Answer:

The energies are

$$E_{x1} = \frac{\hbar^2 \pi^2}{2m\ell_x^2} \quad E_{y1} = \frac{\hbar^2 \pi^2}{2m\ell_y^2} \quad E_{z1} = \frac{\hbar^2 \pi^2}{2m\ell_z^2}.$$

If ℓ_y and ℓ_z are ten times smaller than ℓ_x then E_{y1} and E_{z1} are each 100 times larger than E_{x1} . So the one-dimensional ground state energy E_{x1} is smaller than the true ground state energy $E_{111} = E_{x1} + E_{y1} + E_{z1}$ by a factor 201. Which means it is off by 20 000%.

3.5.8.2 Solution pipeg-b

Question:

At what ratio of ℓ_y/ℓ_x does the energy E_{121} become higher than the energy E_{311} ?

Answer:

Using the given expression for $E_{n_x n_y n_z}$,

$$E_{n_x n_y n_z} = \frac{n_x^2 \hbar^2 \pi^2}{2m\ell_x^2} + \frac{n_y^2 \hbar^2 \pi^2}{2m\ell_y^2} + \frac{n_z^2 \hbar^2 \pi^2}{2m\ell_z^2},$$

$E_{121} = E_{311}$ when

$$\frac{\hbar^2 \pi^2}{2m\ell_x^2} + \frac{4\hbar^2 \pi^2}{2m\ell_y^2} + \frac{\hbar^2 \pi^2}{2m\ell_z^2} = \frac{9\hbar^2 \pi^2}{2m\ell_x^2} + \frac{\hbar^2 \pi^2}{2m\ell_y^2} + \frac{\hbar^2 \pi^2}{2m\ell_z^2}$$

Canceling the terms that both sides have in common:

$$\frac{3\hbar^2 \pi^2}{2m\ell_y^2} = \frac{8\hbar^2 \pi^2}{2m\ell_x^2}$$

and canceling the common factors and rearranging:

$$\frac{\ell_y^2}{\ell_x^2} = \frac{3}{8}.$$

So when $\ell_y/\ell_x = \sqrt{3/8} = 0.61$ or more, the third lowest energy state is given by E_{121} rather than E_{311} . Obviously, it will look more like a box than a pipe then, with the y -dimension 61% of the x -dimension.

3.5.8.3 Solution pipeg-c

Question:

Shade the regions where the particle is likely to be found in the ψ_{322} energy eigenstate.

Answer:

The wave function is

$$\psi_{322} = \sqrt{\frac{8}{\ell_x \ell_y \ell_z}} \sin\left(\frac{3\pi}{\ell_x}x\right) \sin\left(\frac{2\pi}{\ell_y}y\right) \sin\left(\frac{2\pi}{\ell_z}z\right)$$

Now the trick is to realize that the wave function is zero when any of the three sines is zero. Looking along the z -direction, you will see an array of 3 times 2 blobs, or 6 blobs:

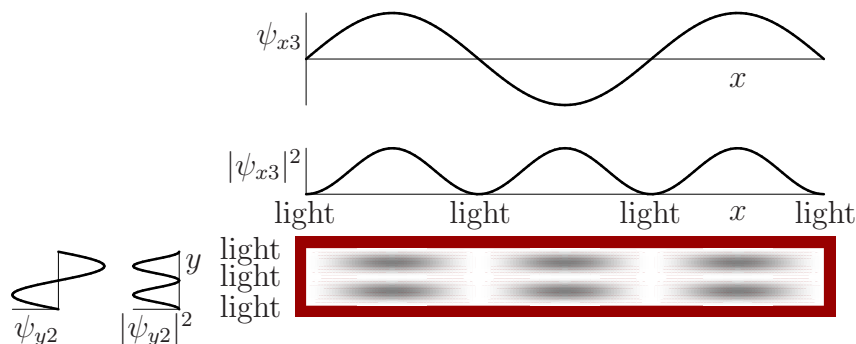


Figure 3.2: Eigenstate ψ_{322} .

The white horizontal centerline line along the pipe corresponds to $\sin(2\pi y/\ell_y)$ being zero at $y = \frac{1}{2}\ell_y$, and the two white vertical white lines correspond to $\sin(3\pi x/\ell_x)$ being zero at $x = \frac{1}{3}\ell_x$ and $x = \frac{2}{3}\ell_x$. The $\sin(2\pi z/\ell_z)$ factor in the wave function will split it further into six blobs front and 6 blobs rear, but that is not visible when looking along the z -direction; the front blobs cover the rear ones. Seen from the top, you would again see an array of 3 times 2 blobs, the top blobs hiding the bottom ones.

3.5.9 Quantum confinement

Chapter 4

Single-Particle Systems

4.1 The Harmonic Oscillator

4.1.1 The Hamiltonian

4.1.2 Solution using separation of variables

4.1.2.1 Solution harmb-a

Question:

Write out the ground state energy.

Answer:

| | |
|---|--|
| $h_0(x) = \frac{1}{(\pi\ell^2)^{1/4}} e^{-\xi^2/2}$ | $\omega = \sqrt{\frac{c}{m}}$ $\ell = \sqrt{\frac{\hbar}{m\omega}}$ $\xi = \frac{x}{\ell}$ |
| $h_1(x) = \frac{2\xi}{(4\pi\ell^2)^{1/4}} e^{-\xi^2/2}$ | |
| $h_2(x) = \frac{2\xi^2 - 1}{(4\pi\ell^2)^{1/4}} e^{-\xi^2/2}$ | |
| $h_3(x) = \frac{2\xi^3 - 3\xi}{(9\pi\ell^2)^{1/4}} e^{-\xi^2/2}$ | |
| $h_4(x) = \frac{4\xi^4 - 12\xi^2 + 3}{(576\pi\ell^2)^{1/4}} e^{-\xi^2/2}$ | |

Table 4.1: First few one-dimensional eigenfunctions of the harmonic oscillator.

Taking the generic expression

$$E_{n_x n_y n_z} = \frac{2n_x + 2n_y + 2n_z + 3}{2} \hbar\omega$$

and substituting the lowest possible value, 0, for each of n_x , n_y , and n_z , you get the ground state energy

$$E_{000} = \frac{3}{2} \hbar\omega$$

4.1.2.2 Solution harmb-b

Question:

Write out the ground state wave function fully.

Answer:

Taking the generic expression

$$\psi_{n_x n_y n_z} = h_{n_x}(x)h_{n_y}(y)h_{n_z}(z)$$

and substituting $n_x = n_y = n_z = 0$, you get the ground state eigenfunction

$$\psi_{000} = h_0(x)h_0(y)h_0(z).$$

Now substitute for h_0 from table 4.1:

$$\psi_{000} = \frac{1}{(\pi\ell^2)^{3/4}} e^{-x^2/2\ell^2} e^{-y^2/2\ell^2} e^{-z^2/2\ell^2}$$

where the constant ℓ is as given in table 4.1. You can multiply out the exponentials:

$$\psi_{000} = \frac{1}{(\pi\ell^2)^{3/4}} e^{-(x^2+y^2+z^2)/2\ell^2}.$$

4.1.2.3 Solution harmb-c

Question:

Write out the energy E_{100} .

Answer:

Taking the generic expression

$$E_{n_x n_y n_z} = \frac{2n_x + 2n_y + 2n_z + 3}{2} \hbar\omega$$

and substituting $n_x = 1$, $n_y = n_z = 0$, you get

$$E_{100} = \frac{5}{2} \hbar\omega$$

4.1.2.4 Solution harmb-d

Question:

Write out the eigenstate ψ_{100} fully.

Answer:

Taking the generic expression

$$\psi_{n_x n_y n_z} = h_{n_x}(x)h_{n_y}(y)h_{n_z}(z)$$

and substituting $n_x = 1$, $n_y = n_z = 0$, you get

$$\psi_{100} = h_1(x)h_0(y)h_0(z).$$

Now substitute for h_0 and h_1 from table 4.1:

$$\psi_{100} = \frac{\sqrt{2}x/\ell}{(\pi\ell^2)^{3/4}} e^{-x^2/2\ell^2} e^{-y^2/2\ell^2} e^{-z^2/2\ell^2}$$

where the constant ℓ is as given in table 4.1. You can multiply out the exponentials:

$$\psi_{100} = \frac{\sqrt{2}x/\ell}{(\pi\ell^2)^{3/4}} e^{-(x^2+y^2+z^2)/2\ell^2}.$$

4.1.3 Discussion of the eigenvalues

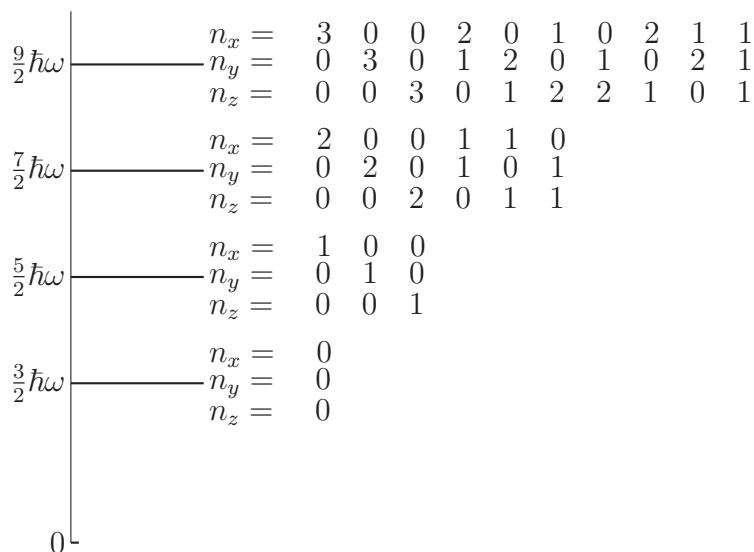


Figure 4.1: The energy spectrum of the harmonic oscillator.

4.1.3.1 Solution harmc-a

Question:

Verify that the sets of quantum numbers shown in the spectrum figure 4.1 do indeed produce the indicated energy levels.

Answer:

The generic expression for the energy is

$$E_{n_x n_y n_z} = \frac{2n_x + 2n_y + 2n_z + 3}{2} \hbar\omega$$

or defining $N = n_x + n_y + n_z$,

$$E_{n_x n_y n_z} = \frac{2N + 3}{2} \hbar\omega$$

Now for the bottom level, $n_x = n_y = n_z = 0$, so $N = n_x + n_y + n_z = 0$, this state has energy $\frac{3}{2}\hbar\omega$.

Similarly, in each of the three sets of the second energy level in figure 4.1, the three quantum numbers n_x , n_y , and n_z add up to $N = 1$, giving this state energy $\frac{5}{2}\hbar\omega$.

For the third energy level, the three quantum numbers of each set add up to $N = 2$, giving energy $\frac{7}{2}\hbar\omega$, and for the fourth set, the quantum numbers in each of the ten sets add up to $N = 3$ for an energy $\frac{9}{2}\hbar\omega$.

4.1.3.2 Solution harmc-b

Question:

Verify that there are no sets of quantum numbers missing in the spectrum figure 4.1; the listed ones are the only ones that produce those energy levels.

Answer:

The generic expression for the energy is

$$E_{n_x n_y n_z} = \frac{2n_x + 2n_y + 2n_z + 3}{2} \hbar\omega$$

or defining $N = n_x + n_y + n_z$,

$$E_{n_x n_y n_z} = \frac{2N + 3}{2} \hbar\omega$$

Now for the bottom level, $N = 0$, and since the three quantum numbers n_x , n_y , and n_z cannot be negative, the only way that $N = n_x + n_y + n_z$ can be zero is if all three numbers are zero. If any one of n_x , n_y , or n_z would be positive, then so would be N . So there is only one state $n_x = n_y = n_z = 0$.

For the second energy level, $N = 1$. To get a nonzero sum N , you must have one of n_x , n_y , and n_z to be nonzero, but not more than 1, or N would be more than 1 too. Also, if one of n_x , n_y , and n_z is 1, then the other two must be 0 or their sum N would still be greater than 1. That means that precisely one of n_x , n_y , and n_z must be 1 and the other two 0. There are three possibilities for the one that is 1, n_x , n_y , or n_z , resulting in the three different sets of quantum numbers shown in the spectrum figure 4.1.

For the third energy level, $N = 2$, the maximum value any one of n_x , n_y , and n_z could possibly have is 2, but then the other two must be zero. That leads to the first three sets of quantum numbers shown in the spectrum. If the maximum value among n_x , n_y , and n_z is not 2 but 1, then a second one must also be 1, or they would not add up to 2. So in this case you have two of them 1 and the third 0. There are three possibilities for the one that is 0, producing the last three sets of quantum numbers shown in the spectrum 4.1 at this energy level.

For the fourth energy level, $N = 3$, the maximum value value that any one of n_x , n_y , and n_z could have is 3, with the other two 0, producing the first three sets of quantum numbers. If the maximum value is 2, then the other two quantum numbers must add up to 1, which means one of them is 1 and the other 0. There are three possibilities for which quantum number is 2, and for each of these there are two possibilities for which of the other two is 1. That produces the next six sets of quantum numbers. Finally, if the maximum value is 1, then both other numbers will have to be 1 too to add up to $N = 3$. That gives the tenth set.

A less intuitive, but more general, procedure is to simply derive the number of different eigenstates S for a given N mathematically and show that it agrees with the figure: The possible values that the quantum number n_x can have in order for $n_x + n_y + n_z$ not to exceed N are in the range from 0 to N , and for each such value of n_x , n_y must be in the range from 0 to $N - n_x$ for $n_x + n_y + n_z$ no to exceed N . For each such acceptable pair of values n_x and n_y , there is exactly one allowed value $n_z = N - n_x - n_y$. So there is exactly one state for each acceptable pair of values n_x and n_y . Which means that the number of states is, using summation symbols,

$$S = \sum_{n_x=0}^N \left(\sum_{n_y=0}^{N-n_x} 1 \right)$$

The sum within the parentheses is $(N - n_x + 1) \times 1$, and then the remaining sum is an arithmetic series [1, 21.1], producing

$$S = (N + 1)(N + 2)/2.$$

Substituting in $N = 0$, you get $S = 1$, a single state, for $N = 1$, $S = 3$, three states, for $N = 2$ six states and for $N = 3$ ten states. So the spectrum 4.1 shows all states.

4.1.4 Discussion of the eigenfunctions

4.1.4.1 Solution harmd-a

Question:

Write out the ground state wave function and show that it is indeed spherically symmetric.

Answer:

Repeating an earlier exercise, taking the generic expression

$$\psi_{n_x n_y n_z} = h_{n_x}(x)h_{n_y}(y)h_{n_z}(z)$$

and substituting $n_x = n_y = n_z = 0$, you get the ground state eigenfunction

$$\psi_{000} = h_0(x)h_0(y)h_0(z).$$

Now substitute for h_0 from table 4.1:

$$\psi_{000} = \frac{1}{(\pi\ell^2)^{3/4}} e^{-x^2/2\ell^2} e^{-y^2/2\ell^2} e^{-z^2/2\ell^2}$$

where the constant ℓ is as given in table 4.1. You can multiply out the exponentials:

$$\psi_{000} = \frac{1}{(\pi\ell^2)^{3/4}} e^{-(x^2+y^2+z^2)/2\ell^2}.$$

According to the Pythagorean theorem, $\sqrt{x^2 + y^2 + z^2}$ is the distance from the origin r , so

$$\psi_{000} = \frac{1}{(\pi\ell^2)^{3/4}} e^{-r^2/2\ell^2}.$$

It follows that the wave function only depends on the *distance* r from the origin, not on the angular orientation compared to it. That is the definition of spherically symmetric: it looks the same from any angle.

4.1.4.2 Solution harmd-b

Question:

Show that the ground state wave function is maximal at the origin and, like all the other energy eigenfunctions, becomes zero at large distances from the origin.

Answer:

According to the answer to the previous question, the ground state is

$$\psi_{000} = \frac{1}{(\pi\ell^2)^{3/4}} e^{-r^2/2\ell^2}.$$

where r is the distance from the origin. Now according to the qualitative properties of exponentials, an exponential is one when its argument is zero, and becomes less than one when its argument becomes negative. So the maximum is at the origin $r = 0$.

The other eigenfunctions do not necessarily have their maximum magnitude at the origin: for example, the shown states ψ_{100} and ψ_{010} are zero at the origin.

For large negative values of its argument, an exponential becomes very small very quickly. So if the distance from the origin is large compared to ℓ , the wave function will be negligible, and it will be zero in the limit of infinite distance.

For example, if the distance from the origin is just 10 times ℓ , the exponential above is already as small as 0.000 000 000 002 which is clearly negligible.

As far as the value of the other eigenfunctions at large distance from the origin is concerned, note from table 4.1 that all eigenfunctions take the generic form

$$\psi_{n_x n_y n_z} = \frac{\text{polynomial in } x}{e^{x^2/2\ell^2}} \frac{\text{polynomial in } y}{e^{y^2/2\ell^2}} \frac{\text{polynomial in } z}{e^{z^2/2\ell^2}}.$$

For the distance from the origin to become large, at least one of x , y , or z must become large, and then the blow up of the corresponding exponential in the bottom makes the eigenfunctions become zero. (Whatever the polynomials in the top do is irrelevant, since an exponential includes, according to its Taylor series, always powers higher than can be found in any given polynomial, hence is much larger than any given polynomial at large values of its argument.)

It may be noted that the eigenfunctions do extend farther from the nominal position when the energy increases. The polynomials get nastier when the energy increases, but far enough away they must eventually always lose from the exponentials.

4.1.4.3 Solution harmd-c

Question:

Write down the explicit expression for the eigenstate ψ_{213} using table 4.1, then verify that it looks like figure 4.2 when looking along the z -axis, with the x -axis horizontal and the y -axis vertical.

Answer:

The generic expression for the eigenfunctions is

$$\psi_{n_x n_y n_z} = h_{n_x}(x)h_{n_y}(y)h_{n_z}(z)$$

and substituting $n_x = 2$, $n_y = 1$ and $n_z = 3$, you get

$$\psi_{213} = h_2(x)h_1(y)h_3(z).$$

Now substitute for those functions from table 4.1:

$$\psi_{213} = \frac{[2(x/\ell)^2 - 1][2y/\ell][2(z/\ell)^3 - 3(z/\ell)]}{2\sqrt{3}(\pi\ell^2)^{3/4}} e^{-x^2/2\ell^2} e^{-y^2/2\ell^2} e^{-z^2/2\ell^2}$$

where the constant ℓ is as given in table 4.1.

The first polynomial within square brackets in the expression above is zero at $x = \ell/\sqrt{2}$ and $x = -\ell/\sqrt{2}$, producing the two vertical white lines along which there is zero probability of finding the particle. Similarly, the second polynomial within square brackets is zero at $y = 0$, producing the horizontal white line. Hence looking along the z -direction, you see the distribution:

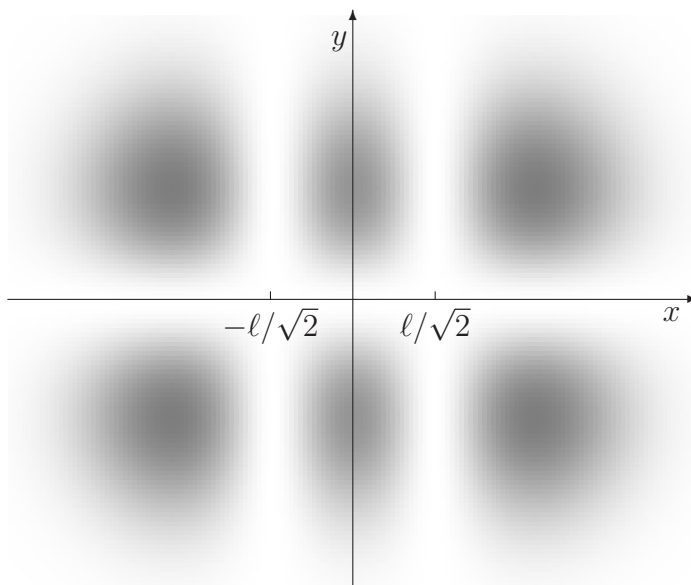


Figure 4.2: Energy eigenfunction ψ_{213} .

Seen from above, you would see four rows of three patches, as the third polynomial between brackets produces zero probability of finding the particle at $z = -\sqrt{3}/2\ell$, $z = 0$, and $z = \sqrt{3}/2\ell$, splitting the distribution into four in the z -direction.

This example illustrates that there is one more set of patches in a given direction each time the corresponding quantum number increases by one unit.

4.1.5 Degeneracy

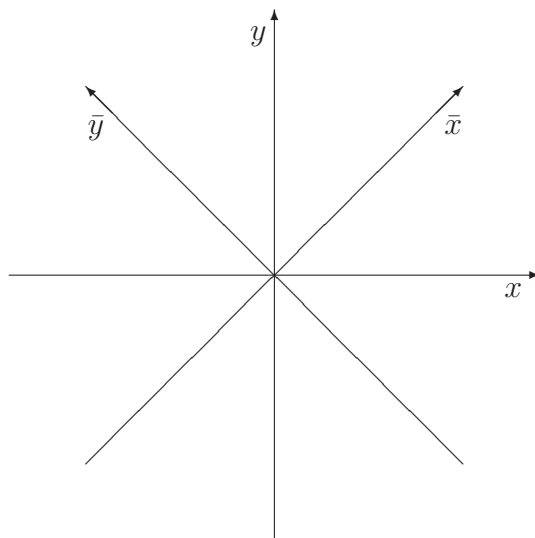
4.1.5.1 Solution harme-a

Question:

Just to check that this book is not lying, (you cannot be too careful), write down the analytical expression for ψ_{100} and ψ_{010} using table 4.1. Next write down $(\psi_{100} + \psi_{010})/\sqrt{2}$ and $(\psi_{010} - \psi_{100})/\sqrt{2}$. Verify that the latter two are the functions ψ_{100} and ψ_{010} in a coordinate system (\bar{x}, \bar{y}, z) that is rotated 45 degrees counter-clockwise around the z -axis compared to the original (x, y, z) coordinate system.

Answer:

Take the rotated coordinates to be \bar{x} and \bar{y} as shown:



A vector displacement of magnitude x in the x -direction has a component along the \bar{x} -axis of magnitude $x \cos 45^\circ$, equivalent to $x/\sqrt{2}$. Similarly, a vector displacement of magnitude y in the y -direction has a component along the \bar{x} -axis of magnitude $y \cos 45^\circ$, equivalent to $y/\sqrt{2}$. So in general, for any point (x, y) ,

$$\bar{x} = \frac{x + y}{\sqrt{2}}.$$

Similarly you get

$$\bar{y} = \frac{y - x}{\sqrt{2}}.$$

Turning now to the eigenfunctions, taking the generic expression

$$\psi_{n_x n_y n_z} = h_{n_x}(x)h_{n_y}(y)h_{n_z}(z)$$

and substituting $n_x = 1$, $n_y = n_z = 0$, you get

$$\psi_{100} = h_1(x)h_0(y)h_0(z).$$

Now substitute for h_0 and h_1 from table 4.1:

$$\psi_{100} = \frac{\sqrt{2}x/\ell}{(\pi\ell^2)^{3/4}} e^{-x^2/2\ell^2} e^{-y^2/2\ell^2} e^{-z^2/2\ell^2}$$

where the constant ℓ is as given in table 4.1. You can multiply out the exponentials:

$$\psi_{100} = \frac{\sqrt{2}x/\ell}{(\pi\ell^2)^{3/4}} e^{-(x^2+y^2+z^2)/2\ell^2}.$$

The same way, you get

$$\psi_{010} = \frac{\sqrt{2}y/\ell}{(\pi\ell^2)^{3/4}} e^{-(x^2+y^2+z^2)/2\ell^2}.$$

So, the combination $(\psi_{100} + \psi_{010})/\sqrt{2}$ is

$$\frac{\psi_{100} + \psi_{010}}{\sqrt{2}} = \frac{(x+y)/\ell}{(\pi\ell^2)^{3/4}} e^{-(x^2+y^2+z^2)/2\ell^2}.$$

Now $x^2 + y^2 + z^2$ is according to the Pythagorean theorem the square distance from the origin, which is the same as $\bar{x}^2 + \bar{y}^2 + z^2$. And since $\bar{x} = (x+y)/\sqrt{2}$, the sum $x+y$ in the combination eigenfunction above is $\sqrt{2}\bar{x}$. So the combination eigenfunction is

$$\frac{\psi_{100} + \psi_{010}}{\sqrt{2}} = \frac{\sqrt{2}\bar{x}/\ell}{(\pi\ell^2)^{3/4}} e^{-(\bar{x}^2 + \bar{y}^2 + z^2)/2\ell^2}.$$

which is exactly the same as ψ_{100} above, except in terms of \bar{x} and \bar{y} . So it is ψ_{100} in the rotated frame.

The other combination goes the same way.

4.1.6 Noneigenstates

4.2 Angular Momentum

4.2.1 Definition of angular momentum

4.2.2 Angular momentum in an arbitrary direction

4.2.2.1 Solution angub-a

Question:

If the angular momentum in a given direction is a multiple of $\hbar = 1.054\,57\,10^{-34}$ J s, then \hbar should have units of angular momentum. Verify that.

Answer:

Angular momentum is linear momentum, (mass times velocity,) times normal distance from the axis. So its units are kg (m/s) m. Conversely J s is N m s and N, a Newton, is kg m/s², so J s is kg m²/s, the same as the units of \hbar .

4.2.2.2 Solution angub-b

Question:

What is the magnetic quantum number of a macroscopic, 1 kg, particle that is encircling the z -axis at a distance of 1 m at a speed of 1 m/s? Write out as an integer, and show digits you are not sure about as a question mark.

Answer:

Showing all digits as a question mark is not acceptable, of course.

The classical angular momentum is 1 m distance times 1 kg times 1 m/s, or 1 J s. Since that should be $m\hbar$ with m the magnetic quantum number, you get

$$m = \frac{1 \text{ J s}}{1.05457 \cdot 10^{-34} \text{ J s}} = 9482371 \dots$$

4.2.2.3 Solution angub-c

Question:

Actually, based on the derived eigenfunction, $C(r, \theta)e^{im\phi}$, would any macroscopic particle ever be at a single magnetic quantum number in the first place? In particular, what can you say about where the particle can be found in an eigenstate?

Answer:

The square magnitude of the wave function gives the probability of finding the particle. The square magnitude,

$$|C(r, \theta)e^{im\phi}|^2 = |C(r, \theta)|^2,$$

is independent of ϕ . So to be in a state of definite angular momentum, the particle must be at all sides of the axis with equal probability. A macroscopic particle will at any given time be at a single angle compared to the axis, not at all angles at once. So, a macroscopic particle will have indeterminacy in angular momentum, just like it has indeterminacy in position, linear momentum, energy, etcetera.

Since the probability distribution of an eigenstate is independent of ϕ , it is called “axisymmetric around the z -axis”. Note that the wave function itself is only axisymmetric if $m = 0$, in other words, if the angular momentum in the z -direction is zero. Eigenstates with different angular momentum look the same if you just look at the probability distribution.

4.2.3 Square angular momentum

4.2.3.1 Solution anguc-a

Question:

The general wave function of a state with azimuthal quantum number l and magnetic quantum number m is $\Psi = R(r)Y_l^m(\theta, \phi)$, where $R(r)$ is some further arbitrary function of r .

Show that the condition for this wave function to be normalized, so that the total probability of finding the particle integrated over all possible positions is one, is that

$$\int_{r=0}^{\infty} R(r)^* R(r) r^2 dr = 1.$$

Answer:

You need to have $\langle \Psi | \Psi \rangle = \int \Psi^* \Psi d^3\vec{r} = 1$ for the wave function to be normalized. Now the volume element $d^3\vec{r}$ is in spherical coordinates given by $r^2 \sin \theta dr d\theta d\phi$, so you must have

$$\int_{r=0}^{\infty} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} R(r)^* Y_l^m(\theta, \phi)^* R(r) Y_l^m(\theta, \phi) r^2 \sin \theta dr d\theta d\phi = 1.$$

Taking this apart into two separate integrals:

$$\int_{r=0}^{\infty} R(r)^* R(r) r^2 dr \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} Y_l^m(\theta, \phi)^* Y_l^m(\theta, \phi) \sin \theta d\theta d\phi = 1.$$

The second integral is one on account of the normalization of the spherical harmonics, so you must have

$$\int_{r=0}^{\infty} R(r)^* R(r) r^2 dr = 1.$$

4.2.3.2 Solution anguc-b

Question:

Can you invert the statement about zero angular momentum and say: if a particle can be found at all angular positions compared to the origin with equal probability, it will have zero angular momentum?

Answer:

No. To be at zero angular momentum, not just the probability $|\Psi|^2$, but Ψ itself must be independent of the spherical coordinate angles θ and ϕ . As an arbitrary example, $\Psi = R(r)e^{i\phi \sin \theta}$ would have a probability of finding the particle independent of θ and ϕ , but not zero angular momentum.

4.2.3.3 Solution anguc-c

Question:

What is the minimum amount that the total square angular momentum is larger than just the square angular momentum in the z -direction for a given value of l ?

Answer:

The total square angular momentum is $l(l+1)\hbar^2$ and the square angular z -momentum is $m^2\hbar^2$. Since for a given value of l , the largest that $|m|$ can be is l , the difference is at least

$$l(l+1)\hbar^2 - l^2\hbar^2 = l\hbar^2.$$

4.2.4 Angular momentum uncertainty

4.3 The Hydrogen Atom

4.3.1 The Hamiltonian

4.3.2 Solution using separation of variables

4.3.2.1 Solution hydb-a

Question:

Use the tables for the radial wave functions and the spherical harmonics to write down the wave function

$$\psi_{nlm} = R_{nl}(r)Y_l^m(\theta, \phi)$$

for the case of the ground state ψ_{100} .

Check that the state is normalized. Note: $\int_0^\infty e^{-2u}u^2 du = \frac{1}{4}$.

Answer:

The tables show that $R_{10} = 2e^{-r/a_0}/\sqrt{a_0^3}$ and that $Y_0^0 = 1/\sqrt{4\pi}$, so

$$\psi_{100} = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

The total probability of finding the particle integrated over all possible positions is, using the techniques of volume integration in spherical coordinates:

$$\int |\psi_{100}|^2 d^3\vec{r} = \int_{r=0}^\infty \int_{\theta=0}^\pi \int_{\phi=0}^{2\pi} \frac{1}{\pi a_0^3} e^{-2r/a_0} r^2 \sin \theta dr d\theta d\phi$$

or rearranging

$$\frac{1}{\pi} \int_{r/a_0=0}^\infty e^{-2r/a_0} \frac{r^2}{a_0^2} d\frac{r}{a_0} \int_{\theta=0}^\pi \sin \theta d\theta \int_{\phi=0}^{2\pi} 1 d\phi$$

giving

$$\frac{1}{\pi} \times \frac{1}{4} \times 2 \times 2\pi$$

which is one as required.

4.3.2.2 Solution hydb-b

Question:

Use the generic expression

$$\psi_{nlm} = -\frac{2}{n^2} \sqrt{\frac{(n-l-1)!}{[(n+l)!a_0]^3}} \left(\frac{2\rho}{n}\right)^l L_{n+l}^{2l+1} \left(\frac{2\rho}{n}\right) e^{-\rho/n} Y_l^m(\theta, \phi)$$

with $\rho = r/a_0$ and Y_l^m from the spherical harmonics table to find the ground state wave function ψ_{100} . Note: the Laguerre polynomial $L_1(x) = 1 - x$ and for any p , L_1^p is just its p -th derivative.

Answer:

You get, substituting $n = 1$, $l = 0$, $m = 0$:

$$\psi_{100} = -\frac{2}{1^2} \sqrt{\frac{0!}{[1!a_0]^3}} \left(\frac{2\rho}{1}\right)^0 L_1^1 \left(\frac{2\rho}{1}\right) e^{-\rho/1} Y_0^0(\theta, \phi)$$

where $0! = 1! = 1$, $L_1^1(x)$ is the first derivative of $L_1(x) = 1 - x$ with respect to x , which is -1 , and $Y_0^0 = 1/\sqrt{4\pi}$ according to the table. So you get

$$\psi_{100} = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}.$$

as in the previous question.

4.3.2.3 Solution hydb-c

Question:

Plug numbers into the generic expression for the energy eigenvalues,

$$E_n = -\frac{\hbar^2}{2m_e a_0^2} \frac{1}{n^2},$$

where $a_0 = 4\pi\epsilon_0\hbar^2/m_e e^2$, to find the ground state energy. Express in eV, where 1 eV equals $1.6022 \cdot 10^{-19}$ J. Values for the physical constants can be found at the start of this section and in the notations section.

Answer:

First verify the Bohr radius

$$a_0 = \frac{4\pi \cdot 8.854 \cdot 10^{-12} \text{ C}^2/\text{J m} \cdot (1.0546 \cdot 10^{-34} \text{ J s})^2}{9.109 \cdot 10^{-31} \text{ kg} \cdot (1.6022 \cdot 10^{-19} \text{ C})^2} = 0.5292 \cdot 10^{-10} \text{ m}$$

Next, taking $n = 1$ for the ground state,

$$E_1 = -\frac{(1.0546 \cdot 10^{-34} \text{ J s})^2}{2 \cdot 9.109 \cdot 10^{-31} \text{ kg} \cdot (0.5292 \cdot 10^{-10} \text{ m})^2} \frac{1}{1^2} = -2.1799 \cdot 10^{-18} \text{ J} \frac{1 \text{ eV}}{1.6022 \cdot 10^{-19} \text{ J}}$$

which gives $E_1 = -13.61 \text{ eV}$

4.3.3 Discussion of the eigenvalues

4.3.3.1 Solution hydc-a

Question:

If there are infinitely many energy levels $E_1, E_2, E_3, E_4, E_5, E_6, \dots$, where did they all go in the energy spectrum?

Answer:

The E_n for large values of n are all graphically indistinguishable from zero energy. The electron is almost free from the nucleus in those energy states.

4.3.3.2 Solution hydc-b

Question:

What is the value of energy level E_2 ? And E_3 ?

Answer:

No need to put all the numbers into

$$E_n = -\frac{\hbar^2}{2m_e a_0^2} \frac{1}{n^2}$$

because the only difference between E_2 and E_1 is just a final factor $\frac{1}{4}$. So $E_2 = \frac{1}{4}E_1 = -3.4$ eV. Similarly, $E_3 = \frac{1}{9}E_1 = -1.51$ eV.

4.3.3.3 Solution hydc-c

Question:

Based on the results of the previous question, what is the color of the light emitted in a Balmer transition from energy E_3 to E_2 ? The Planck-Einstein relation says that the angular frequency ω of the emitted photon is its energy divided by \hbar , and the wave length of light is $2\pi c/\omega$ where c is the speed of light. Typical wave lengths of visible light are: violet 400 nm, indigo 445 nm, blue 475 nm, green 510 nm, yellow 570 nm, orange 590 nm, red 650 nm.

Answer:

The energy carried away by the photon is the energy lost by the electron, which is

$$E_3 - E_2 = -1.51 \text{ eV} + 3.4 \text{ eV} = 1.89 \text{ eV} \frac{1.602 \cdot 10^{-19} \text{ J}}{1 \text{ eV}} = 3.026 \cdot 10^{-19} \text{ J}$$

Dividing by $\hbar = 1.054 \cdot 10^{-34} \text{ J s}$ gives the angular frequency to be $2.87 \cdot 10^{15}/\text{s}$, and then the wave length is 656 nm, using $c = 3 \cdot 10^8 \text{ m/s}$. That will be red light.

4.3.3.4 Solution hyd-c-d

Question:

What is the color of the light emitted in a Balmer transition from an energy level E_n with a high value of n to E_2 ?

Answer:

It is like the previous question, except E_n will be approximately zero at high values of n .

$$E_n - E_2 = 0 \text{ eV} + 3.4 \text{ eV} = 3.4 \text{ eV} \frac{1.602 \cdot 10^{-19} \text{ J}}{1 \text{ eV}} = 5.45 \cdot 10^{-19} \text{ J}$$

Dividing by $\hbar = 1.054 \cdot 10^{-34} \text{ J s}$ gives the angular frequency to be $5.17 \cdot 10^{15} / \text{s}$, and then the wave length is 364 nm. That will be near ultraviolet. The transition from E_4 will produce blue-green light, from E_5 indigo, and from E_6 violet.

4.3.4 Discussion of the eigenfunctions

4.3.4.1 Solution hydd-a

Question:

At what distance r from the nucleus does the square of the ground state wave function become less than one percent of its value at the nucleus? Express it both as a multiple of the Bohr radius a_0 and in Å.

Answer:

The square wave function is

$$|\psi_{100}(r)|^2 = \frac{1}{\pi a_0^3} e^{-2r/a_0}$$

and the value at the nucleus $r = 0$ is then

$$|\psi_{100}(0)|^2 = \frac{1}{\pi a_0^3}$$

For the value at r above to be one percent of this, you must have

$$e^{-2r/a_0} = 0.01$$

or taking logarithm, $r = 2.3 a_0$. Expressed in Å, $a_0 = 0.53 \text{ Å}$, so $r = 1.22 \text{ Å}$.

4.3.4.2 Solution hydd-b

Question:

Check from the conditions

$$n > l \geq |m|$$

that ψ_{200} , ψ_{211} , ψ_{210} , and ψ_{21-1} are the only states of the form ψ_{nlm} that have energy E_2 . (Of course, all their combinations, like $2p_x$ and $2p_y$, have energy E_2 too, but they are not simply of the form ψ_{nlm} , but combinations of the “basic” solutions ψ_{200} , ψ_{211} , ψ_{210} , and ψ_{21-1} .)

Answer:

Since the energy is given to be $E_n = E_2$, you have $n = 2$. The azimuthal quantum number l must be a smaller nonnegative integer, so it can only be 0 or 1. In case $l = 0$, the absolute value of the magnetic quantum number m cannot be more than zero, allowing only $m = 0$. That is the ψ_{200} state. In the case that $l = 1$, the absolute value of m can be up to one, allowing $m = 1, 0$, and -1 .

4.3.4.3 Solution hydd-c

Question:

Check that the states

$$2p_x = \frac{1}{\sqrt{2}}(-\psi_{211} + \psi_{21-1}) \quad 2p_y = \frac{i}{\sqrt{2}}(\psi_{211} + \psi_{21-1})$$

are properly normalized.

Answer:

Find the square norm:

$$\langle 2p_x | 2p_x \rangle = \frac{1}{2} \langle -\psi_{211} + \psi_{21-1} | -\psi_{211} + \psi_{21-1} \rangle$$

or multiplying out

$$\langle 2p_x | 2p_x \rangle = \frac{1}{2} (\langle \psi_{211} | \psi_{211} \rangle + \langle -\psi_{211} | \psi_{21-1} \rangle + \langle \psi_{21-1} | -\psi_{211} \rangle + \langle \psi_{21-1} | \psi_{21-1} \rangle)$$

or using the orthonormality of ψ_{211} and ψ_{21-1} .

$$\langle 2p_x | 2p_x \rangle = \frac{1}{2} (1 + 0 + 0 + 1) = 1.$$

For the state $2p_y$, remember that i comes out of the left side of the inner product as $-i$:

$$\langle 2p_y | 2p_y \rangle = \frac{-i^2}{2} \langle \psi_{211} + \psi_{21-1} | \psi_{211} + \psi_{21-1} \rangle$$

The rest goes the same way.

4.4 Expectation Value and Standard Deviation

4.4.1 Statistics of a die

4.4.1.1 Solution esda-a

Question:

Suppose you toss a coin a large number of times, and count heads as one, tails as two. What will be the expectation value?

Answer:

For a fair coin, the probability of heads or tails is the same; each will have a probability of 50% or $\frac{1}{2}$. So the expectation value is $\frac{1}{2} \times 1 + \frac{1}{2} \times 2 = 1.5$. This will be the average value you obtain in a large number of throws.

4.4.1.2 Solution esda-b

Question:

Continuing this example, what will be the maximum deviation?

Answer:

If you throw a 1, the deviation is $|1 - 1.5|$ or 0.5. If you throw a 2, the deviation is $|2 - 1.5|$, also 0.5. So the maximum deviation is 0.5.

4.4.1.3 Solution esda-c

Question:

Continuing this example, what will be the standard deviation?

Answer:

The average square deviation from 1.5 is:

$$\frac{1}{2}(1 - 1.5)^2 + \frac{1}{2}(2 - 1.5)^2 = \frac{1}{4}$$

Taking a square root, the standard deviation is 0.5. In this case the standard deviation is the same as the maximum deviation, since the deviation from 1.5 is always 0.5 regardless what you throw.

4.4.1.4 Solution esda-d

Question:

Have I got a die for you! By means of a small piece of lead integrated into its light-weight structure, it does away with that old-fashioned uncertainty. It comes up six every time! What will be the expectation value of your throws? What will be the standard deviation?

Answer:

The expectation value will, of course, be 6, every throw is a 6;

$$0 \cdot 1 + 0 \cdot 2 + 0 \cdot 3 + 0 \cdot 4 + 0 \cdot 5 + 1 \cdot 6 = 6,$$

and the standard deviation will, of course, be zero, no throw will deviate from the value 6;

$$\begin{aligned} \sigma &= [0(1 - 6)^2 + 0(2 - 6)^2 + 0(3 - 6)^2 + \\ &\quad 0(4 - 6)^2 + 0(5 - 6)^2 + 1(6 - 6)^2]^{1/2} \\ &= 0 \end{aligned}$$

4.4.2 Statistics of quantum operators

4.4.2.1 Solution esdb-a

Question:

The $2p_x$ pointer state of the hydrogen atom was defined as

$$\frac{1}{\sqrt{2}}(-\psi_{211} + \psi_{21-1}).$$

What are the expectation values of energy, square angular momentum, and z angular momentum for this state?

Answer:

Note that the square coefficients of the eigenfunctions ψ_{211} and ψ_{21-1} are each $\frac{1}{2}$, so each has a probability $\frac{1}{2}$ in the $2p_x$ state.

Eigenfunction ψ_{211} has an energy eigenvalue E_2 , and so does ψ_{21-1} , so the expectation value of energy in the $2p_x$ state is

$$\langle E \rangle = \frac{1}{2}E_2 + \frac{1}{2}E_2 = E_2 = -3.4 \text{ eV}.$$

This is as expected since the only value that can be measured in this state is E_2 .

Similarly, eigenfunction ψ_{211} has a square angular momentum eigenvalue $2\hbar^2$, and so does ψ_{21-1} , so the expectation value of square angular momentum in the $2p_x$ state is that value,

$$\langle L^2 \rangle = \frac{1}{2}2\hbar^2 + \frac{1}{2}2\hbar^2 = 2\hbar^2.$$

Eigenfunction ψ_{211} has a z angular momentum eigenvalue \hbar , and ψ_{21-1} has $-\hbar$, so the expectation value of z angular momentum in the $2p_x$ state is

$$\langle L_z \rangle = \frac{1}{2}\hbar - \frac{1}{2}\hbar = 0$$

Measurements in which the z angular momentum is found to be \hbar average out against those where it is found to be $-\hbar$.

4.4.2.2 Solution esdb-b

Question:

Continuing the previous question, what are the standard deviations in energy, square angular momentum, and z angular momentum?

Answer:

Since the expectation value in energy is E_2 , as are the eigenvalues of each state, the standard deviation is zero.

$$\sigma_E = \sqrt{\frac{1}{2}(E_2 - E_2)^2 + \frac{1}{2}(E_2 - E_2)^2} = 0.$$

This is expected since every measurement produces E_2 ; there is no deviation from that value.

Similarly the standard deviation in L^2 is zero:

$$\sigma_{L^2} = \sqrt{\frac{1}{2}(2\hbar^2 - 2\hbar^2)^2 + \frac{1}{2}(2\hbar^2 - 2\hbar^2)^2} = 0.$$

For the z angular momentum, the expectation value is zero but the two states have eigenvalues \hbar and $-\hbar$, so

$$\sigma_{L_z} = \sqrt{\frac{1}{2}(\hbar - 0)^2 + \frac{1}{2}(-\hbar - 0)^2} = \hbar.$$

Whether \hbar or $-\hbar$ is measured, the deviation from zero has magnitude \hbar .

4.4.3 Simplified expressions

4.4.3.1 Solution esdb2-a

Question:

The $2p_x$ pointer state of the hydrogen atom was defined as

$$\frac{1}{\sqrt{2}}(-\psi_{211} + \psi_{21-1}).$$

where both ψ_{211} and ψ_{21-1} are eigenfunctions of the total energy Hamiltonian H with eigenvalue E_2 and of square angular momentum \hat{L}^2 with eigenvalue $2\hbar^2$; however, ψ_{211} is an eigenfunction of z angular momentum \hat{L}_z with eigenvalue \hbar , while ψ_{21-1} is one with eigenvalue $-\hbar$. Evaluate the expectation values of energy, square angular momentum, and z angular momentum in the $2p_x$ state using inner products. (Of course, since $2p_x$ is already written out in terms of the eigenfunctions, there is no simplification in this case.)

Answer:

For energy you have,

$$\langle E \rangle = \frac{1}{2} \langle -\psi_{211} + \psi_{21-1} | H | -\psi_{211} + \psi_{21-1} \rangle.$$

By the definition of eigenfunction, the products with H simplify:

$$\langle E \rangle = \frac{1}{2} \langle -\psi_{211} + \psi_{21-1} | -E_2\psi_{211} + E_2\psi_{21-1} \rangle.$$

Multiplying out further, while noting that on account of orthonormality of the eigenstates,

$$\langle \psi_{211} | \psi_{211} \rangle = \langle \psi_{21-1} | \psi_{21-1} \rangle = 1, \quad \langle \psi_{211} | \psi_{21-1} \rangle = \langle \psi_{21-1} | \psi_{211} \rangle = 0,$$

you get $\langle E \rangle = E_2$.

Similarly, for the square angular momentum,

$$\langle L^2 \rangle = \frac{1}{2} \langle -\psi_{211} + \psi_{21-1} | \widehat{L}^2 | -\psi_{211} + \psi_{21-1} \rangle.$$

or multiplying out

$$\langle L^2 \rangle = \frac{1}{2} \langle -\psi_{211} + \psi_{21-1} | -2\hbar^2\psi_{211} + 2\hbar^2\psi_{21-1} \rangle.$$

multiplying out further to $\langle L^2 \rangle = 2\hbar^2$.

For the z angular momentum,

$$\langle L_z \rangle = \frac{1}{2} \langle -\psi_{211} + \psi_{21-1} | \widehat{L}_z | -\psi_{211} + \psi_{21-1} \rangle.$$

or multiplying out

$$\langle L_z \rangle = \frac{1}{2} \langle -\psi_{211} + \psi_{21-1} | -\hbar\psi_{211} - \hbar\psi_{21-1} \rangle.$$

multiplying out further to $\langle L_z \rangle = 0$.

4.4.3.2 Solution esdb2-b

Question:

Continuing the previous question, evaluate the standard deviations in energy, square angular momentum, and z angular momentum in the $2p_x$ state using inner products.

Answer:

For energy you have,

$$\sigma_E^2 = \langle (H - E_2)^2 \rangle = \frac{1}{2} \langle -\psi_{211} + \psi_{21-1} | (H - E_2)^2 | -\psi_{211} + \psi_{21-1} \rangle.$$

or multiplying out, noting that $H\psi_{21\pm 1} = E_2\psi_{21\pm 1}$, so that $(H - E - 2)\psi_{21\pm 1} = 0$,

$$\sigma_E^2 = \frac{1}{2} \langle -\psi_{211} + \psi_{21-1} | -0\psi_{211} + 0\psi_{21-1} \rangle.$$

which is zero. The same way, $\sigma_{L^2} = 0$.

For z angular momentum, you have, since the expectation value is zero,

$$\sigma_{L_z}^2 = \langle (\hat{L}_z - 0)^2 \rangle = \frac{1}{2} \langle -\psi_{211} + \psi_{21-1} | (\hat{L}_z - 0)^2 | -\psi_{211} + \psi_{21-1} \rangle.$$

or multiplying out,

$$\sigma_{L_z}^2 = \frac{1}{2} \langle -\psi_{211} + \psi_{21-1} | -\hbar^2\psi_{211} + \hbar^2\psi_{21-1} \rangle$$

which multiplies out to \hbar^2 , so σ_{L_z} itself is \hbar .

4.4.4 Some examples

4.5 The Commutator

4.5.1 Commuting operators

4.5.1.1 Solution commutator

Question:

The pointer state

$$2p_x = \frac{1}{\sqrt{2}} (-\psi_{211} + \psi_{21-1}).$$

is one of the eigenstates that H , \hat{L}^2 , and \hat{L}_x have in common. Check that it is not an eigenstate that H , \hat{L}^2 , and \hat{L}_z have in common.

Answer:

It is an eigenstate of H and \widehat{L}^2 , but not of \widehat{L}_z . Since the z angular momentum of a ψ_{nlm} state is $m\hbar$, the combination above has a 50%/50% probability that the z angular momentum is \hbar or $-\hbar$.

4.5.2 Noncommuting operators and their commutator

4.5.3 The Heisenberg uncertainty relationship

4.5.3.1 Solution commutec-a

Question:

This sounds serious! If I am driving my car, the police requires me to know my speed (linear momentum). Also, I would like to know where I am. But neither is possible according to quantum mechanics.

Answer:

On second thought, maybe I can relax.

According to the uncertainty relationship, the uncertainties could be as small as, for example, $0.5 \cdot 10^{-10}$ m in position and 10^{-24} kg m/s for linear momentum. I am not going to miss my exit if I am mistaken by half an Å in where the car really is.

Also, 10^{-24} kg m/s of linear momentum for a 1 100 kg car corresponds to an uncertainty in velocity of $2 \cdot 10^{-27}$ mph. I don't think the police is going to ticket me for going $2 \cdot 10^{-27}$ mph over the speed limit, since their laser displays do not have the 29 digits required to read off 75.000 000 000 000 000 000 000 000 002 mph.

The requirements of uncertainty that give rise to the very size of the atoms are immeasurably small for the objects that populate the macroscopic world.

4.5.4 Commutator reference

4.6 The Hydrogen Molecular Ion

4.6.1 The Hamiltonian

4.6.2 Energy when fully dissociated

4.6.3 Energy when closer together

4.6.4 States that share the electron

4.6.5 Comparative energies of the states

4.6.6 Variational approximation of the ground state

4.6.6.1 Solution hione-a

Question:

The solution for the hydrogen molecular ion requires elaborate evaluations of inner product integrals and a computer evaluation of the state of lowest energy. As a much simpler example, you can try out the variational method on the one-dimensional case of a particle stuck inside a pipe, as discussed in chapter 3.5. Take the approximate wave function to be:

$$\psi = ax(\ell - x)$$

Find a from the normalization requirement that the total probability of finding the particle integrated over all possible x positions is one. Then evaluate the energy $\langle E \rangle$ as $\langle \psi | H | \psi \rangle$, where according to chapter 3.5.3, the Hamiltonian is

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

Compare the ground state energy with the exact value,

$$E_1 = \hbar^2 \pi^2 / 2m\ell^2$$

(Hints: $\int_0^\ell x(\ell - x) dx = \ell^3/6$ and $\int_0^\ell x^2(\ell - x)^2 dx = \ell^5/30$)

Answer:

To satisfy the normalization requirement that the particle must be somewhere, you need $\langle \psi | \psi \rangle = 1$, or substituting for ψ ,

$$1 = \langle ax(\ell - x) | ax(\ell - x) \rangle = |a|^2 \langle x(\ell - x) | x(\ell - x) \rangle$$

And by definition, chapter 2.3, the final inner product is just the integral $\int_0^\ell x^2(\ell - x)^2 dx$ which is given to be $\ell^5/30$. So you must have

$$|a|^2 = \frac{30}{\ell^5}$$

Now evaluate the expectation energy:

$$\langle E \rangle = \langle ax(\ell - x) | H | ax(\ell - x) \rangle = |a|^2 \left\langle x(\ell - x) \left| -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right| x(\ell - x) \right\rangle$$

You can substitute in the value of $|a|^2$ from the normalization requirement above and apply the Hamiltonian on the function to its right:

$$\langle E \rangle = \frac{30 \hbar^2}{\ell^5 m} \langle x(\ell - x) | 1 \rangle$$

The inner product is by definition the integral $\int_0^\ell x(\ell - x) dx$, which was given to be $\ell^3/6$. So the final expectation energy is

$$\langle E \rangle = \frac{\hbar^2 10}{2m\ell^2} \text{ versus } \frac{\hbar^2 \pi^2}{2m\ell^2} \text{ exact.}$$

The error in the approximation is only 1.3%! That is a surprisingly good result, since the parabola $ax(\ell - x)$ and the sine $a' \sin(\pi x/\ell)$ are simply different functions. While they may have superficial resemblance, if you scale each to unit height by taking $a = 4/\ell^2$ and $a' = 1$, then the derivatives at $x = 0$ and ℓ are $4/\ell$ respectively π/ℓ , off by as much as 27%.

If you go the next logical step, approximating the ground state with two functions as

$$\psi = ax(\ell - x) + bx^2(\ell - x)^2$$

where a and b are related by the normalization requirement $\langle \psi | \psi \rangle = 1$, you find a ground state energy to a stunning, (for a two term approximation,) accuracy of 0.0015%! However, the algebra becomes impossibly messy, so it was left out of the questions list. Similarly, a two point, linear interpolation, finite element version was left out, since there is so much baggage, it would distract from the true purpose of this book, to bring across the basic ideas of quantum mechanics to engineers.

Now, if you read the next subsection, you will see that in real-life, multi-dimensional, problems, getting results this accurate is difficult. Still, if you are desperate for a good solution of these very complex problems by a simple and reliable means, variational methods are hard to beat.

4.6.7 Comparison with the exact ground state

Chapter 5

Multiple-Particle Systems

5.1 Wave Function for Multiple Particles

5.1.1 Solution complex-a

Question:

A simple form that a six-dimensional wave function can take is a product of two three-dimensional ones, as in $\psi(\vec{r}_1, \vec{r}_2) = \psi_1(\vec{r}_1)\psi_2(\vec{r}_2)$. Show that if ψ_1 and ψ_2 are normalized, then so is ψ .

Answer:

This is a direct consequence of the fact that integrals can be factored if their integrands can be and the limits of integration are independent of the other variable:

$$\int_{\text{all } \vec{r}_1} \int_{\text{all } \vec{r}_2} \left| \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) \right|^2 d^3\vec{r}_1 d^3\vec{r}_2 = \int_{\text{all } \vec{r}_1} \left| \psi_1(\vec{r}_1) \right|^2 d^3\vec{r}_1 \int_{\text{all } \vec{r}_2} \left| \psi_2(\vec{r}_2) \right|^2 d^3\vec{r}_2 = 1$$

5.1.2 Solution complex-b

Question:

Show that for a simple product wave function as in the previous question, the relative probabilities of finding particle 1 near a position \vec{r}_a versus finding it near another position \vec{r}_b is the same regardless where particle 2 is. (Or rather, where particle 2 is likely to be found.)

Note: This is the reason that a simple product wave function is called “uncorrelated.” For particles that interact with each other, an uncorrelated wave function is often not a good approximation. For example, two electrons repel each other. All else being the same, the electrons would rather be at positions where the other electron is nowhere close. As a result, it really makes a difference for electron 1 where electron 2 is likely to be and vice-versa. To handle such situations, usually *sums* of product wave functions are used. However, for some cases, like for the helium atom, a single product wave function is a perfectly acceptable first approximation. Real-life electrons are crowded together around attracting nuclei and learn to live with each other.

Answer:

The probability of finding particle 1 within a vicinity $d^3\vec{r}_1$ of \vec{r}_a and particle 2 within a vicinity $d^3\vec{r}_2$ of \vec{r}_2 is:

$$\psi_1(\vec{r}_a)^*\psi_2(\vec{r}_2)^*\psi_1(\vec{r}_a)\psi_2(\vec{r}_2) d^3\vec{r}_1 d^3\vec{r}_2$$

while the corresponding probability of finding particle 1 within a vicinity $d^3\vec{r}_1$ of \vec{r}_b and particle 2 within a vicinity $d^3\vec{r}_2$ of \vec{r}_2 is:

$$\psi_1(\vec{r}_b)^*\psi_2(\vec{r}_2)^*\psi_1(\vec{r}_b)\psi_2(\vec{r}_2) d^3\vec{r}_1 d^3\vec{r}_2.$$

Taking the ratio of the two probabilities, the chances of finding particle 1 at \vec{r}_a versus finding it at \vec{r}_b are the same wherever particle 2 is likely to be found.

5.2 The Hydrogen Molecule

5.2.1 The Hamiltonian

5.2.1.1 Solution hmola-a

Question:

Verify that the repulsive potential between the electrons is infinitely large when the electrons are at the same position.

Note: You might therefore think that the wave function needs to be zero at the locations in six-dimensional space where $\vec{r}_1 = \vec{r}_2$. Some authors refer to that as a “Coulomb hole.” But the truth is that in quantum mechanics, electrons are smeared out due to uncertainty. That causes electron 1 to “see electron 2 at all sides”, and vice-versa, and they do therefore not encounter any unusually large potential when the wave function is nonzero at $\vec{r}_1 = \vec{r}_2$. In general, it is just not worth the trouble for the electrons to stay away from the same position: that would reduce their uncertainty in position, increasing their uncertainty-demanded kinetic energy.

Answer:

The repulsive potential is the term

$$\frac{e^2}{4\pi\epsilon_0} \frac{1}{|\vec{r}_1 - \vec{r}_2|}$$

and when $\vec{r}_1 = \vec{r}_2$, you are dividing by zero.

5.2.1.2 Solution hmola-b

Question:

Note that the total kinetic energy term is simply a multiple of the six-dimensional Laplacian operator. It treats all Cartesian position coordinates exactly the same, regardless of which direction or which electron it is. Is this still the case if other particles are involved?

Answer:

The kinetic energy of the two electrons is

$$-\frac{\hbar^2}{2m_e} \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial y_1^2} + \frac{\partial^2}{\partial z_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial y_2^2} + \frac{\partial^2}{\partial z_2^2} \right).$$

and the terms within the parentheses are the six-dimensional Laplacian. But if other particles would be involved, they would have a different value of $\hbar^2/2m$ and the total operator would no longer be the normal Laplacian.

All else being the same, heavier particles would have less kinetic energy. But, of course, all else is usually *not* the same. For example, the atoms in noble gases have the same kinetic energy at the same temperature regardless of atom mass.

5.2.2 Initial approximation to the lowest energy state

5.2.2.1 Solution hmolb-a

Question:

If electron 2 does not affect where electron 1 is likely to be, how would a grey-scale picture of the probability of finding electron 1 look?

Answer:

It would be a blob around the left proton, exactly like the one of a lone hydrogen atom at that position.

5.2.2.2 Solution hmolb-b

Question:

When the protons are close to each other, the electrons do affect each other, and the wave function above is no longer valid. But suppose you were given the true wave function, and you were once again asked to draw the blob showing the probability of finding electron 1 (using a plotting package, say). What would the big problem be?

Answer:

Since electron 2 now affects where electron 1 is, you would have to draw a different blob for every possible position of electron 2, an impossible task.

5.2.3 The probability density

5.2.3.1 Solution hmolc-a

Question:

Suppose, given the wave function $\psi_1(\vec{r}_1)\psi_r(\vec{r}_2)$, that you found an electron near the left proton. What electron would it probably be? Suppose you found an electron at the point halfway in between the protons. What electron would that likely be?

Answer:

The total probability of finding electron 1 at a position \vec{r} is

$$\int |\Psi(\vec{r}, \vec{r}_2)|^2 d^3\vec{r}_2 = |\psi_1(\vec{r})|^2 \int |\psi_r(\vec{r}_2)|^2 d^3\vec{r}_2 = |\psi_1(\vec{r})|^2$$

since ψ_r is normalized. Similarly, the probability of finding electron 2 at position \vec{r} is $|\psi_r(\vec{r})|^2$.

If \vec{r} is close to the left proton, $|\psi_1(\vec{r})|^2$ is significant, but $|\psi_r(\vec{r})|^2$ is small, so you are much more likely to find electron 1 there than electron 2.

But at the point halfway in between the protons, $|\psi_1(\vec{r})|^2$ and $|\psi_r(\vec{r})|^2$ are equal by symmetry, and you are just as likely to find electron 1 there as electron 2.

5.2.4 States that share the electrons

5.2.4.1 Solution hmold-a

Question:

Obviously, the visual difference between the various states is minor. It may even seem counter-intuitive that there is any difference at all: the states $\psi_1\psi_r$ and $\psi_r\psi_1$ are exactly the same physically, with one electron around each proton. So why would their combinations be any different?

The quantum difference would be much more clear if you could see the full six-dimensional wave function, but visualizing six-dimensional space just does not work. However, if you restrict yourself to only looking on the z -axis through the nuclei, you get a drawable z_1, z_2 -plane describing near what *axial* combinations of positions you are most likely to find the two electrons. In other words: what would be the chances of finding electron 1 near some axial position z_1 and electron 2 at the same time near some other axial position z_2 ?

Try to guess these probabilities in the z_1, z_2 -plane as grey tones, (darker if more likely), and then compare with the answer.

Answer:

Here are the pictures, assuming the origin is halfway in between the protons:

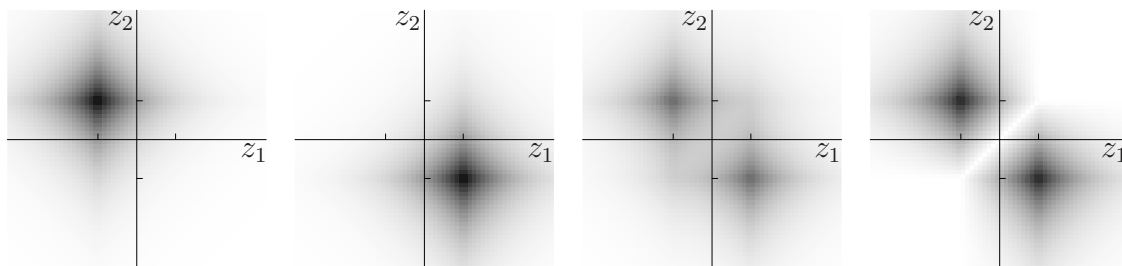


Figure 5.1: Wave functions on the z -axis through the nuclei. From left to right: $\psi_l\psi_r$, $\psi_r\psi_l$, the symmetric combination $a(\psi_l\psi_r + \psi_r\psi_l)$, and the antisymmetric one $a(\psi_l\psi_r - \psi_r\psi_l)$.

These results can be explained as follows: For the state $\psi_l\psi_r$, electron 1 is around the left proton, so its likely z_1 positions are clustered around the position z_{lp} of that proton, indicated by a tick mark on the negative z_1 -axis in figure 5.1. Similarly electron 2 is around the right proton, so its z_2 positions are clustered around the positive value z_{rp} indicated by the tick mark on the positive z_2 axis. This means the wave function, $\Psi(0, 0, z_1, 0, 0, z_2)$, will look as shown in the left picture of figure 5.1. It will be mostly in the quadrant of negative z_1 and positive z_2 .

Similarly $\psi_r\psi_l$ will look as the second picture. Here the positions of electron 1 cluster around the positive position of the right proton and those of electron 2 around the negative position of the left proton.

When you average the two states symmetrically, you get a two-blob picture like the third picture. Now it is electron 1 around the left proton and electron 2 around the right one or vice-versa. But there is still almost no probability of finding both protons in the first quadrant, both near the right proton. Nor are you likely to find them in the third quadrant, both near the left proton.

If you average the first two states antisymmetrically, you get the fourth picture. In the antisymmetric combination, the wave function is zero on the symmetry line between the blobs.

You see that the states are really different when looked at in the full six-dimensional space.

5.2.4.2 Solution hmold-b

Question:

Based on the previous question, how would you think the probability density $n(z)$ would look on the axis through the nuclei, again ignoring the existence of positions beyond the axis?

Answer:

For any state, the probability of finding electron 1 near a given z , regardless of where electron 2 is, is found by setting z_1 equal to z and integrating over all possible positions z_2 for electron 2. For the two-dimensional state $\psi_l\psi_r$ shown in the left column of figure 5.2, you are then integrating over vertical lines in the top picture; imagine moving all blank ink vertically towards the z_1 axis and then setting $z_1 = z$. The resulting curve is shown immediately below. As expected, electron 1 is in this state most likely to be found somewhere around z_l , the negative position of the left proton. Regardless of where electron 2 is.

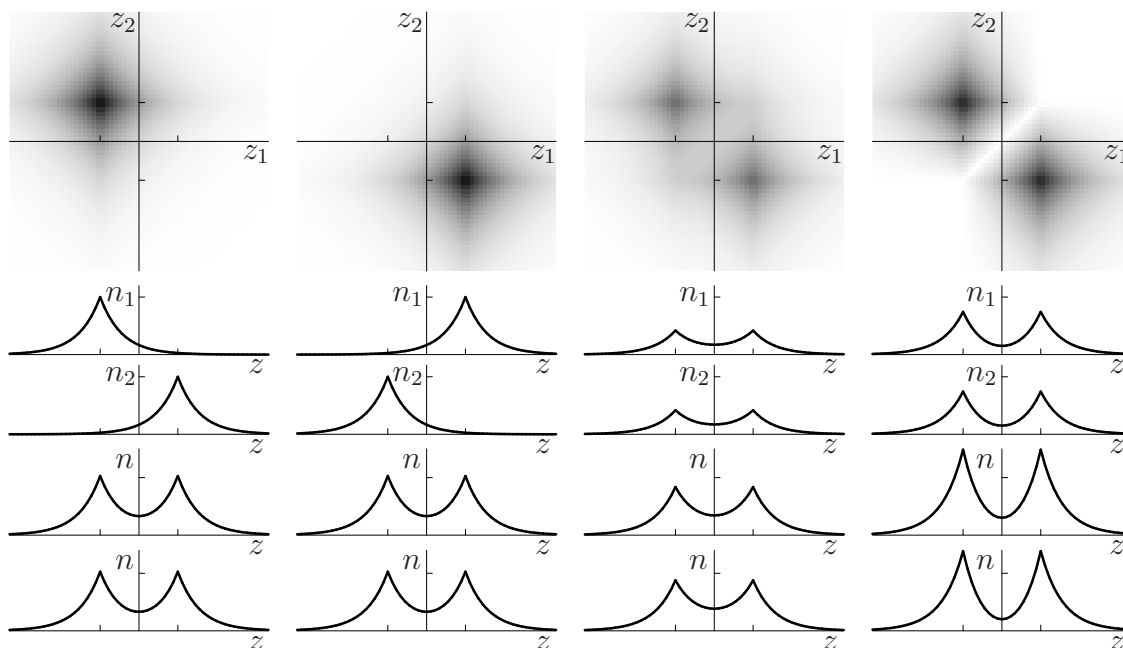


Figure 5.2: Probability density functions on the z -axis through the nuclei. From left to right: $\psi_l\psi_r$, $\psi_r\psi_l$, the symmetric combination $a(\psi_l\psi_r + \psi_r\psi_l)$, and the antisymmetric one $a(\psi_l\psi_r - \psi_r\psi_l)$. From top to bottom, the top row of curves show the probability of finding electron 1 near z regardless where electron 2 is. The second row shows the probability of finding electron 2 near z regardless where electron 1 is. The third row shows the total probability of finding either electron near z , the sum of the previous two rows. The fourth row shows the same as the third, but assuming the true three-dimensional world rather than just the line through the nuclei.

(Note that all possible positions of electron 2 should really be found by integrating over all possible positions in three dimensions, not just axial ones. The final row in the figure gives the total probabilities when corrected for that. But the *idea* is the same, just harder to visualize.)

The probability density at a given value of z also needs to include the possibility of finding electron 2 there. That probability is found by setting $z_2 = z$ and then integrating over all possible values of z_1 . You are now moving the blank ink horizontally towards the z_2 axis, and then setting $z_2 = z$. The resulting curve is shown in the second graph in the left column of figure 5.2. As expected, electron 2 is most likely to be found somewhere around z_{rp} , the positive position of the right proton.

To get the probability density, the chance of finding either proton near z , you need to add the two curves together. That is done in the third graph in the left column of figure 5.2. An electron is likely to be somewhere around each proton. This graph looks exactly like the correct three-dimensional curve shown in the bottom graph, but that is really just a coincidence.

The states $\psi_r\psi_l$ and $a(\psi_l\psi_r \pm \psi_r\psi_l)$ can be integrated similarly; they are shown in the subsequent columns in figure 5.2. Note how the line of zero wave function in the antisymmetric case disappears during the integrations. Also note that really, the probability density functions of the symmetric and antisymmetric states are quite different, though they look qualitatively the same.

5.2.5 Variational approximation of the ground state

5.2.6 Comparison with the exact ground state

5.3 Two-State Systems

5.3.1 Solution 2state-a

Question:

The effectiveness of mixing states was already shown by the hydrogen molecule and molecular ion examples. But the generalized story above restricts the “basis” states to be orthogonal, and the states used in the hydrogen examples were not.

Show that if ψ_1 and ψ_2 are not orthogonal states, but are normalized and produce a real and positive value for $\langle\psi_1|\psi_2\rangle$, like in the hydrogen examples, then orthogonal states can be found in the form

$$\bar{\psi}_1 = \alpha(\psi_1 - \varepsilon\psi_2) \quad \bar{\psi}_2 = \alpha(\psi_2 - \varepsilon\psi_1).$$

For normalized ψ_1 and ψ_2 the Cauchy-Schwartz inequality implies that $\langle\psi_1|\psi_2\rangle$ will be less than one. If the states do not overlap much, it will be much less than one and ε will be small.

(If ψ_1 and ψ_2 do not meet the stated requirements, you can always redefine them by factors ae^{ic} and be^{-ic} , with a , b , and c real, to get states that do.)

Answer:

The inner product of $\bar{\psi}_1$ and $\bar{\psi}_2$ must be zero for them to be orthogonal:

$$\alpha^2 \langle\psi_1 - \varepsilon\psi_2|\psi_2 - \varepsilon\psi_1\rangle = 0$$

and this can be multiplied out, dropping the common factor α^2 and noting that $\langle\psi_1|\psi_1\rangle$ and $\langle\psi_2|\psi_2\rangle$ are one, as

$$\langle\psi_1|\psi_2\rangle\varepsilon^2 - 2\varepsilon + \langle\psi_1|\psi_2\rangle = 0$$

for which the smallest root can be written as

$$\varepsilon = \frac{\langle\psi_1|\psi_2\rangle}{1 + \sqrt{1 - \langle\psi_1|\psi_2\rangle^2}}.$$

That is less than $\langle\psi_1|\psi_2\rangle$, hence ε is small if the overlap is small.

The constant α follows from the requirement that the new states must still be normalized, and is found to be

$$\alpha = \frac{1}{\sqrt{1 - 2\varepsilon\langle\psi_1|\psi_2\rangle + \varepsilon^2}}.$$

Note that the denominator is nonzero; the argument of the square root exceeds $(1 - \varepsilon)^2$.

5.3.2 Solution 2state-b

Question:

Show that it does not have an effect on the solution whether or not the basic states ψ_1 and ψ_2 are normalized, like in the previous question, before the state of lowest energy is found.

This requires no detailed analysis; just check that the same solution can be described using the nonorthogonal and orthogonal basis states. It is however an important observation for various numerical solution procedures: your set of basis functions can be cleaned up and simplified without affecting the solution you get.

Answer:

Using the original basis states, the solution, say the ground state of lowest energy, can be written in the form

$$c_1\psi_1 + c_2\psi_2$$

for some values of the constants c_1 and c_2 . Now the expression for the orthogonalized functions,

$$\bar{\psi}_1 = \alpha(\psi_1 - \varepsilon\psi_2) \quad \bar{\psi}_2 = \alpha(\psi_2 - \varepsilon\psi_1),$$

can for given $\bar{\psi}_1$ and $\bar{\psi}_2$ be thought of as two equations for ψ_1 and ψ_2 that can be solved. In particular, adding ε times the second equation to the first gives

$$\psi_1 = \frac{\bar{\psi}_1 + \varepsilon\bar{\psi}_2}{\alpha(1 - \varepsilon^2)}.$$

Similarly, adding ε times the first equation to the second gives

$$\psi_2 = \frac{\bar{\psi}_2 + \varepsilon\bar{\psi}_1}{\alpha(1 - \varepsilon^2)}.$$

If this is plugged into the expression for the solution, $c_1\psi_1 + c_2\psi_2$, it takes the form

$$\bar{c}_1\bar{\psi}_1 + \bar{c}_2\bar{\psi}_2$$

where

$$\bar{c}_1 = \frac{c_1 + \varepsilon c_2}{\alpha(1 - \varepsilon^2)} \quad \bar{c}_2 = \frac{c_2 + \varepsilon c_1}{\alpha(1 - \varepsilon^2)}.$$

So, while the constants \bar{c}_1 and \bar{c}_2 are different from c_1 and c_2 , the same solution can be found equally well in terms of $\bar{\psi}_1$ and $\bar{\psi}_2$ as in terms of ψ_1 and ψ_2 .

In the terms of linear algebra, $\bar{\psi}_1$ and $\bar{\psi}_2$ “span the same function space” as ψ_1 and ψ_2 : any wave function that can be described as a combination of ψ_1 and ψ_2 can also be described in terms of $\bar{\psi}_1$ and $\bar{\psi}_2$, although with different constants. This is true as long as the definitions of the new functions can be solved for the old functions as above. The matrix of coefficients, here

$$\begin{pmatrix} \alpha & -\alpha\varepsilon \\ -\alpha\varepsilon & \alpha \end{pmatrix}$$

must have a nonzero determinant.

5.4 Spin

5.4.1 Solution spin-a

Question:

Delta particles have spin $\frac{3}{2}$. What values can their spin angular momentum in a given direction have?

Answer:

$$-\frac{3}{2}\hbar, -\frac{1}{2}\hbar, \frac{1}{2}\hbar, \frac{3}{2}\hbar.$$

Reread the text if you got this wrong, because spin is really, really, important in quantum mechanics.

5.4.2 Solution spin-b

Question:

Delta particles have spin $\frac{3}{2}$. What is their square spin angular momentum?

Answer:

$$s(s + 1)\hbar^2 = \frac{15}{4}\hbar^2.$$

5.5 Multiple-Particle Systems Including Spin

5.5.1 Wave function for a single particle with spin

5.5.1.1 Solution complexsa-a

Question:

What is the normalization requirement of the wave function of a spin $\frac{1}{2}$ particle in terms of Ψ_+ and Ψ_- ?

Answer:

The particle must be found somewhere, either with spin up or with spin down. The total probability of finding it somewhere with spin up is $\int |\Psi_+|^2 d^3\vec{r}$, and the total probability of finding it somewhere with spin down is $\int |\Psi_-|^2 d^3\vec{r}$. The sum of the two integrals must be one to express the fact that the probability of finding the particle somewhere, either with spin up or spin down, must be one, certainty.

5.5.2 Inner products including spin

5.5.2.1 Solution complexsaia

Question:

Show that the normalization requirement for the wave function of a spin $\frac{1}{2}$ particle in terms of Ψ_+ and Ψ_- requires its norm $\sqrt{\langle\Psi|\Psi\rangle}$ to be one.

Answer:

As a corresponding question in the previous subsection discussed; the total probability of finding the particle somewhere with spin up is $\int |\Psi_+|^2 d^3\vec{r}$, and the total probability of finding it somewhere with spin down is $\int |\Psi_-|^2 d^3\vec{r}$. The sum of the two integrals must be one to express the fact that the probability of finding the particle somewhere, either with spin up or spin down, must be one, certainty.

Compare that with the square norm of the wave function, which is by definition the inner product of the wave function with itself:

$$\langle\Psi|\Psi\rangle = \langle\Psi_+\uparrow + \Psi_-\downarrow|\Psi_+\uparrow + \Psi_-\downarrow\rangle = \langle\Psi_+|\Psi_+\rangle + \langle\Psi_-|\Psi_-\rangle$$

and the final two inner products are by definition the two integrals above. Since their sum must be one, it follows that the norm of the wave function $\sqrt{\langle\Psi|\Psi\rangle}$ must be one even if there is spin.

5.5.2.2 Solution complexsai-b

Question:

Assume that ψ_l and ψ_r are normalized spatial wave functions. Now show that a combination of the two like $(\psi_l\uparrow + \psi_r\downarrow)/\sqrt{2}$ is a normalized wave function with spin.

Answer:

You have

$$\left\langle \frac{\psi_l\uparrow + \psi_r\downarrow}{\sqrt{2}} \left| \frac{\psi_l\uparrow + \psi_r\downarrow}{\sqrt{2}} \right. \right\rangle = \left(\frac{1}{\sqrt{2}} \right)^2 \langle \psi_l\uparrow + \psi_r\downarrow | \psi_l\uparrow + \psi_r\downarrow \rangle,$$

and multiplying out the inner product according to the rule spin-up components together and spin-down components together,

$$= \frac{1}{2} \left(\langle \psi_l | \psi_l \rangle + \langle \psi_r | \psi_r \rangle \right),$$

and since it is given that ψ_l and ψ_r are normalized

$$= \frac{1}{2} (1 + 1) = 1.$$

5.5.3 Commutators including spin

5.5.3.1 Solution complexsac-a

Question:

Are not some commutators missing from the fundamental commutation relationship? For example, what is the commutator $[\widehat{S}_y, \widehat{S}_x]$?

Answer:

Since the commutator is antisymmetric, $[\widehat{S}_y, \widehat{S}_x]$ is the negative of $[\widehat{S}_x, \widehat{S}_y]$, so it is $-i\hbar\widehat{S}_z$.

5.5.4 Wave function for multiple particles with spin

5.5.4.1 Solution complexsb-a

Question:

As an example of the orthonormality of the two-particle spin states, verify that $\langle \uparrow\uparrow | \downarrow\uparrow \rangle$ is zero, so that $\uparrow\uparrow$ and $\downarrow\uparrow$ are indeed orthogonal. Do so by explicitly writing out the sums over S_{z1} and S_{z2} .

Answer:

The inner product is by definition

$$\langle \uparrow\uparrow | \downarrow\uparrow \rangle = \sum_{S_{z1}=\pm\frac{1}{2}\hbar} \sum_{S_{z2}=\pm\frac{1}{2}\hbar} \uparrow(S_{z1})\uparrow(S_{z2}) \downarrow(S_{z1})\uparrow(S_{z2})$$

or writing out the second sum explicitly

$$\langle \uparrow\uparrow | \downarrow\uparrow \rangle = \sum_{S_{z1}=\pm\frac{1}{2}\hbar} [\uparrow(S_{z1})\uparrow(+\frac{1}{2}\hbar) \downarrow(S_{z1})\uparrow(+\frac{1}{2}\hbar) + \uparrow(S_{z1})\uparrow(-\frac{1}{2}\hbar) \downarrow(S_{z1})\uparrow(-\frac{1}{2}\hbar)]$$

or writing out the first sum also explicitly

$$\begin{aligned} \langle \uparrow\uparrow | \downarrow\uparrow \rangle = & \uparrow(+\frac{1}{2}\hbar)\uparrow(+\frac{1}{2}\hbar) \downarrow(+\frac{1}{2}\hbar)\uparrow(+\frac{1}{2}\hbar) + \uparrow(+\frac{1}{2}\hbar)\uparrow(-\frac{1}{2}\hbar) \downarrow(+\frac{1}{2}\hbar)\uparrow(-\frac{1}{2}\hbar) + \\ & \uparrow(-\frac{1}{2}\hbar)\uparrow(+\frac{1}{2}\hbar) \downarrow(-\frac{1}{2}\hbar)\uparrow(+\frac{1}{2}\hbar) + \uparrow(-\frac{1}{2}\hbar)\uparrow(-\frac{1}{2}\hbar) \downarrow(-\frac{1}{2}\hbar)\uparrow(-\frac{1}{2}\hbar) \end{aligned}$$

and noting that $\uparrow(-\frac{1}{2}\hbar) = 0$ and $\downarrow(+\frac{1}{2}\hbar) = 0$, you see that all terms are zero.

5.5.4.2 Solution complexsb-b

Question:

A more concise way of understanding the orthonormality of the two-particle spin states is to note that an inner product like $\langle \uparrow\uparrow | \downarrow\uparrow \rangle$ equals $\langle \uparrow | \downarrow \rangle \langle \uparrow | \uparrow \rangle$, where the first inner product refers to the spin states of particle 1 and the second to those of particle 2. The first inner product is zero because of the orthogonality of \uparrow and \downarrow , making $\langle \uparrow\uparrow | \downarrow\uparrow \rangle$ zero too.

To check this argument, write out the sums over S_{z1} and S_{z2} for $\langle \uparrow | \downarrow \rangle \langle \uparrow | \uparrow \rangle$ and verify that it is indeed the same as the written out sum for $\langle \uparrow\uparrow | \downarrow\uparrow \rangle$ given in the answer for the previous question.

The underlying mathematical principle is that sums of products can be factored into separate sums as in:

$$\sum_{\text{all } S_{z1}} \sum_{\text{all } S_{z2}} f(S_{z1})g(S_{z2}) = \left[\sum_{\text{all } S_{z1}} f(S_{z1}) \right] \left[\sum_{\text{all } S_{z2}} g(S_{z2}) \right]$$

This is similar to the observation in calculus that integrals of products can be factored into separate integrals:

$$\int_{\text{all } \vec{r}_1} \int_{\text{all } \vec{r}_2} f(\vec{r}_1)g(\vec{r}_2) d^3\vec{r}_1 d^3\vec{r}_2 = \left[\int_{\text{all } \vec{r}_1} f(\vec{r}_1) d^3\vec{r}_1 \right] \left[\int_{\text{all } \vec{r}_2} g(\vec{r}_2) d^3\vec{r}_2 \right]$$

Answer:

$$\langle \uparrow\downarrow | \uparrow\uparrow \rangle = \left[\sum_{S_{z1}=\pm\frac{1}{2}\hbar} \uparrow(S_{z1})\downarrow(S_{z1}) \right] \left[\sum_{S_{z2}=\pm\frac{1}{2}\hbar} \uparrow(S_{z2})\uparrow(S_{z2}) \right]$$

and written out

$$\langle \uparrow\downarrow | \uparrow\uparrow \rangle = [\uparrow(+\frac{1}{2}\hbar)\downarrow(+\frac{1}{2}\hbar) + \uparrow(-\frac{1}{2}\hbar)\downarrow(-\frac{1}{2}\hbar)] [\uparrow(+\frac{1}{2}\hbar)\uparrow(+\frac{1}{2}\hbar) + \uparrow(-\frac{1}{2}\hbar)\uparrow(-\frac{1}{2}\hbar)]$$

and multiplying out, and reordering the second and third factor in each term, you see it is the same as the expression obtained in the answer to the previous question,

$$\begin{aligned} \langle \uparrow\uparrow | \downarrow\downarrow \rangle &= \uparrow(+\frac{1}{2}\hbar)\uparrow(+\frac{1}{2}\hbar) \downarrow(+\frac{1}{2}\hbar)\uparrow(+\frac{1}{2}\hbar) + \uparrow(+\frac{1}{2}\hbar)\uparrow(-\frac{1}{2}\hbar) \downarrow(+\frac{1}{2}\hbar)\uparrow(-\frac{1}{2}\hbar) + \\ &\quad \uparrow(-\frac{1}{2}\hbar)\uparrow(+\frac{1}{2}\hbar) \downarrow(-\frac{1}{2}\hbar)\uparrow(+\frac{1}{2}\hbar) + \uparrow(-\frac{1}{2}\hbar)\uparrow(-\frac{1}{2}\hbar) \downarrow(-\frac{1}{2}\hbar)\uparrow(-\frac{1}{2}\hbar). \end{aligned}$$

5.5.5 Example: the hydrogen molecule

5.5.5.1 Solution complexsc-a

Question:

Show that the normalization requirement for ψ_{gs} means that

$$|a_{++}|^2 + |a_{+-}|^2 + |a_{-+}|^2 + |a_{--}|^2 = 1$$

Answer:

For brevity, write

$$\psi_{\text{gs},0} = a [\psi_1(\vec{r}_1)\psi_r(\vec{r}_2) + \psi_r(\vec{r}_1)\psi_1(\vec{r}_2)]$$

so that

$$\psi_{\text{gs}} = a_{++}\psi_{\text{gs},0}\uparrow\uparrow + a_{+-}\psi_{\text{gs},0}\uparrow\downarrow + a_{-+}\psi_{\text{gs},0}\downarrow\uparrow + a_{--}\psi_{\text{gs},0}\downarrow\downarrow.$$

For ψ_{gs} to be normalized, its square norm must be one:

$$\langle \psi_{\text{gs}} | \psi_{\text{gs}} \rangle = 1.$$

According to the previous subsection, this inner product evaluates as the sum of the inner products of the matching spin components:

$$\langle a_{++}\psi_{\text{gs},0} | a_{++}\psi_{\text{gs},0} \rangle + \langle a_{+-}\psi_{\text{gs},0} | a_{+-}\psi_{\text{gs},0} \rangle + \langle a_{-+}\psi_{\text{gs},0} | a_{-+}\psi_{\text{gs},0} \rangle + \langle a_{--}\psi_{\text{gs},0} | a_{--}\psi_{\text{gs},0} \rangle = 1$$

Now the constants $a_{\pm\pm}$ can be pulled out of the inner products as $|a_{\pm\pm}|^2$, and the inner products that are left, all $\langle \psi_{\text{gs},0} | \psi_{\text{gs},0} \rangle$, are one since $\psi_{\text{gs},0}$ was normalized through the choice of the constant a . So the claimed expression results.

5.5.6 Triplet and singlet states

5.5.6.1 Solution complexse-a

Question:

Like the states $\uparrow\uparrow$, $\uparrow\downarrow$, $\downarrow\uparrow$, and $\downarrow\downarrow$; the triplet and singlet states are an orthonormal quartet. For example, check that the inner product of $|1\ 0\rangle$ and $|0\ 0\rangle$ is zero.

Answer:

By definition, the inner product is

$$\left\langle \frac{1}{\sqrt{2}} (\uparrow\downarrow + \downarrow\uparrow) \left| \frac{1}{\sqrt{2}} (\uparrow\downarrow - \downarrow\uparrow) \right. \right\rangle = \frac{1}{2} \langle \uparrow\downarrow + \downarrow\uparrow | \uparrow\downarrow - \downarrow\uparrow \rangle$$

and multiplying out, that becomes

$$\frac{1}{2} (\langle \uparrow\downarrow | \uparrow\downarrow \rangle - \langle \uparrow\downarrow | \downarrow\uparrow \rangle + \langle \downarrow\uparrow | \uparrow\downarrow \rangle - \langle \downarrow\uparrow | \downarrow\uparrow \rangle)$$

and using orthonormality of the arrow combinations, that is

$$\frac{1}{2} (1 - 0 + 0 - 1) = 0$$

5.6 Identical Particles

5.6.1 Solution ident-a

Question:

Check that indeed any linear combination of the triplet states is unchanged under particle exchange.

Answer:

In the notations of the previous section, the most general linear combination of the triplet states takes the form:

$$a_1|1\ 1\rangle + a_2|1\ 0\rangle + a_3|1\ -1\rangle$$

or writing out their definitions as found there,

$$a_1\uparrow\uparrow + a_2\frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow) + a_3\downarrow\downarrow.$$

Exchanging the two particles involved means to interchange the order of each pair of arrows, since by definition the first arrow refers to particle 1 and the second to particle 2. A look at the expression above shows that such an interchange of order does absolutely nothing to these states.

5.6.2 Solution ident-b

Question:

Suppose the electrons of the hydrogen molecule are in the excited antisymmetric spatial state

$$a [\psi_1(\vec{r}_1)\psi_r(\vec{r}_2) - \psi_r(\vec{r}_1)\psi_1(\vec{r}_2)].$$

In that case what can you say about the spin state?

Yes, in this case the spin would be less restricted if the electrons were bosons. But antisymmetric spatial states themselves are pretty restrictive in general. The precise sense in which the antisymmetrization requirement is more restrictive than the symmetrization requirement will be explored in the next section.

Answer:

Since the excited spatial state takes care of the sign change, the spin state should remain unchanged under the electron exchange. That is true for the three triplet states, but not for the singlet state, so the spin state can be any combination of the three triplet states. The complete wave function must therefore be of the form

$$a [\psi_1(\vec{r}_1)\psi_r(\vec{r}_2) - \psi_r(\vec{r}_1)\psi_1(\vec{r}_2)] [a_1|1\ 1\rangle + a_2|1\ 0\rangle + a_3|1\ -1\rangle]$$

You can also derive this using the arrow combinations like was done in the text for the ground state. Then the requirements are that $a_{++} = a_{++}$ and $a_{--} = a_{--}$, which is trivial, and that $a_{+-} = a_{-+}$, which restricts the mixed spin states to the triplet combination. In those terms the constants above are $a_1 = a_{++}$, $a_3 = a_{--}$, and $a_2 = \sqrt{2}a_{+-}$.

5.7 Ways to Symmetrize the Wave Function

5.7.1 Solution symways-a

Question:

How many single-particle states would a basic Hartree-Fock approximation use to compute the electron structure of an arsenic atom? How many Slater determinants would that involve?

Answer:

Hartree-Fock would use 33 single-particle states, combining into a single Slater determinant.

5.7.2 Solution symways-b

Question:

If two more single-particle states would be used to improve the accuracy for the arsenic atom, (one more normally does not help), how many Slater determinants could be formed with those states?

Answer:

The 34-th state would introduce 33 more Slater determinants, and the 35-th another 561, for a total of 595.

5.8 Matrix Formulation

5.8.1 Solution matfor-a

Question:

As a relatively simple example, work out the above ideas for the $Q = 2$ hydrogen molecule spatial states $\psi_1^S = \psi_l\psi_r$ and $\psi_2^S = \psi_l\psi_r$. Write the matrix eigenvalue problem and identify the two eigenvalues and eigenvectors. Compare with the results of section 5.3.

Assume that ψ_l and ψ_r have been slightly adjusted to be orthonormal. Then so are ψ_1^S and ψ_2^S orthonormal, since the various six-dimensional inner product integrals, like

$$\begin{aligned} \langle \psi_1^S | \psi_2^S \rangle &\equiv \langle \psi_l\psi_r | \psi_r\psi_l \rangle \equiv \\ &\int_{\text{all } \vec{r}_1} \int_{\text{all } \vec{r}_2} \psi_l(\vec{r}_1)\psi_r(\vec{r}_2) \psi_r(\vec{r}_1)\psi_l(\vec{r}_2) d^3\vec{r}_1 d^3\vec{r}_2 \end{aligned}$$

can according to the rules of calculus be factored into three-dimensional integrals as

$$\begin{aligned} \langle \psi_1^S | \psi_2^S \rangle &= \left[\int_{\text{all } \vec{r}_1} \psi_l(\vec{r}_1) \psi_r(\vec{r}_1) d^3\vec{r}_1 \right] \left[\int_{\text{all } \vec{r}_2} \psi_r(\vec{r}_2) \psi_l(\vec{r}_2) d^3\vec{r}_2 \right] \\ &= \langle \psi_l | \psi_r \rangle \langle \psi_r | \psi_l \rangle \end{aligned}$$

which is zero if ψ_l and ψ_r are orthonormal.

Also, do not try to find actual values for H_{11} , H_{12} , H_{21} , and H_{22} . As section 5.2 noted, that can only be done numerically. Instead just refer to H_{11} as J and to H_{12} as $-L$:

$$\begin{aligned} H_{11} &\equiv \langle \psi_1^S | H \psi_1^S \rangle \equiv \langle \psi_l\psi_r | H \psi_l\psi_r \rangle \equiv J \\ H_{12} &\equiv \langle \psi_1^S | H \psi_2^S \rangle \equiv \langle \psi_l\psi_r | H \psi_r\psi_l \rangle \equiv -L. \end{aligned}$$

Next note that you also have

$$\begin{aligned} H_{22} &\equiv \langle \psi_2^S | H \psi_2^S \rangle \equiv \langle \psi_r\psi_l | H \psi_r\psi_l \rangle = J \\ H_{21} &\equiv \langle \psi_2^S | H \psi_1^S \rangle \equiv \langle \psi_r\psi_l | H \psi_l\psi_r \rangle = -L \end{aligned}$$

because they are the exact same inner product integrals; the difference is just which electron you number 1 and which one you number 2 that determines whether the wave functions are listed as $\psi_1\psi_r$ or $\psi_r\psi_1$.

Answer:

Using the abbreviations J and L , the matrix eigenvalue problem becomes

$$\begin{aligned} Ja_1 - La_2 &= Ea_1 \\ -La_1 + Ja_2 &= Ea_2 \end{aligned}$$

or taking everything to the left hand side,

$$\begin{aligned} (J - E)a_1 - La_2 &= 0 \\ -La_1 + (J - E)a_2 &= 0 \end{aligned} .$$

For this homogeneous system of equations to have a solution other than the trivial one $a_1 = a_2 = 0$, the determinant of the matrix must be zero:

$$\begin{vmatrix} (J - E) & -L \\ -L & (J - E) \end{vmatrix} = 0 \quad \implies \quad (J - E)^2 - L^2 = 0$$

which allows for the two possibilities

$$J - E = L \quad \text{or} \quad J - E = -L.$$

So there are two energy eigenvalues:

$$E_1 = J - L \quad \text{and} \quad E_2 = J + L.$$

In the first case, since according to the equations above

$$(J - E_1)a_1 - La_2 = 0 \quad \implies \quad La_1 - La_2 = 0$$

it follows that a_1 and a_2 must be equal, producing the eigenfunction

$$a_1 (\psi_1^S + \psi_2^S) = a_1 (\psi_1\psi_r + \psi_r\psi_1)$$

and normalization shows that $a_1 = 1/\sqrt{2}$, assuming you take it real and positive, (and assuming that ψ_1 and ψ_r are really adjusted to be orthonormal as assumed in this particular question).

So the first energy eigenstate is

$$\text{eigenfunction: } \frac{1}{\sqrt{2}} (\psi_1\psi_r + \psi_r\psi_1) \quad \text{eigenvalue: } E_1 = J - L$$

Similarly the second energy eigenstate is

$$\text{eigenfunction: } \frac{1}{\sqrt{2}} (\psi_1\psi_r - \psi_r\psi_1) \quad \text{eigenvalue: } E_2 = J + L.$$

Comparing with section 5.3, the first eigenstate can be recognized as the ground state in which the nuclei share the electrons symmetrically. The second eigenstate is the excited-energy antisymmetric state in which the electrons share the electrons antisymmetrically. Other states of this type, like simply $\psi_1\psi_r$, say, have *expectation* energy somewhere in between E_1 and E_2 , but they are not eigenstates and do not have definite energy.

Of course, the analysis here is approximate. But as discussed more in the earlier section 5.2, the true ground state is really symmetric, and the excited energy eigenstate really is antisymmetric. After all, the Hamiltonian commutes with the operation of swapping the electrons, (swapping the electrons does not do anything physically,) so the energy eigenstates must also be eigenstates of the swapping operator. The symmetric state is an eigenstate of the swapping operator with eigenvalue 1, it stays the same, and the antisymmetric state is an eigenstate with eigenvalue -1 ; it changes sign under the swap.

5.8.2 Solution matfor-b

Question:

Find the eigenstates for the same problem, but now including spin.

As section 5.7 showed, the antisymmetric wave function with spin consists of a sum of six Slater determinants. Ignoring the highly excited first and sixth determinants that have the electrons around the same nucleus, the remaining $C = 4$ Slater determinants can be written out explicitly to give the two-particle states

$$\begin{aligned} \psi_1^S &= \frac{\psi_1\psi_r\uparrow\uparrow - \psi_r\psi_1\uparrow\uparrow}{\sqrt{2}} & \psi_2^S &= \frac{\psi_1\psi_r\uparrow\downarrow - \psi_r\psi_1\downarrow\uparrow}{\sqrt{2}} \\ \psi_3^S &= \frac{\psi_1\psi_r\downarrow\uparrow - \psi_r\psi_1\uparrow\downarrow}{\sqrt{2}} & \psi_4^S &= \frac{\psi_1\psi_r\downarrow\downarrow - \psi_r\psi_1\downarrow\downarrow}{\sqrt{2}} \end{aligned}$$

Note that the Hamiltonian does not involve spin, to the approximation used in most of this book, so that, following the techniques of section 5.5, an inner product like $H_{23} = \langle \psi_2^S | H \psi_3^S \rangle$ can be written out like

$$\begin{aligned} H_{23} &= \frac{1}{2} \langle \psi_1\psi_r\uparrow\downarrow - \psi_r\psi_1\downarrow\uparrow | H (\psi_1\psi_r\downarrow\uparrow - \psi_r\psi_1\uparrow\downarrow) \rangle \\ &= \frac{1}{2} \langle \psi_1\psi_r\uparrow\downarrow - \psi_r\psi_1\downarrow\uparrow | (H\psi_1\psi_r)\downarrow\uparrow - (H\psi_r\psi_1)\uparrow\downarrow \rangle \end{aligned}$$

and then multiplied out into inner products of matching spin components to give

$$H_{23} = -\frac{1}{2}\langle\psi_l\psi_r|H\psi_r\psi_l\rangle - \frac{1}{2}\langle\psi_r\psi_l|H\psi_l\psi_r\rangle = L.$$

The other 15 matrix coefficients can be found similarly, and most will be zero.

If you do not have experience with linear algebra, you may want to skip this question, or better, just read the solution. However, the four eigenvectors are not that hard to guess; maybe easier to guess than correctly derive.

Answer:

Evaluating all 16 inner products H_{kk} as above, the matrix eigenvalue problem is found to be

$$\begin{aligned} (J+L)a_1 + 0a_2 + 0a_3 + 0a_4 &= Ea_1 \\ 0a_1 + Ja_2 + La_3 + 0a_4 &= Ea_2 \\ 0a_1 + La_2 + Ja_3 + 0a_4 &= Ea_3 \\ 0a_1 + 0a_2 + 0a_3 + (J+L)a_4 &= Ea_4 \end{aligned}$$

After bringing everything to the left hand side, the determinant of the resulting matrix can again be set to zero, and the possible energy values found. From those the eigenvectors can be deduced. It turns out that the larger eigenvalue is triply degenerate, so the three corresponding eigenvectors are not unique; more than one acceptable choice exists for them. However, you do have to normalize them to unit length and ensure that they are mutually orthogonal.

Rather than going through that math, it is quicker just to guess the eigenvectors. One guess that works is

$$(a_1, a_2, a_3, a_4) = (1, 0, 0, 0).$$

Just substitute $a_1 = 1$ and $a_2 = a_3 = a_4 = 0$ into the equations above and see that they are satisfied provided that the energy E has the excited value $J + L$. The corresponding eigenfunction $\psi_1 = \psi_1^S$ has, according to its definition above, both electrons spin-up and in the excited antisymmetric spatial state $(\psi_l\psi_r - \psi_r\psi_l)/\sqrt{2}$.

A similar guess that works is

$$(a_1, a_2, a_3, a_4) = (0, 0, 0, 1).$$

This corresponds to the eigenfunction $\psi_2 = \psi_4^S$ in which both electrons are spin-down, and again in the antisymmetric spatial state. The third one that works is

$$(a_1, a_2, a_3, a_4) = (0, 1, 1, 0)/\sqrt{2}$$

where the scale factor $\sqrt{2}$ is only needed to ensure that the vector is of unit length. The eigenstate $\psi_3 = (\psi_2^S + \psi_3^S)/\sqrt{2}$ corresponds, according to the definitions of ψ_2^S and ψ_3^S above,

to the electrons being in the antisymmetric spatial state times the $|1\ 0\rangle$ triplet state of section 5.5.6. The energy is again the elevated value $J + L$.

The final eigenvector

$$(a_1, a_2, a_3, a_4) = (0, 1, -1, 0)/\sqrt{2},$$

gives the eigenstate $\psi_4 = (\psi_2^S - \psi_3^S)/\sqrt{2}$. This corresponds to the electrons being in the symmetric spatial state times the singlet spin state. The energy is the ground state value $J - L$.

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Time Evolution

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7.1.1 The equation

7.1.2 Solution of the equation

7.1.2.1 Solution schrodsol-a

Question:

The energy of a photon is $\hbar\omega$ where ω is the classical frequency of the electromagnetic field produced by the photon. So what is $e^{-iE_{\pi}t/\hbar}$ for a photon? Are you surprised by the result?

Answer:

The exponential $e^{-iE_n t/\hbar}$ becomes $e^{-i\omega t}$. That is the classical time dependence of the electromagnetic field.

The result is not really surprising, because of the wave-particle dualism of quantum mechanics. Classical physics understands the wave nature of light well, and not its particle nature. This is the opposite of the situation for an electron, where classical physics understands the particle nature, and not the wave nature.

7.1.2.2 Solution schrodsol-b

Question:

For the one-dimensional harmonic oscillator, the energy eigenvalues are

$$E_n = \frac{2n + 1}{2}\omega$$

Write out the coefficients $c_n(0)e^{-iE_n t/\hbar}$ for those energies.

Now classically, the harmonic oscillator has a natural frequency ω . That means that whenever ωt is a whole multiple of 2π , the harmonic oscillator is again in the same state as it started out with. Show that the coefficients of the energy eigenfunctions have a natural frequency of $\frac{1}{2}\omega$; $\frac{1}{2}\omega t$ must be a whole multiple of 2π for the coefficients to return to their original values.

Answer:

The coefficients are

$$c_n(0)e^{-i\frac{(2n+1)}{2}\omega t}$$

Now if ωt is 2π , the argument of the exponential equals i times an odd multiple of π . That makes the exponential equal to minus one. It takes until $\omega t = 4\pi$ until the exponential returns to its original value one.

7.1.2.3 Solution schrodsol-c

Question:

Write the full wave function for a one-dimensional harmonic oscillator. Formulae are in chapter 4.1.2.

Answer:

Using the give formulae

$$\Psi(x, t) = \sum_{n=0}^{\infty} c_n(0) e^{-i\frac{(2n+1)\omega t}{2}} h_n(x)$$

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A.28 WKB Theory of Nearly Classical Motion

A.28.1 Solution wkb-a

Question:

Use the equation

$$\frac{1}{\hbar} \int_{\underline{x}=x_1}^{x_2} p_c(\underline{x}) d\underline{x} = n\pi$$

to find the WKB approximation for the energy levels of a particle stuck in a pipe of chapter 3.5.5. The potential V is zero inside the pipe, given by $0 \leq x \leq \ell_x$

In this case, the WKB approximation produces the exact result, since the classical momentum really is constant. If there was a force field in the pipe, the solution would only be approximate.

Answer:

Substituting in $p_c = \sqrt{2mE}$, $x_1 = 0$ and $x_2 = \ell_x$,

$$\frac{1}{\hbar} \sqrt{2mE} \ell_x = n\pi$$

and squaring both sides, the energy is found as $E = n^2 \hbar^2 \pi^2 / 2m\ell_x^2$. That is the same result as in chapter 3.5.5, but obtained in a much easier way.

A.28.2 Solution wkb-b

Question:

Use the equation

$$\frac{1}{\hbar} \int_{x=x_1}^{x_2} p_c(x) dx = (n - \frac{1}{2})\pi$$

to find the WKB approximation for the energy levels of the harmonic oscillator. The potential energy is $\frac{1}{2}m\omega x^2$ where the constant ω is the classical natural frequency. So the total energy, expressed in terms of the turning points $x_2 = -x_1$ at which $E = V$, is $E = \frac{1}{2}m\omega x_2^2$.

In this case too, the WKB approximation produces the exact energy eigenvalues. That, however, is just a coincidence; the classical WKB wave functions are certainly not exact; they become infinite at the turning points. As the example h_{50} above shows, the true wave functions most definitely do not.

Answer:

Substituting in $p_c = \sqrt{2m(E - V)}$, with $V = \frac{1}{2}m\omega^2 x^2$ and $E = \frac{1}{2}m\omega^2 x_2^2$, produces

$$\frac{1}{\hbar} \int_{x=-x_2}^{x_2} m\omega \sqrt{x_2^2 - x^2} dx = (n - \frac{1}{2})\pi$$

The integral can be done by making the substitution $x = x_2 \sin(\alpha)$:

$$\frac{1}{\hbar} m\omega x_2^2 \int_{\alpha=-\pi/2}^{\pi/2} \cos^2 \alpha d\alpha = (n - \frac{1}{2})\pi$$

and the remaining integral is $\frac{1}{2}\pi$:

$$\frac{1}{\hbar} m\omega x_2^2 \frac{1}{2}\pi = (n - \frac{1}{2})\pi$$

So, since $E = \frac{1}{2}m\omega^2 x_2^2$, the energy levels are found to be $E_n = (n - \frac{1}{2})\hbar\omega$. That is exact; the fact that in this case the values of n are counted from one instead of zero is just a matter of notations. Despite the imperfect wave functions, it sure is a lot simpler than the exact derivation of chapter 4.1 as found in its note.

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D.59 Analysis of the ideal gas Carnot cycle

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D.61 Chemical potential in the distributions

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D.64 Spherical harmonics by ladder operators

D.65 How to make Clebsch-Gordan tables

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D.68 Awkward questions about spin

D.69 More awkwardness about spin

D.70 Emergence of spin from relativity

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D.72.1 Existence of a potential

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D.75 Solving the NMR equations

D.76 Harmonic oscillator revisited

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D.80 Hydrogen ground state Stark effect

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D.84 Band gap explanation derivations

Appendix N

Notes

N.1 Why this book?

N.2 History and wish list

N.3 Nature and real eigenvalues

N.4 Are Hermitian operators really like that?

N.5 Why boundary conditions are tricky

N.6 Is the variational approximation best?

N.7 Shielding approximation limitations

N.8 Why the s states have the least energy

N.9 Explanation of the band gaps

N.10 A less fishy story

N.11 Better description of two-state systems

N.12 Second quantization in other books

N.13 Combining angular momentum factors

N.14 The electric multipole problem

N.15 A tenth of a googol in universes

N.16 A single Slater determinant is not exact

N.17 Generalized orbitals

N.18 “Correlation energy”

N.19 Ambiguities in electron affinity

N.20 Why Floquet theory should be called so

N.21 Superfluidity versus BEC

N.22 The mechanism of ferromagnetism

N.23 Fundamental assumption of statistics

N.24 A problem if the energy is given

N.25 The recipe of life

N.26 **Physics of the fundamental commutators**

N.27 **Magnitude of components of vectors**

N.28 **Adding angular momentum components**

N.29 **Clebsch-Gordan tables are bidirectional**

N.30 **Machine language Clebsch-Gordan tables**

N.31 **Existence of magnetic monopoles**

N.32 **More on Maxwell's third law**

N.33 Setting the record straight on alignment

N.34 NuDat 2 data selection

N.35 Auger discovery

N.36 Draft: Cage-of-Faraday proposal

Web Pages

Below is a list of relevant web pages.

1. ENSDF data¹

The Nuclear Data Sheets are an authoritative and comprehensive data source on nuclei. The corresponding Nuclear Data Sheets policies² have been used repeatedly in this book to decide what conventions to take as standard.

2. NIST data³

Authoritative values of physical constants from NIST.

3. NuDat 2 database⁴

Extensive information about nuclei provided by the National Nuclear Data Center.

4. Anthony Stone's Wigner coefficient calculators⁵

The calculator on this site gives exact values for the Wigner 3j, 6j, and 6j symbols. The 3j symbols are readily converted to Clebsch-Gordan coefficients, {N.13}.

5. TUNL Nuclear Data Evaluation Group⁶

Extensive data on light nuclei from $A = 3$ to 20.

6. Wikipedia⁷

Probably this book's primary source of information on about every loose end, though somewhat uneven. Some great, some confusing, some overly technical.

¹<http://www-nds.iaea.org/relnsd/NdsEnsf/QueryForm.html>

²<http://www.nndc.bnl.gov/nds/NDSPolicies.pdf>

³<http://www.nist.gov/pml/data/>

⁴<http://www.nndc.bnl.gov/nudat2/>

⁵<http://www-stone.ch.cam.ac.uk/wigner.html>

⁶<http://www.tunl.duke.edu/nucldata/>

⁷<http://wikipedia.org>

References

- [1] M.R. Spiegel and J. Liu. *Mathematical Handbook of Formulas and Tables*. Schaum's Outline Series. McGraw-Hill, second edition, 1999. 11, 12, 13, 17, 18, 19, 34