Interpretation of the wave function

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One particle without spin in 1 dimension

$\Psi(x)$: Wave function of one particle without the spin coordinate in 1D
$\hookrightarrow x$: coordinate defining the position of the particle in the 1D space

As an example of wave function of one particle in 1 dimension without spin, we can consider the particle in a box of width **L**:

```
In[1]:= psi[x_] = Sqrt[2/L] Sin[ Pi x / L]
```

Out[1]= $\sqrt{2}\sqrt{\frac{1}{L}}\,\text{Sin}\left[\frac{\pi x}{L}\right]$

We assume the wave function to be **normalized**:

$$\int_{\tau} |\Psi(x)|^2 dx = \int_{\tau} \Psi^*(x)\Psi(x) dx = 1$$

The dimension of the wave function is $\mathsf{L}^{-1/2}$.

One particle without spin in 1 dimension

- $|\Psi(x)|^2$: **Probability density** of finding the particle in x
- $|\Psi(x)|^2 dx$: **Probability** of finding the particle in the length element dx around the position x

  $\hookrightarrow$ **Probability** P in a space region $-x_1 \leq x \leq x_2$

$$P = \int_{-x_1}^{x_2} |\Psi(x)|^2 dx = \int_{-x_1}^{x_2} \Psi^*(x)\Psi(x) dx$$

  $\hookrightarrow$ **Probability** P in all the space $\Rightarrow P = 1$

One particle without spin in 3 dimensions

$\Psi(x, y, z)$: Wave function of one particle without spin in 3D
$\hookrightarrow (x, y, z)$: coordinates defining the position of the particle in the 3D space

As an example of wave function of one particle in 3 dimensions without spin, we can consider the particle in a box of dimensions Lx, Ly, Lz:

```
In[3]:= psi3d[x_, y_, z_] = (Sqrt[2/Lx] Sin[Pi x /Lx]) (Sqrt[2/Ly] Sin[Pi y /Ly])
          (Sqrt[2/Lz] Sin[Pi z /Lz])
```

Out[3]= $2\sqrt{2}\sqrt{\frac{1}{Lx}}\sqrt{\frac{1}{Ly}}\sqrt{\frac{1}{Lz}}\,\mathrm{Sin}\left[\frac{\pi x}{Lx}\right]\mathrm{Sin}\left[\frac{\pi y}{Ly}\right]\mathrm{Sin}\left[\frac{\pi z}{Lz}\right]$

We assume the wave function to be **normalized**:

$$\int_{\tau_x}\int_{\tau_y}\int_{\tau_z} |\Psi(x, y, z)|^2 dx\, dy\, dz = 1$$

The dimension of the wave function is $\mathsf{L}^{-3/2}$.

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One particle without spin in 3 dimensions

- $|\Psi(x,y,z)|^2$: **Probability density** of finding the particle in the position (x,y,z)
- $|\Psi(x,y,z)|^2 dx\,dy\,dz$: **Probability** of finding the particle in the volume element $dx\,dy\,dz$ around the position (x,y,z)

  $\hookrightarrow$ **Probability** P in a space region V

$$P = \int\int\int_V |\Psi(x,y,z)|^2 dx\,dy\,dz$$

  $\hookrightarrow$ **Probability** P in all the space $\Rightarrow P = 1$

One particle without spin in 3 dimensions

What if we do not integrate over all coordinates?

$$D(z) = \int_{\tau_x} \int_{\tau_y} |\Psi(x, y, z)|^2 dx\, dy$$

For example, the following function could be defined, in which **we are not integrating over the z coordinate**:

In[7]:= $\mathrm{Dd}[z\_] = \int_0^{Ly} \int_0^{Lx} \mathrm{psi3d}[x, y, z]^2 \, dx \, dy$

Out[7]= $\dfrac{2\,\mathrm{Sin}\left[\frac{\pi z}{Lz}\right]^2}{Lz}$

One particle without spin in 3 dimensions

$$D(z) = \int_{\tau_x} \int_{\tau_y} |\Psi(x, y, z)|^2 dx\, dy$$

Probability density of finding the particle with an specific value of z and every value of x and y.
Physical dimension: L^{-1}.

$D(z)\, dz$: **Probability** of finding the particle in a dz interval around z (for every value of x and y).

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One particle without spin in 3 dimensions

In spherical coordinates (r, θ, ϕ):

For example, we define this function for the particle in all the 3D space, in spherical coordinates:

```
In[9]:= psiesf[r_, t_, p_] = Sqrt[1/(Pi a^3)] Exp[-r/a]
```

Out[9]= $\dfrac{\sqrt{\frac{1}{a^3}}\, e^{-\frac{r}{a}}}{\sqrt{\pi}}$

Physical dimension of $\Psi(r, \theta, \phi)$: $L^{-3/2}$

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One particle without spin in 3 dimensions

- $|\Psi(r,\theta,\phi)|^2$: **Probability density** at the point (r,θ,ϕ)
- $|\Psi(r,\theta,\phi)|^2\, r^2\, \sin\theta\, dr\, d\theta\, d\phi$: **Probability** in a volume element $r^2\, \sin\theta\, dr\, d\theta\, d\phi$

  $\hookrightarrow$ **Probability** P in a space region V

$$P = \int\int\int_V |\Psi(r,\theta,\phi)|^2 r^2\, \sin\theta\, dr\, d\theta\, d\phi$$

What if we do **not** integrate over the radial distance from the origin?

$$P(r) = \int_0^{2\pi} \int_0^{\pi} |\Psi(r,\theta,\phi)|^2 \; r^2 \; \sin\theta \, d\theta \, d\phi$$

If we integrate over the directions in space except for the radial distance to the origin, we get this probability function:

In[13]:= $\text{Pp}[r\_] = \int_0^{2\,\text{Pi}} \int_0^{\text{Pi}} \text{psiesf}[r, t, p]^2 \, r^2 \, \text{Sin}[t] \, d t \, d p$

Out[13]= $\frac{4\, e^{-\frac{2r}{a}} r^2}{a^3}$

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One particle without spin in 3 dimensions

$$P(r) = \int_0^{2\pi} \int_0^{\pi} |\Psi(r,\theta,\phi)|^2 \; r^2 \; \sin\theta \, d\theta \, d\phi$$

Probability density of finding the particle at a specific distance r and in all directions (value of θ and ϕ).
Physical dimension: L^{-1}.
$\hookrightarrow$ **Radial distribution function** $P(r)$

$P(r)\,dr$: **Probability** of finding the particle at a distance from the origin between r and $r+dr$, and in every direction of the space.

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N particles without spin in a 1D space

$\Psi(x_1, x_2, ..., x_N)$: Wave function of the system
$\hookrightarrow$ x_1: coordinate determining the position of the first particle
$\hookrightarrow$ x_2: coordinate determining the position of the second particle
$\hookrightarrow$ ...

If for example now we consider 4 particles in a one-dimensional box of width L:

```
In[15]:= psiN[x1_, x2_, x3_, x4_] =
  Sqrt[2 / L] Sin[Pi x1 / L] Sqrt[2 / L] Sin[Pi x2 / L]
   Sqrt[2 / L] Sin[Pi x3 / L] Sqrt[2 / L] Sin[Pi x4 / L]
```

Out[15]= $\frac{4 \, \text{Sin}\left[\frac{\pi \, x1}{L}\right] \text{Sin}\left[\frac{\pi \, x2}{L}\right] \text{Sin}\left[\frac{\pi \, x3}{L}\right] \text{Sin}\left[\frac{\pi \, x4}{L}\right]}{L^2}$

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N particles without spin in a 1D space

Normalization condition of the wave function

$$\underbrace{\int\int\int\ldots\int}_{\text{All space}} |\Psi(x_1, x_2, ..., x_N)|^2 \, dx_1 \, dx_2 \ldots dx_N = 1$$

involves a multidimensional integral over the N dimensions of the space. The physical dimension of this function is $\mathsf{L}^{-N/2}$

N particles without spin in a 1D space

- $|\Psi(x_1, x_2, ..., x_N)|^2$: **Probability density** of finding the particle 1 in x_1, the particle 2 in x_2, etc.
- $|\Psi(x_1, x_2, ..., x_N)|^2 \, dx_1 \, dx_2 ... dx_N$: **probability** of finding the particle 1 along the length element dx_1 around the position x_1, the particle 2 along the length element dx_2 around the position x_2, etc.

  $\hookrightarrow$ **Probability** P within a distance l of the N-dimensional space

$$P = \underbrace{\int \int \int \dots \int_l}_{N \text{ integrals}} |\Psi(x_1, x_2, ..., x_N)|^2 \, dx_1 \, dx_2 ... dx_N$$

N particles without spin in a 1D space

What if we integrate only over the coordinate of a single particle?

$$D_1(x_2, x_3, ..., x_N) = \int |\Psi(x_1, x_2, ..., x_N)|^2 \, dx_1$$

For example, integrating only over the coordinates of the particle 1, the following function could be defined, which will be a function of the coordinates of the other three particles:

```
In[19]:= Dn[x2_, x3_, x4_] = ∫_0^L psiN[x1, x2, x3, x4]^2 dx1
```

$$\text{Out[19]=} \frac{8\,\mathrm{Sin}\left[\frac{\pi\,x2}{L}\right]^2 \mathrm{Sin}\left[\frac{\pi\,x3}{L}\right]^2 \mathrm{Sin}\left[\frac{\pi\,x4}{L}\right]^2}{L^3}$$

N particles without spin in a 1D space

$$D_1(x_2, x_3, ..., x_N) = \int |\Psi(x_1, x_2, ..., x_N)|^2 \, dx_1$$

Probability density of finding the particle 2 in x_2, and the 3 in x_3, etc., when the particle 1 is at any position of the space.
Physical dimension: L^{-N+1}.

$$D_1(x_2, x_3, ..., x_N) \, dx_2 \, dx_3 \, ...dx_N$$

Probability of finding the particle 2 in a length element dx_2 around the position x_2, the particle 3 in a length element dx_3 around the position x_3, etc., when the particle 1 is at any position of the space.

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N particles without spin in a 1D space

What if we do not integrate over the coordinate of one particle?

$$D(x_1) = \underbrace{\int\int\int\dots\int}_{N-1 \text{ integrals}} |\Psi(x_1, x_2, ..., x_N)|^2 \, dx_2 \dots dx_N$$

Integrating over all the coordinates except those of the particle 1, the following function could be defined, which will be a function only of the coordinates of particle 1:

In[20]:= Dnn[x1_] = $\int_0^L \int_0^L \int_0^L$ psiN[x1, x2, x3, x4]^2 dx2 dx3 dx4

Out[20]= $\frac{2\,\text{Sin}\left[\frac{\pi\, x1}{L}\right]^2}{L}$

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N particles without spin in a 1D space

$$D(x_1) = \underbrace{\int\int\int\dots\int}_{N-1 \text{ integrals}} |\Psi(x_1, x_2, ..., x_N)|^2 \, dx_2 \dots dx_N$$

Probability density of finding the particle 1 in x_1 when the rest of the particles are at any position of the space.
Physical dimension: L^{-1}.

$$D(x_1)\, dx_1$$

Probability of finding the particle 1 at a length element dx_1 around the position x_1 when the rest of the particles are at any position of the space.

N particles without spin in a 1D space

What if we do not integrate over the coordinates of two particles?

$$D'(x_1, x_2) = \underbrace{\int\int\int \ldots \int}_{N-2 \text{ integrals}} |\Psi(x_1, x_2, ..., x_N)|^2 \, dx_3 \, dx_4 \, ... \, dx_N$$

Probability density of finding the particle 1 in x_1 and the particle 2 in x_2 when the rest of the particles are at any position of the space.
Physical dimension: L^{-2}.

$$D'(x_1, x_2) \, dx_1 \, dx_2$$

Probability of finding the particle 1 in a length element dx_1 around x_1 and the particle 2 in a length element dx_2 around x_2, when the rest of the particles are at any position of the space.

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N particles without spin in a 1D space

What if now we integrate over the coordante of the particle 2?

$$D(x_1) = \int D'(x_1, x_2) dx_2$$

Probability density of finding the particle 1 in x_1 when the rest of the particles are at any position of the space.
Physical dimension: L^{-1}.

N particles without spin in a 1D space

We recover the previous expression!!

$$
\begin{aligned}
D(x_1) &= \int D'(x_1, x_2) dx_2 = \\
&= \int \underbrace{\int\int\int \ldots \int}_{N-2} |\Psi(x_1, x_2, ..., x_N)|^2 \, dx_3 \, dx_4 \ldots dx_N \, dx_2 \\
&= \underbrace{\int\int\int \ldots \int}_{N-1} |\Psi(x_1, x_2, ..., x_N)|^2 \, dx_2 \, dx_3 \, dx_4 \ldots dx_N
\end{aligned}
$$

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N particles without spin in a 3D space

$\Psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N)$: Wave function of the system
$\hookrightarrow$ $\vec{r}_1$: position vector of the first particle
$\hookrightarrow$ $\vec{r}_2$: position vector of the second particle
$\hookrightarrow$ ...

If we now consider 2 particles in a three-dimensional box of dimensions Lx, Ly, Lz, we can define the following wave function for the system:

```
In[22]:= psiN3d[x1_, y1_, z1_, x2_, y2_, z2_] =
  Sqrt[2/Lx] Sin[Pi x1 /Lx] Sqrt[2/Ly] Sin[Pi y1 /Ly] Sqrt[2/Lz]
   Sin[Pi z1 /Lz] Sqrt[2/Lx] Sin[Pi x2 /Lx] Sqrt[2/Ly] Sin[Pi y2 /Ly]
   Sqrt[2/Lz] Sin[Pi z2 /Lz]
```

Out[22]= $$\frac{8\,\mathrm{Sin}\left[\frac{\pi\,x1}{Lx}\right]\mathrm{Sin}\left[\frac{\pi\,x2}{Lx}\right]\mathrm{Sin}\left[\frac{\pi\,y1}{Ly}\right]\mathrm{Sin}\left[\frac{\pi\,y2}{Ly}\right]\mathrm{Sin}\left[\frac{\pi\,z1}{Lz}\right]\mathrm{Sin}\left[\frac{\pi\,z2}{Lz}\right]}{Lx\,Ly\,Lz}$$

N particles without spin in a 3D space

Normalization condition of the wave function

$$\underbrace{\int\int\int\dots\int}_{\text{All the space}} |\Psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N)|^2 \, d\vec{r}_1 \, d\vec{r}_2 \dots d\vec{r}_N = 1$$

involves a multidimensional integral over the $3N$-dimensional space. The physical dimension of this function is $\mathsf{L}^{-3N/2}$

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N particles without spin in a 3D space

- $|\Psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N)|^2$: **Probability density** of finding the particle 1 in $\vec{r}_1$, the particle 2 in $\vec{r}_2$, etc.
- $|\Psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N)|^2 \, d\vec{r}_1 \, d\vec{r}_2 \dots d\vec{r}_N$: **Probability** of finding the particle in a volume element $d\vec{r}_1$ around $\vec{r}_1$, and the partcile 2 in a volume element $d\vec{r}_2$ around $\vec{r}_2$, etc.

  $\hookrightarrow$ **Probability** P in the volume V of the $3N$-dimensional space.

$$P = \underbrace{\int \int \int \dots \int_V}_{3N \text{ integrals}} |\Psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N)|^2 \, d\vec{r}_1 \, d\vec{r}_2 \dots d\vec{r}_N$$

N particles without spin in a 3D space

What if we do not integrate over the coordinates of one particle?

$$D(\vec{r}_1) = \underbrace{\int\int\int\dots\int}_{3N-3 \text{ integrals}} |\Psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N)|^2 \, d\vec{r}_2 \, d\vec{r}_3 \, d\vec{r}_4 \dots d\vec{r}_N$$

Probability density of finding the particle 1 in the position $\vec{r}_1$ when the rest of the particles are in any position of the space.
Physical dimension: L^{-3}.

$D(\vec{r}_1)\, d\vec{r}_1$: **Probability density** of finding the particle 1 in a volume element $d\vec{r}_1$ centered around $\vec{r}_1$ when the rest of the particles are in any position of the space.

N particles without spin in a 3D space

What if we do not integrate over the coordinates of two particles?

$$D'(\vec{r}_1, \vec{r}_2) = \underbrace{\int\int\int \dots \int}_{3N-6 \text{ integrals}} |\Psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N)|^2 \, d\vec{r}_3 \, d\vec{r}_4 \dots d\vec{r}_N$$

Probability density of finding the particle 1 in $\vec{r}_1$ and the particle 2 in $\vec{r}_2$ when the rest of the particles are in any position of the space.
Physical dimension: L^{-6}.

$D'(\vec{r}_1, \vec{r}_2) \, d\vec{r}_1 \, d\vec{r}_2$: **Probability** of finding the particle 1 in a volume element $d\vec{r}_1$ centered around $\vec{r}_1$ and the particle 2 in a volume element $d\vec{r}_2$ centered around $\vec{r}_2$ when the rest of the particles are in any position of the space.

N particles without spin in a 3D space

What if we integrate now over the coordinates of particle 2?

$$D(\vec{r}_1) = \int\int\int D'(\vec{r}_1, \vec{r}_2) d\vec{r}_2$$

Probability density of finding the particle 1 in the position $\vec{r}_1$ when the rest of the particles are in any position of the space.
Physical dimension: L^{-3}.

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N particles without spin in a 3D space

We recover the previous expression!!

$$
\begin{aligned}
D(\vec{r}_1) &= \int\int\int D'(\vec{r}_1, \vec{r}_2) d\vec{r}_2 = \\
&= \int\int\int \underbrace{\int\int\int \dots \int}_{3N-6} |\Psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N)|^2 \, d\vec{r}_3 \, d\vec{r}_4 \dots d\vec{r}_N \, d\vec{r}_2 \\
&= \underbrace{\int\int\int \dots \int}_{3N-3} |\Psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N)|^2 \, d\vec{r}_2 \, d\vec{r}_3 \, d\vec{r}_4 \dots d\vec{r}_N
\end{aligned}
$$

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