Chapter 3: Observables with Continuous Eigenvalues

In the last chapter we worked with QM observables with discrete eigenvalue spectra. Let us now try to incorporate observables with continuous eigenvalues. The simplest examples of such observables are, for instance, $\hat{z}$, the $z-$component of position, or $\hat{p}_x$, the $x-$component of momentum, etc. Such observables are also represented by hermitian matrices whose eigenvalues can assume any real values, in general, within $-\infty$ and ∞. The dimensionality of the vector space spanned by the eigenkets of these observables is therefore (uncountably) infinite. As such the rigorous mathematics of such a vector space is rather treacherous. Fortunately however, most of the results that we worked out for the discrete spectra in the previous chapter can immediately be generalized to the continuous spectra. The cases where such straight forward generalizations may not hold and may lead to errors will be indicated specifically.

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The transition from the discrete to the continuous eigen-spectra is the main topic of this chapter. For this, first let us talk briefly about the continuous analogue of the Kronecker-Delta δ_{ij}, namely the Dirac δ-Function.

Dirac δ-Function

The Dirac δ-function in one dimension is defined by

$$\delta(x) = \begin{cases} 0 & x \neq 0 \\ \infty & x = 0 \end{cases}$$

together with

$$\int_{x_1}^{x_2} \delta(x) dx = 1,$$

provided $0 \in [x_1, x_2]$ (and zero otherwise). It is an even function which is infinitely peaked at $x = 0$ and has unit total area. The most important property of the δ-function that immediately follows from its definition is

$$\int_{-\infty}^{\infty} \delta(x) f(x) dx = f(0), = f(0) \underbrace{\int_{-\infty}^{+\infty} \delta(x) dx}_{1}$$

for any function $f(x)$. This is easy to understand as it does not matter what values the function $f(x)$ take except at $x = 0$, since the δ-function itself is non-vanishing only at this point. So in effect $\delta(x) f(x) \equiv \delta(x) f(0)$, so that $f(0)$ can be pulled outside the integral. The right hand side of the above relation is then reached. This relation can also be generalised as

$$\int_{-\infty}^{\infty} \delta(x - x') f(x) dx = f(x'),$$

where $\delta(x - x')$ is the delta function which peaks at $x = x'$. Mathematically the δ-function is too singular to be called a proper function; many prefer instead call it the δ-distribution. As long as the δ-distribution appears inside an integral which is eventually integrated, it is well-defined and can be viewed as a generalised function. There are however caveats, for example, when a product of two δ-distributions, whose arguments become zero simultaneously, appear as an integral. We will talk about such situations if and when they occur.

警告

There are a number of ways to visualise the δ-distribution mathematically. One can, for example, view it as the limit of a Gaussian

$$\delta(x) = \lim_{\sigma \to 0} \frac{1}{\sqrt{2\pi}\sigma} e^{-x^2/2\sigma^2},$$

or a Lorentzian

$$\delta(x) = \lim_{\epsilon \to 0} \frac{1}{\pi} \frac{\epsilon}{x^2 + \epsilon^2}.$$

An extremely useful integral representation of the δ-distribution can be derived from the Fourier transformation of functions. Recall the Fourier transformation $\tilde{f}(k)$ of a general function $f(x)$

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} f(x) dx.$$

The transformation being reversible we can also write

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} \tilde{f}(k) dk.$$

Reusing the first relation on the right hand side of the above equation one arrives at

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ik(x-x')} f(x') dk dx',$$

which, when identified with the basic definition of the δ-distribution, immediately yields

$\delta(x-x') = \langle x | x' \rangle$

$$\delta(x - x') = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-x')} dk.$$

From this relation one can also derive yet another representation by carrying out the integration as a limit,

$$\delta(x - x') = \lim_{N \to \infty} \frac{\sin N(x - x')}{\pi(x - x')}.$$

Below we list some of the properties of the δ-distribution which we will use very often in the next sections and also later. Students are therefore recommended to try to derive each of the following relations as an exercise.

- $\int_{-\infty}^{+\infty} f(x)\delta(x)dx = f(0),$
- $\delta(ax) = \frac{1}{|a|}\delta(x),$
- $\int_{-\infty}^{+\infty} \delta(x-y)\delta(x)dx = \delta(y),$
- $\int_{-\infty}^{+\infty} f(x)\frac{d^n\delta(x)}{dx^n}dx = (-1)^n \frac{d^n f(x)}{dx^n}\bigg|_{x=0},$
- $\delta(f(x)) = \sum_i \frac{\delta(x-x_i)}{|f'(x_i)|},$
- $\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{ikx}dk,$
- $\frac{d\theta(x)}{dx} = \delta(x).$

Position Operator and Position Space

Recall the Stern-Gerlach experiment discussed in chapter 2, where we saw that an arbitrary spin state jumps into one of the $|S_z;\pm\rangle$ states, the eigenstates of the $\hat{S}_Z$ operator, when subjected to an SG$_z$ apparatus. In this sense a measurement in quantum mechanics is essentially a filtering process. We now extend this idea to measurements of observables with continuous eigen-spectra, for example the position (or co-ordinate) operator in one dimension, $\hat{x}$. An eigenket $|x'\rangle$ of this operator satisfies the eigenvalue equation,

$$\hat{x}|x'\rangle = x'|x'\rangle,$$

where x' is just a number (eigenvalue) with the dimension of length. To understand this relation, consider a highly idealised selective measurement of $\hat{x}$, in which we place a tiny detector that clicks only when a QM particle is precisely at the location x' and *nowhere else*. Immediately after the detector clicks we can therefore say that the state of the particle is described by $|x'\rangle$. This in turn also means that any other eigenket of $\hat{x}$, for example, $|x''\rangle$, is automatically orthogonal to $|x'\rangle$, as it should be. Just as in the case of discrete eigenkets, the position eigenkets are postulated to form a complete set. These are the basis kets describing the infinite dimensional Hilbert space known as the position space.

In the following table we summarise the generalizations of the relations for the observables with discrete eigen-spectra to those for the position operator in one dimension. Make sure that the conventions for the representations of numbers, kets and operators in the continuous basis are clearly understood.

	Discrete Spectra	Continuous Spectra
Eigenvalue Eqn.	$\hat{O}\lvert e_i\rangle = \lambda_i \lvert e_i\rangle$ $\hat{O} = \hat{O}^\dagger$ $\lambda_i \in \mathbb{R}$ $\{\lvert e_i\rangle\} \to$ basis	$\hat{x}\lvert x\rangle = x\lvert x\rangle$ $\hat{x} = \hat{x}^\dagger$ $x \in \mathbb{R}$ $\{\lvert x\rangle\} \to$ basis
Completeness	$\sum_{i=1}^{n} \lvert e_i\rangle\langle e_i\rvert = \hat{I}$	$\int_{-\infty}^{\infty} dx\, \lvert x\rangle\langle x\rvert = \hat{I}$
Orthonormality	$\langle e_i \vert e_j\rangle = \delta_{ij}$	$\langle x \vert x'\rangle = \delta(x-x')^{(*)}$
Decomposition of		
(i) Statevectors	$\lvert\psi\rangle = \sum_{i=1}^{n} \psi_i \lvert e_i\rangle$ $\psi_i = \langle e_i\vert\psi\rangle$ $\sum_{i=1}^{n} \lvert\psi_i\rvert^2 = 1$	$\lvert\psi\rangle = \int_{-\infty}^{\infty} dx\, \psi(x)\lvert x\rangle$ $\psi(x) = \langle x\vert\psi\rangle$ $\int_{-\infty}^{\infty} dx\, \lvert\psi(x)\rvert^2 = 1^{(**)}$
(ii) Operators	$\langle e_i\vert\hat{M}\vert e_j\rangle = M_{ij}$ $\langle e_i\vert\hat{O}\vert e_j\rangle = \lambda_i\delta_{ij}$	$\langle x\vert\hat{M}\vert x'\rangle = M(x,x')^{(***)}$ $\langle x\vert\hat{x}\vert x'\rangle = x\delta(x-x')$
Expectation Value	$\langle\hat{O}\rangle = \langle\psi\vert\hat{O}\vert\psi\rangle$ $= \sum_{i=1}^{n} \lambda_i \lvert\psi_i\rvert^2$	$\langle\hat{x}\rangle = \langle\psi\vert\hat{x}\vert\psi\rangle$ $= \int_{-\infty}^{\infty} dx\, x\lvert\psi(x)\rvert^2$

Note especially the relations marked with asterisk(s).
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First compare the orthonormality relations in discrete and continuous spaces marked with $^{(*)}$. While for the former we easily get $\langle e_i|e_i\rangle = 1$, for the later the basis-kets $|x\rangle$ are simply not normalisable due to the presence of the δ-distribution on the right hand side. In other words the inner product of a position eigenket with itself is not defined. This means that such kets do not actually belong to the usual Hilbert that we talked about in the last chapter. One actually has to build up a whole new framework (the notion of a Rigged Hilbert Space) to not only incorporate such kets, but also to be able to build an arbitrary normalised QM state ($|\psi\rangle$ for example) out of the continuous superposition of these kets. The rigorous mathematics involved here is highly non trivial and beyond the scope of this course. So for the time being we will simply accept that all the relations in the table above are mathematically realisable.

Next take a look at the decomposition of an arbitrary normalised state vector, especially at the component of $|\psi\rangle$ along a basis state (ψ_i in discrete basis and $\psi(x)$ in continuous basis). The quantity $|\psi_i|^2$ is interpreted as the probability that $|\psi\rangle$ will be thrown into the state $|e_i\rangle$ when $\hat{O}$ is measured. For the continuous case however $|\psi(x)|^2\, dx$ is interpreted as the probability that the particle described by $|\psi\rangle$ will be found within a narrow interval dx around x, when we measure its position (i.e.~$\hat{x}$). The relation marked with $^{(**)}$ in the table is therefore the probability to finding the particle anywhere between $-\infty$ and ∞, which should be 1. The function $\psi(x)$ is known as the wave function in position space for the particle described by $|\psi\rangle$.

Finally consider the matrix element $M(x,x')$ of an arbitrary operator $\hat{M}$ in the position space marked by (***) in the table, which, as such, is a function of two variables x and x'. This means the quantity $\langle\psi_1|\hat{M}|\psi_2\rangle$ can be written in terms of the wavefunctions of $|\psi_1\rangle$ and $|\psi_2\rangle$ as follows:

$$\begin{aligned}\langle\psi_1|\hat{M}|\psi_2\rangle &= \int\limits_{-\infty}^{\infty} dx \int\limits_{-\infty}^{\infty} dx' \, \langle\psi_1|x\rangle\langle x|\hat{M}|x'\rangle\langle x'|\psi_2\rangle \\ &= \int\limits_{-\infty}^{\infty} dx \int\limits_{-\infty}^{\infty} dx' \, \psi_1^*(x) M(x,x')\psi_2(x').\end{aligned}$$

An enormous simplification of the above expression takes place if $\hat{M}$ is a function of $\hat{x}$. The position operator itself is just a multiplicative factor $x \in \mathbb{R}$ in the position space as is clear from its eigenvalues equation. 倍增的 Utilising this, if, for example, $\hat{M} = \hat{x}^n$, leading to $M(x,x') = x^n\delta(x-x')$, then the double integral reduces to a single integral

$$\langle\psi_1|\hat{M}|\psi_2\rangle = \int\limits_{-\infty}^{\infty} dx \, \psi_1^*(x) x^n \psi_2(x).$$

In general, if $\hat{M} = f(\hat{x})$, then

$$\langle\psi_1|f(\hat{x})|\psi_2\rangle = \int\limits_{-\infty}^{\infty} dx \, \psi_1^*(x) f(x) \psi_2(x).$$

Note especially that while $f(\hat{x})$ is an operator, $f(x)$ is just a function of x. At this point we can also ask, how the momentum operator $\hat{p}$ looks when written in position space. A such $\langle x|\hat{p}|x'\rangle$ is to be derived utilising the basic definition of momentum as a generator of infinitesimal translation. We will derive this explicitly as an exercise for this chapter later. However you can easily check yourself that $p(x) = -i\hbar\frac{d}{dx} + f(x)$, where $f(x)$ is any function of x, is consistent with the commutation relation $[\hat{x},\hat{p}] = i\hbar$. You can show this consistency for an arbitrary state vector $|\psi\rangle$ in the position space by showing that the following relation holds:

$$\langle x|[\hat{x},\hat{p}]|\psi\rangle = i\hbar\langle x|\psi\rangle = i\hbar\psi(x).$$

We choose the simplest possibility where $f(x) = 0$ so that

$$\langle x|\hat{p}|x'\rangle = -i\hbar\frac{d}{dx}\,\delta(x-x').$$

This leads to the identity

$$\langle\psi_1|\hat{p}|\psi_2\rangle = \int\limits_{-\infty}^{\infty} dx \, \psi_1^*(x)\left(-i\hbar\frac{d}{dx}\right)\psi_2(x).$$

By applying this identity repeatedly one can also show that

$$\langle x|\hat{p}^n|x'\rangle = -i\hbar\frac{d^n}{dx^n}\,\delta(x-x'),$$

leading to

$$\langle\psi_1|\hat{p}^n|\psi_2\rangle = \int\limits_{-\infty}^{\infty} dx \, \psi_1^*(x)(-i\hbar)^n\left(\frac{d^n}{dx^n}\right)\psi_2(x).$$

You are recommended to check yourself that you are able to derive all of these relations by yourself.

Momentum Space and Change of Basis

The momentum space, in an exactly similar way as the position space, is described by the continuous eigenkets $|p\rangle$ of the momentum operator $\hat{p}$. Here $\hat{p}$ represents the momentum operator in one dimension ($\hat{p_x}$ for example). We can get all the relevant relations for the momentum space by simply replacing x with p in the corresponding relations for position space that we listed in the table in the previous section. *The only change that is necessary to incorporate* is the representation of the momentum space wavefunction for an arbitrary state vector ψ as

$$\langle p|\psi\rangle = \tilde{\psi}(p),$$

since the actual functional form of $\psi(x)$ is not necessarily the same as that of $\tilde{\psi}(p)$. In fact we will soon see that $\psi(x)$ and $\tilde{\psi}(p)$ are Fourier transforms of each other. The quantity $|\tilde{\psi}(p)|^2\, dp$ is to be interpreted as the probability to finding the momentum of the system described by $|\psi\rangle$ within a narrow interval dp around p.
The matrix elements of any general operator $\hat{M}$ in the momentum space have a simpler form if $\hat{M} = f(\hat{p})$. This can be shown in an exactly similar way as we did for the position space. The position operator $\hat{x}$ in the momentum-space is given as $x(p) = i\hbar\frac{d}{dp}$.
Finally, just as in the discrete case, let us talk about the change of basis from $\{|x\rangle\} \to \{|p\rangle\}$. For this we need to construct the matrix elements $\langle x|p\rangle$ of the Hopping-matrix in the following way. We start with the eigenvalue equation for the momentum operator $\hat{p}|p\rangle = p|p\rangle$. Multiplying this relation with $\langle x|$ from left and introducing the completeness relation in the position space in between $\hat{p}$ and $|p\rangle$ we get,

$\int_{-\infty}^{+\infty} |x\rangle\langle x|\, dx = \mathbb{1}$

$$\langle x|\hat{p}|p\rangle = \int_{-\infty}^{\infty} dx'\, \langle x|\hat{p}|x'\rangle\langle x'|p\rangle = p\langle x|p\rangle.$$

Recall that $\langle x|\hat{p}|x'\rangle = -i\hbar\frac{d}{dx}\,\delta(x-x')$. Utilising this and carrying out the integaration over x' we finally get

$$\frac{d}{dx}\langle x|p\rangle = \frac{ip}{\hbar}\langle x|p\rangle.$$

This is a first-order linear differential equation in $\langle x|p\rangle$ which can be solved with an exponential ansatz yielding

$$\langle x|p\rangle = C\exp\left(\frac{ixp}{\hbar}\right).$$

The constant C is $\frac{1}{\sqrt{2\pi\hbar}}$, which can be evaluated from

$= \int_{-\infty}^{+\infty} \langle x|p\rangle\langle p|x'\rangle\, dp = \int_{-\infty}^{+\infty} dp\, C\exp\left(\frac{ixp}{\hbar}\right) C^*\exp\left(\frac{-ix'p}{\hbar}\right)$

$$\delta(x-x') = \langle x|x'\rangle = \int_{-\infty}^{\infty} dp\, \langle x|p\rangle\langle p|x'\rangle,$$

$= |C|^2 \int_{-\infty}^{+\infty} dp\, \exp\left(\frac{i(x-x')p}{\hbar}\right)$

if we choose it to be real without any loss of generality. Note that you have to utilise the relation $p = \hbar k$ to deduce the above. Similarly,

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp\left(-\frac{ixp}{\hbar}\right).$$

Utilising these two relations we also have

$$\psi(x) = \langle x|\psi\rangle = \int_{-\infty}^{\infty} dp\, \langle x|p\rangle\langle p|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dp\, \exp\left(\frac{ixp}{\hbar}\right)\tilde{\psi}(p)$$

and

$$\tilde{\psi}(p) = \langle p|\psi\rangle = \int_{-\infty}^{\infty} dx\ \langle p|x\rangle\langle x|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx\ \exp\left(-\frac{ixp}{\hbar}\right)\psi(x).$$

This clearly shows, as we already mentioned before, that $\psi(x)$ and $\tilde{\psi}(p)$ are Fourier transforms of each other.

Generalisation to Three Dimensions

So far we concentrated only on position and momentum operators in one dimension. We now generalise those results to three dimensions in the following way.
In three dimensions we can associate three different position operators $\hat{x}$, $\hat{y}$ and $\hat{z}$ associated to the measurement of the components of the position-vector $\vec{x}$ of a particle along the directions x, y and z. For convenienece of representation we generalise these operators as $\hat{x}_i$, by identifying $\hat{x}_1 = \hat{x}$, $\hat{x}_2 = \hat{y}$ and $\hat{x}_3 = \hat{z}$ respectively. Each of these operators satisfy $\hat{x}_i|x_i\rangle = x_i|x_i\rangle$. Since they also mutually commute with each other,

$$[\hat{x}_i, \hat{x}_j] = \hat{0},\ \ \forall\, i, j,$$

one can conceive of a simultaneous eigenket of these. We express this simultaneous eigenket as $|\mathbf{x}\rangle \equiv |x_1, x_2, x_3\rangle$, which satisfies $\hat{x}_i|\mathbf{x}\rangle = x_i|\mathbf{x}\rangle\ \forall\, i$. Additionally, we can combine the three $\hat{x}_i$'s to form the so-called vector-operator, which is nothing other than a collection of three one dimensional operators. We express this vector-operator as $\hat{\vec{x}}$. The eigenvalue equation for $\hat{\vec{x}}$ can then be written as

$$\hat{\vec{x}}|\mathbf{x}\rangle = \vec{x}|\mathbf{x}\rangle,$$

where the eigenvalue now is the three dimesional vector $\vec{x}$ with components x_1, x_2 and x_3. The orthonormality and the completeness relations for these eigenkets are

$$\langle \mathbf{x}|\mathbf{x}'\rangle = \delta^3(\vec{x} - \vec{x}'),\ \ \int d^3x\ |\mathbf{x}\rangle\langle\mathbf{x}| = \hat{I}$$

respectively, where $\delta^3(\vec{x} - \vec{x}')$ is the three-diemnsional δ-function

$$\delta^3(\vec{x} - \vec{x}') = \delta(x_1 - x_1')\delta(x_2 - x_2')\delta(x_3 - x_3').$$

For the momentum space we simply replace x's with p's in all of the relations written above:

- Mutual Commutation: $[\hat{p}_i, \hat{p}_j] = \hat{0},\ \ \forall\, i, j$
- Eigenvalue Eqn. for $\hat{p}_i$: $\hat{p}_i|\mathbf{p}\rangle = p_i|\mathbf{p}\rangle$
- Eigenvalue Eqn. for $\hat{\vec{p}}$: $\hat{\vec{p}}|\mathbf{p}\rangle = \vec{p}|\mathbf{p}\rangle$
- Orthonormality: $\langle\mathbf{p}|\mathbf{p}'\rangle = \delta^3(\vec{p} - \vec{p}')$
- Completeness: $\int d^3p\ |\mathbf{p}\rangle\langle\mathbf{p}| = \hat{I}$.

The non-commutivity of the position and momentum operators, which exists only between the same components of these operators, can now be generalised with the help of δ_{ij} as

$$[\hat{x}_i, \hat{p}_j] = (i\hbar\delta_{ij})\,\hat{I},\ \ \forall\, i, j.$$

This relation together with the previous two commutators, $[\hat{x}_i, \hat{x}_j] = \hat{0}$ and $[\hat{p}_i, \hat{p}_j] = \hat{0}$, form the cornerstone of quantum mechanics. They are often known as the fundamental quantum conditions or the fundamental commutation relations.

Next we write down the decomposition of an arbitrary state vector in terms of the simultaneous eigenkets of the position space as

$$|\psi\rangle = \int d^3x\, |\mathbf{x}\rangle\langle\mathbf{x}|\psi\rangle = \int d^3x\, \psi(\mathbf{x})|\mathbf{x}\rangle,$$

and of the momentum space as

$$|\psi\rangle = \int d^3p\, |\mathbf{p}\rangle\langle\mathbf{p}|\psi\rangle = \int d^3p\, \tilde{\psi}(\mathbf{p})|\mathbf{p}\rangle.$$

The $\psi(\mathbf{x})$ and the $\tilde{\psi}(\mathbf{p})$ are identified as the wave functions in the position and momentum space respectively. These are, as before, Fourier transforms of each other:

$$\psi(\mathbf{x}) = \left(\frac{1}{2\pi\hbar}\right)^{3/2} \int d^3p\, \exp\left(\frac{i\vec{p}\cdot\vec{x}}{\hbar}\right)\tilde{\psi}(\mathbf{p})$$
$$\tilde{\psi}(\mathbf{p}) = \left(\frac{1}{2\pi\hbar}\right)^{3/2} \int d^3x\, \exp\left(-\frac{i\vec{p}\cdot\vec{x}}{\hbar}\right)\psi(\mathbf{x}).$$

These expressions can be obtained utilising the three-dimensional analog of the function $\langle x|p\rangle$, namely

$$\langle\mathbf{x}|\mathbf{p}\rangle = \left(\frac{1}{2\pi\hbar}\right)^{3/2} \exp\left(\frac{i\vec{p}\cdot\vec{x}}{\hbar}\right).$$

As for the vector-operators, the momentum operator, for example, can be generalised as

$$\langle\mathbf{x}|\hat{\vec{p}}|\mathbf{x}'\rangle = \left(-i\hbar\vec{\nabla}\right)\delta^3(\vec{x}-\vec{x}'),$$

in the position space, leading to

$$\langle\psi_1|\hat{\vec{p}}|\psi_2\rangle = \int d^3x\, \psi_1^*(\mathbf{x})\left(-i\hbar\vec{\nabla}\right)\psi_2(\mathbf{x})$$

for two arbitrary state-vectors $|\psi_1\rangle$ and $|\psi_2\rangle$. In momentum space the same looks like

$$\langle\psi_1|\hat{\vec{p}}|\psi_2\rangle = \int d^3p\, \tilde{\psi}_1{}^*(\mathbf{p})\,(\vec{p})\,\tilde{\psi}_2(\mathbf{p}).$$

Finally, it is interesting to take a look at the dimesion of the wavefunctions (position as well as momentum) of an arbitray state-vector $|\psi\rangle$ in one- and three-dimensions. Provided $|\psi\rangle$ is normalised, the normalisation condition in one-dimension, $\int dx\, |\psi(x)|^2 = 1$, clearly indicates that the dimension of $\psi(x)$ must be $(\mathrm{length})^{-1/2}$. On the other hand, the same condition in three-dimensions, $\int d^3x\, |\psi(\mathbf{x})|^2 = 1$, indicates that the dimension of $\psi(\mathbf{x})$ is $(\mathrm{length})^{-3/2}$.

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