# Quantum Mechanics 2 (PHY 4423) Lecture 1 (Jan 19) Spring 2021

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**Abstract**

REVIEW: (a) inner product of two vectors in the Hilbert space; (b) matrix representations of Dirac ket and bra vectors, matrix representations of operators; (c) outer product of ket and bra vectors; (d) position and momentum operators in position and momentum representations; (e) Schroedinger equation in position and momentum representations. Background assumed from previous course on Quantum Mechanics 1: time-independent Schroedinger equation; operator methods, and the postulates of quantum mechanics; one-dimensional potentials; quantum harmonic oscillator; angular momentum and spin; entanglement and its applications; quantum mechanics in three dimensions and the hydrogen atom.

## 1. Review

Quantum Mechanics was born from the realization that Classical Physics could not describe several experiments in which the measurement outcome was discrete rather than continuous as expected. This rendered, among other formulations, Schroedinger's Equation, a description of this new Physics in terms of Eigenvalue Problems, finding then a natural language in which to model the experimental findings as a set of discrete eigenvalues. The natural space for Quantum Mechanics, given this formulation, is then the one for Eigenvalue Problems in PDE's, namely Hilbert Spaces, which are (possibly infinite dimensional) complete vector spaces with inner product (which allows to establish angles between vectors). The field of Mathematics related to the study of Hilbert Spaces is Functional Analysis (which is loosely speaking like Linear Algebra for infinite dimensional spaces). In our case, our points in space (vectors) will be functions $f = f(x), \quad x \in \mathcal{R}$ instead of $(f_1, ..., f_n) = (f(x_1), ..., f(x_n))$ (the number of "components" of our vectors is not finite anymore, but they rather have the cardinality of real numbers).

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*1.1. Inner Product of Two Vectors in the Hilbert Space*

Let's say we have a vector space, called $H$. An inner product is a mapping $\langle\cdot|\cdot\rangle : H \times H \to \mathcal{C}$ to the field of complex numbers such that

1. this mapping $\langle\cdot|\cdot\rangle : H \times H \to \mathcal{C}$ is linear in its second argument, so if $f, g, h \in H, \quad \alpha, \beta \in \mathcal{C}$
$$\langle h|\alpha f + \beta g\rangle = \alpha \langle h|f\rangle + \beta \langle h|g\rangle$$
2. it is conjugate symmetric, so if $f, g \in H$, then
$$\langle f|g\rangle = \overline{\langle g|f\rangle}$$
where $\overline{\langle g|f\rangle} = \langle g|f\rangle^*$ are both notations for the complex conjugate of $\langle g|f\rangle$.
3. $\langle f|f\rangle \geq 0$ for any vector $f \in H$. Moreover, $\langle f|f\rangle = 0$ if and only if $f = 0$.

This type of mapping is called sesquilinear. Notice that mathematicians sometimes have different conventions for inner products in functional analysis: they may attribute the linearity to the first argument, and they might denote the inner product as $(\cdot,\cdot)$. A Hilbert space is a vector space with an inner product where one more condition is satisfied, called completeness. First we notice that the inner product can induce a norm $||f|| = \langle f|f\rangle^{1/2}$ for each element, and we can define a distance between elements in our vector space via $||f - g||$. If we study sequences of points $\{f_n\}_{n=1}^{\infty}$in our vector space such that

$$\lim_{n,m\to\infty} ||f_n - f_m|| = 0$$

(called Cauchy sequences), our space is complete if every one of these type of sequences converges to a vector $f$ in $H$. If that is the case, our vector space is complete and therefore a Hilbert space.

Our Hilbert space will be the set of (possibly complex-valued) square integrable functions over a given interval $(a, b)$, that is, functions $f(x)$ for which

$$\int_a^b |f(x)|^2 dx = \int_a^b f^*(x)f(x)dx < \infty$$

This Hilbert space is called $L_2(a, b)$, the space of square-integrable functions over the interval $(a, b)$.

We can induce a norm by $||f|| = \langle f|f\rangle^{1/2}$ , where

$$\langle f|f\rangle = \int_a^b f^*(x)f(x)dx = \int_a^b |f(x)|^2 dx$$

from the inner product associated to square-integrable functions,

$$\langle f|g\rangle = \int_a^b f^*(x)g(x)dx = \lim_{n\to\infty} \sum_{i=1}^{n} f^*(x_i)g(x_i)\frac{(b-a)}{n}$$

where $\{x_i\}_{i=1}^n$ is a regular partition of $[a,b]$ (this makes clear how the $L_2(a,b)$ inner product is an infinite dimensional extension of the usual inner product for vectors of finite dimension).

The Cauchy-Schwarz Inequality $|\langle f|g\rangle| \leq ||f|| \cdot ||g||$ holds for spaces with inner product, and this is what lets us guarantee that the inner product above is finite for any elements in our $L_2(a,b)$ Hilbert space.

To represent a physical state, $\Psi(x)$ (to be called a wave function) must be normalized, meaning $||\Psi|| = 1$, or equivalently,

$$\langle \Psi|\Psi\rangle = \int_a^b |\Psi(x)|^2 dx = 1.$$

As we mentioned, the inner product of a Hilbert space lets us define angles between vectors. In particular, we can define an orthogonality between two vectors $f, g$ if $\langle f|g\rangle = 0$. We define then an orthonormal set of functions $\{f_n\}$ as one for which

$$\langle f_n|f_m\rangle = \delta_{nm}$$

where $\delta_{nm}$ is the Kronecker delta. A complete set of functions $\{f_n\}_{n=1}^\infty$ is defined as one for which any function $f(x)$ in the Hilbert space can be expressed as a linear combination of elements in the set:

$$f(x) = \sum_{n=1}^{\infty} c_n f_n(x).$$

If it was the case that the complete set of functions $\{f_n\}_{n=1}^\infty$ was also orthonormal, then by inner product properties

$$\langle f_m|f\rangle = \left\langle f_m | \sum_{n=1}^{\infty} c_n f_n \right\rangle = \sum_{n=1}^{\infty} c_n \langle f_m|f_n\rangle = \sum_{n=1}^{\infty} c_n \delta_{mn} = c_m.$$

*1.2. Matrix Representations of Dirac (ket and bra) Vectors and of Operators*

The state of a system in Quantum Mechanics is represented by a vector $|S(t)\rangle$ (this is the Dirac ket-notation for vectors in the Hilbert Space).

This vector can be expressed with respect to different bases. For example, $\Psi(x,t)$ represents the $x-$component in the expansion of $|S(t)\rangle$ in terms of the basis of position eigenfunctions

$$\langle x|S(t)\rangle = \Psi(x,t)$$

where we're performing the inner product with respect to the eigenfunctions $|x\rangle$ of the position operator $\hat{x}$ (such that $\hat{x}\,|x\rangle = x\,|x\rangle$).

This also lets us introduce the Dirac bra-notation for functionals of the Hilbert space. On one hand, $\langle x|\cdot\rangle : H \to \mathcal{C}$ maps vectors of the Hilbert space into the field of complex numbers, and so it is a linear functional, which can be proved continuous by Cauchy-Schwarz. On the other hand, the Riesz Representation

Theorem guarantees that every continuous linear functional $L\{\cdot\} : H \to \mathcal{C}$ from the Hilbert space to the complex numbers can be represented as an inner product $\langle Z|\cdot\rangle$ with respect to a unique vector $|Z\rangle$ of the Hilbert space, namely, for $L$ there exists a unique $|Z\rangle \in H$ such that

$$L\{|S(t)\rangle\} = \langle Z|S(t)\rangle \quad \forall\, |S(t)\rangle \in H$$

So every continuous linear functional $L$ can be represented as a given $\langle Z|$. Notice $\langle Z|$ lives in the space of continuous linear functionals from $H$ to $\mathcal{C}$, whereas $|Z\rangle \in H$ is a vector in the Hilbert space. In the Dirac notation though, elements $\langle Z|$ are called "bra-vectors", because the Riesz map $L_z \leftrightarrow |Z\rangle$ lets us identify uniquely continuous linear functionals with vectors in the Hilbert space, since

$$L_z\{|S\rangle\} = \langle Z|S\rangle \quad \forall\, |S\rangle \in H.$$

The space of continuous linear functionals from $H$ to $\mathcal{C}$ has a name, it's called the dual of $H$, it's denoted as $H^*$, and it's also a vector space.

Going back to our previous discussion, the state $|S(t)\rangle$ can be expressed in terms of different bases, for example also with respect to the momentum eigenfunctions $\{|p\rangle\}$ with eigenvalues $p \in \mathcal{R}$:

$$\langle p|S(t)\rangle = \Phi(p,t)$$

They are just different ways to represent the same state vector $|S(t)\rangle$.

Given an orthonormal basis $\{|e_n\rangle\}$, vectors can be represented by their components with respect to this basis, so

$$|\alpha\rangle = \sum_n a_n\,|e_n\rangle\,, \quad a_n = \langle e_n|\alpha\rangle$$

Regarding operators $\hat{Q}$ representing physical observables, they are linear transformations on the Hilbert space, so

$$|\beta\rangle = \hat{Q}\,|\alpha\rangle$$

and since

$$\sum_n b_n\,|e_n\rangle = |\beta\rangle = \sum_n a_n \hat{Q}\,|e_n\rangle\,, \quad b_n = \langle e_n|\beta\rangle$$

then taking the inner product with $|e_m\rangle$, since the basis is orthonormal,

$$b_m = \sum_n b_n\,\langle e_m|e_n\rangle = \sum_n a_n\,\left\langle e_m|\hat{Q}|e_n\right\rangle = \sum_n a_n Q_{mn}$$

defining

$$Q_{mn} = \left\langle e_m|\hat{Q}|e_n\right\rangle.$$

So, operators representing observables, since they're linear, can be represented with respect to a given basis (like our orthonormal one) by their matrix elements as above. These matrix elements indicate how components are transformed.

If we have an orthonormal basis $\{|e_n\rangle\}$ of ket-vectors, we can represent the identity operator by

$$1 = \sum_n |e_n\rangle \langle e_n|$$

since for any $|\alpha\rangle$ we have

$$\{\sum_n |e_n\rangle \langle e_n|\} |\alpha\rangle = \sum_n |e_n\rangle \langle e_n| |\alpha\rangle = |\alpha\rangle$$

We can represent bra-vectors in terms of $\{\langle e_n|\}$, which is called the dual basis to $\{|e_n\rangle\}$, with the property that $\langle e_m|e_n\rangle = \delta_{mn}$. Since any ket-vector is represented by the orthonormal basis $\{|e_n\rangle\}$ via

$$|\alpha\rangle = \sum_n |e_n\rangle \langle e_n| |\alpha\rangle$$

in order to define $\langle\alpha|$ as a continuous linear functional it's enough to define its action over the elements of the orthonormal basis,

$$\langle\alpha|e_n\rangle = \langle e_n|\alpha\rangle^*$$

so now the functional $\langle\alpha|$ is completely defined and we can represent it in terms of the dual basis as

$$\sum_n \langle\alpha|e_n\rangle \langle e_n|$$

since applying it to $|e_m\rangle$ we have

$$\sum_n \langle\alpha|e_n\rangle \langle e_n| |e_m\rangle = \sum_n \langle\alpha|e_n\rangle \delta_{nm} = \langle\alpha|e_m\rangle$$

so $\sum_n \langle\alpha|e_n\rangle \langle e_n|$ matches $\langle\alpha|$ for all $|e_n\rangle$ and therefore

$$\langle\alpha| = \sum_n \langle\alpha|e_n\rangle \langle e_n| = \sum_n \langle e_n|\alpha\rangle^* \langle e_n| .$$

so if

$$|\alpha\rangle = \sum_n a_n |e_n\rangle$$

then

$$\langle\alpha| = \sum_n a_n^* \langle e_n| .$$

*1.3. Outer Product of ket and bra Vectors*

In the previous sections we studied inner product, Hilbert spaces, and ket and bra vectors. If we have an orthonormal basis $\{|e_n\rangle\}$, we can think of the inner product of an infinite dimensional Hilbert space as an extension of the dot product we know for vectors in a finite dimensional space:

$$|\alpha\rangle = \sum_n a_n |e_n\rangle$$

$$|\beta\rangle = \sum_n b_n |e_n\rangle$$

$$\langle\alpha|\beta\rangle = \sum_n a_n^* \langle e_n| |\beta\rangle = \sum_n a_n^* b_n.$$

Now, for the outer product a similar analogy can be made. We can define the outer product

$$\hat{A} = |\alpha\rangle \langle\beta|$$

which is an operator on the Hilbert space such that for any element $|S\rangle \in H$,

$$\hat{A} |S\rangle = |\alpha\rangle \langle\beta| |S\rangle = \langle\beta|S\rangle |\alpha\rangle \in H$$

so it's clear its effect is to measure the projection of $|S\rangle$ along $|\beta\rangle$ and then multiply it by the vector $|\alpha\rangle$ . The outer product is a linear operator by linearity of the inner product in its second argument. If we have an orthonormal basis we can make the analogy with outer products of finite dimensional spaces. The easiest way is, since it's a linear operator, to find its matrix representation in terms of the orthonormal basis as we did in the previous section. So, given the basis $\{|e_n\rangle\}$, we compute

$$A_{mn} = \langle e_m| |\alpha\rangle \langle\beta| |e_n\rangle = \langle e_m|\alpha\rangle \langle\beta|e_n\rangle = a_m b_n^*$$

So now it's clear: it's analog to the outer product of a column vector (ket) $|\alpha\rangle$ with a row vector (bra) $\langle\beta|$, which generates a matrix by multiplying the component $a_m$ with the conjugate $b_n^*$. It's a linear operator of rank one.

For the simpler case $|\alpha\rangle \langle\alpha|$ , clearly the latter operator simply obtains the projection of its argument along $|\alpha\rangle$, so it's called the projection operator (onto the subspace spanned by $|\alpha\rangle$). In retrospective, the identity operator

$$1 = \sum_n |e_n\rangle \langle e_n|$$

is simply obtaining the projection along each of the basis vectors and then adding them to recover the initial vector argument.

This can be extended to the case where the basis is not countable but rather has the cardinality of the real numbers (with a continous index), as for position or momentum eigenstates. In those cases we replace the sum by an integral and we can write the identity operator as

$$1 = \int dx \,|x\rangle \langle x|$$

or

$$1 = \int dp \,|p\rangle \langle p|$$

*1.4. Position and momentum operators in position and momentum representations*

As abovementioned, the identity operator can be written in terms of the position or momentum eigenstates, so a given state vector $|S(t)\rangle$ can be represented in terms of any of those basis as

$$|S(t)\rangle = \int dx \,|x\rangle \langle x| \,|S(t)\rangle = \int dx \Psi(x,t) \,|x\rangle \,, \quad \Psi(x,t) = \langle x|S(t)\rangle$$

$$|S(t)\rangle = \int dp \,|p\rangle \langle p| \,|S(t)\rangle = \int dp \Phi(p,t) \,|p\rangle \,, \quad \Phi(p,t) = \langle p|S(t)\rangle$$

so the position-space wave function $\Psi(x,t) = \langle x|S(t)\rangle$ is the component of the state vector $|S(t)\rangle$ along $|x\rangle$, and the momentum-space wave function $\Phi(p,t) = \langle p|S(t)\rangle$ is the component of the state vector $|S(t)\rangle$ along $|p\rangle$. These are the position and momentum representations of the state vector $|S(t)\rangle$. Given that both position and momentum are physical observables, we will study now the form of their Hermitian operators in both representations. Operators can be expressed in a given representation by taking the inner product with a corresponding basis vector. For example, for the position operator $\hat{x}$, we have

$$\langle x|\hat{x}|S(t)\rangle = \langle \hat{x}x|S(t)\rangle = x \langle x|S(t)\rangle = x\Psi(x,t)$$

so $\hat{x} = x$ in the position representation. Likewise, the momentum operator in its own (momentum) representation is

$$\langle p|\hat{p}|S(t)\rangle = \langle \hat{p}p|S(t)\rangle = p \langle p|S(t)\rangle = p\Phi(p,t)$$

and in its representation, $\hat{p} = p$. The momentum operator has the form $\hat{p} = -i\hbar\partial_x$ in the position representation. For example, for a free particle with position-space wave function $\Psi(x,t) = e^{i(kx-\omega(k)t)} = e^{i(px-\varepsilon(p)t)/\hbar}$ we have $p\Psi(x,t) = pe^{i(px-\varepsilon(p)t)/\hbar} = -i\hbar\partial_x e^{i(px-\varepsilon(p)t)/\hbar} = \hat{p}\Psi(x,t)$. This points out to the fact that the eigenfunctions of the momentum operator in the position representation are of the form $\langle x|p\rangle = f_p(x) = A_p \exp(ipx/\hbar)$, since

$$\hat{p} \,|p\rangle = p \,|p\rangle$$

$$-i\hbar\partial_x \langle x|p\rangle = \langle x|\hat{p}|p\rangle = p\,\langle x|p\rangle$$

$$-i\hbar\partial_x f_p(x) = \hat{p} f_p(x) = p f_p(x)$$

$$f_p(x) = A_p \exp(ipx/\hbar)$$

The constant $A_p$ is defined by means of a (Dirac) orthonormality condition between the momentum eigenfunctions (with continuous index):

$$\langle p|p'\rangle = \left\langle p|\int |x\rangle \langle x|\, dx|p'\right\rangle = \int \langle p|x\rangle \langle x|p'\rangle\, dx = \int f_p^*(x) f_{p'}(x)dx =$$

$$= \int A_p^* A_{p'} \exp(i(p'-p)x/\hbar)dx = A_p^* A_{p'} 2\pi\hbar\delta(p'-p)$$

so it suffices choosing $A_p = 1/\sqrt{2\pi\hbar}$ for all $p \in \mathcal{R}$ so that $\langle p|p'\rangle = \int f_p^*(x) f_{p'}(x)dx = \delta(p'-p)$. Therefore $\langle x|p\rangle = f_p(x) = \exp(ipx/\hbar)/\sqrt{2\pi\hbar}$ .

We can now transform the position-space wave function to the momentum-space representation. Since we have $\Psi(x,t) = \langle x|S(t)\rangle$ and we want

$\Phi(p,t) = \langle p|S(t)\rangle$, we can obtain it by inserting an identity operator as below:

$$\Phi(p,t) = \langle p|S(t)\rangle = \left\langle p|\int dx\,|x\rangle \langle x|\, S(t)\right\rangle = \int dx\,\langle p\,|x\rangle \langle x|\, S(t)\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int dx \exp(-ipx/\hbar)\Psi(x,t)$$

using the fact that $\langle p|x\rangle = \frac{\exp(-ipx/\hbar)}{\sqrt{2\pi\hbar}}$ . Notice that the momentum-space representation of the wave function, $\Phi(p,t)$, is (except for the $\hbar$'s appearing) the Fourier transform of the position-space representation of the wave function $\Psi(x,t)$. Therefore, using an inverse Fourier transform, we also have

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int \exp(ipx/\hbar)\Phi(p,t)dp$$

What we're interested now is on the form of the position operator in the momentum representation. We can use the Dirac notation to obtain representations of these sort by inserting the identity operator conveniently. So, the position operator in the momentum representation is obtained by

$$\langle p|\hat{x}|S(t)\rangle = \left\langle p|\hat{x}\int dx\,|x\rangle \langle x|\,|S(t)\right\rangle = \int x\,\langle p|x\rangle\, \Psi(x,t)dx = \int x\frac{e^{-\frac{ipx}{\hbar}}}{\sqrt{2\pi\hbar}}\Psi(x,t)dx =$$

$$= i\hbar\partial_p \int \frac{e^{-\frac{ipx}{\hbar}}}{\sqrt{2\pi\hbar}}\Psi(x,t)dx = i\hbar\partial_p\Phi(p,t) = i\hbar\partial_p\,\langle p|S(t)\rangle$$

since $\Phi(p,t) = \int \frac{\exp(-ipx/\hbar)}{\sqrt{2\pi\hbar}}\Psi(x,t)dx = \langle p|S(t)\rangle$ is the wave function in the momentum space representation. Therefore $\hat{x} = i\hbar\partial_p$ in the momentum space representation.

*1.5. Schroedinger equation in position and momentum representations*

The Schroedinger equation establishes the equivalence between the actions of the Hamiltonian operator and the energy operator over a given state

$$\hat{H}\,|S(t)\rangle = \hat{E}\,|S(t)\rangle$$

where the energy operator is

$$\hat{E} = i\hbar\partial_t$$

and the Hamiltonian operator is

$$\hat{H} = \frac{\hat{p}^2}{2m} + V$$

so

$$i\hbar\partial_t\,|S(t)\rangle = \{\frac{\hat{p}^2}{2m} + V\}\,|S(t)\rangle$$

Since the kinetic energy depends on the momentum operator and the potential could depend on the position operator, it's clear that the Schroedinger equation will have a different form in the position and momentum representations.

In the position representation, we know that $\hat{p} = -i\hbar\partial_x$, so $\hat{p}^2 = -\hbar^2\partial_x^2$, and if we assume $V = V(x)$, then

$$i\hbar\partial_t\,\langle x|S(t)\rangle = \left\langle x|\frac{\hat{p}^2}{2m} + V(\hat{x})|S(t)\right\rangle$$

so the Schroedinger equation in the position representation is simply

$$i\hbar\partial_t\Psi(x,t) = \frac{-\hbar^2}{2m}\partial_x^2\Psi(x,t) + V(x)\Psi(x,t)$$

The equivalent representation in the momentum space of the Schroedinger equation would make use of the fact that $\hat{x} = i\hbar\partial_p$, so

$$i\hbar\partial_t\,\langle p|S(t)\rangle = \left\langle p|\frac{\hat{p}^2}{2m} + V(\hat{x})|S(t)\right\rangle$$

and if $V(x)$ can be expanded as a power series in $x$ , then

$$i\hbar\partial_t\Phi(p,t) = \frac{p^2}{2m}\Phi(p,t) + V(i\hbar\partial_p)\{\Phi(p,t)\}$$

but the disadvantage of this expression is that, in general, $V(x)$ will contain terms of all orders in $x$, so the equation above is a PDE of infinite order in $p$. The last term can be expressed in a more convenient way if we apply a Fourier transform to the Schroedinger equation in position-space to obtain an integral equation, and this will be an equivalent expression for the Schroedinger equation in the momentum representation:

$$\frac{1}{\sqrt{2\pi\hbar}}\int dx\exp(-ipx/\hbar)i\hbar\partial_t\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int dx\exp(-ipx/\hbar)\{\frac{-\hbar^2}{2m}\partial_x^2\Psi(x,t)+V(x)\Psi(x,t)\}$$

and integrating by parts twice the second term (we know that in Fourier space there's an equivalence $\hat{p} = -i\hbar\partial_x$ )

$$i\hbar\partial_t\{\frac{1}{\sqrt{2\pi\hbar}}\int dx\exp(-ipx/\hbar)\Psi(x,t)\} = \frac{-\hbar^2}{2m}\frac{1}{\sqrt{2\pi\hbar}}\int dx\Psi(x,t)\partial_x^2\exp(-ipx/\hbar)$$

$$+\frac{1}{\sqrt{2\pi\hbar}}\int dx\exp(-ipx/\hbar)V(x)\Psi(x,t)$$

so

$$i\hbar\partial_t\Phi(p,t) = \frac{p^2}{2m}\Phi(p,t) + \frac{1}{\sqrt{2\pi\hbar}}\int dx\exp(-ipx/\hbar)V(x)\Psi(x,t)$$

and we can express the transform of the product using convolution, so

$$i\hbar\partial_t\Phi(p,t) = \frac{p^2}{2m}\Phi(p,t) + \frac{1}{\sqrt{2\pi\hbar}}\int dp'\Phi(p-p',t)\int dx\frac{\exp(-ip'x/\hbar)}{\sqrt{2\pi\hbar}}V(x)$$

the equation above is a nicer expression for the Schroedinger equation in momentum space (notice the appearance of the Fourier transform of the potential), where we have used

$$\frac{1}{2\pi\hbar}\int\exp(i(p'-p)x/\hbar)dx = \delta(p'-p)$$

Please notice the following remarks by D. Saxon on the Schroedinger equation in momentum space: “unless the potential is a very special function, the momentum space equation is considerably more complicated than that in configuration space... The reason for the complications in momentum space, compared to the utter simplicity of the momentum space equations for a free particle, is that the momentum is no longer a constant of the motion. The presence of external forces means that the state function necessarily contains a broad mixture of pure momentum states and this mixing is explicitly represented by the integral in [the] equation...”

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