Wavelet basis for the Schrödinger equation

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Abstract

The self-similar representation for the Schrödinger equation is derived.

The general form Schrödinger equation

$$\imath\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi, \tag{1}$$

which is the generalization of the free particle wave equation

$$\imath\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2},$$

describes the evolution of the wave function $\psi(\vec{x}, t)$ for the quantum system with a general form of Hamiltonian $\hat{H}$. The solution of the Schrödinger equation (1), if it exists, is not uniquely determined by the Hamiltonian; the symmetry of the problem and/or boundary conditions must be given also.

For this reason, for the problems with spherical symmetry (SO_3) — say, the Hydrogen atom — we look for a solution within the class of spherical functions. For homogeneous problems, i.e. the problems invariant under translations, we suppose the solution to be the superposition of plane waves, the unitary representations of the translation group

$$G : x' = x + b. \tag{2}$$

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To find a solution of the Schrödinger equation (1) with a (Lie) symmetry group G, we have to look for a state vector $|\psi\rangle$ of a Hilbert space $\mathcal{H}$ in the form with respect to G

$$|\psi\rangle = c_v \int_G U(g)|v\rangle d\mu_L(g)\langle v|U^*(g)|\psi\rangle. \tag{3}$$

This means that we suppose it to be a decomposition with respect to a certain representation $U(g)$ of the Lie group G; $d\mu_L(g)$ is the left-invariant measure on G. Here after $v \in \mathcal{H}$ an *admissible* vector of the representation $U(g)$ [1, 2], a vector of the Hilbert space $\mathcal{H}$ satisfying the normalization condition

$$c_v = \int_G |\langle v|U(g)|v\rangle|^2 d\mu_L(g) < \infty \tag{4}$$

is referred to as a basic wavelet [3]. For the group of translations (2) the decomposition (3) is a trivial one $|\psi\rangle = \int |k\rangle dk\langle k|\psi\rangle$ and causes no problem with the particular choice of the admissible vector. For other groups this problem is not always trivial and often requires some physical insight.

In the present paper, following [4], we consider the possibility of self-similar objects in quantum mechanics and related solutions of the Schrödinger equation.

For the case of the one dimensional Schrödinger equation

$$\imath\hbar\frac{\partial\psi}{\partial t} = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + W(x)\right]\psi, \tag{5}$$

(taken for simplicity) the Lie group which pertains to the self-similarity is the affine group

$$G : x' = ax + b; \qquad d\mu(a,b) = \frac{dadb}{a^2} \tag{6}$$

The representation of the affine group (6) apt to the problem ultimately has the form

$$U(a,b)f(x) = \frac{1}{\sqrt{a}}f\left(\frac{x-b}{a}\right), \tag{7}$$

but the particular type of the basic wavelet $v(x)$ is to be chosen from physical consideration.

For the sake of a well defined quasiclassical limit at, large a we have to choose a minimal wave packet

$$v_0(x) = [2\pi(\Delta x)^2]^{-1/4} \exp\left(-\frac{(x-\bar{x})^2}{4(\Delta x)^2} + \imath px\right) \tag{8}$$

as a basic wavelet; since it minimises the uncertainty relation $\Delta x \Delta p \geq \hbar/2$ (See e.g. [6]). Strictly speaking, the minimal wave packet (8) is not an admissible vector, since c_{v_0} is formally equal to infinity. This ambigity, however, is not of principal importance, and in our model we can treat c_{v_0} as a formal constant.

Substituting,

$$\psi(x) = c_v^{-1} \int \frac{1}{\sqrt{a}} v\left(\frac{x-b}{a}\right) \langle v; a, b|\psi\rangle \frac{dadb}{a^2} \tag{9}$$

into the Schrödinger equation (1) we get

$$\imath\hbar \frac{\partial}{\partial t}\langle v; a, b|\psi\rangle = \tag{10}$$
$$\frac{\hbar^2}{2ma^2}\left[\frac{1}{(\Delta x)^2} - \left\{\frac{\imath p}{\hbar} - \frac{\frac{x-b}{a} - \bar{x}}{(\Delta x)^2}\right\}\right]\langle v; a, b|\psi\rangle + W(a,b)\langle v; a, b|\psi\rangle$$

where $W(a, b)$ is the wavelet transform of the potential $W(x)$:

$$W(a,b) = c_v^{-1} \int \frac{1}{\sqrt{a}} v\left(\frac{b-x}{a}\right) W(x)dx$$

This potential, in our opinion, might have a deep physical meaning, since the potential function, which describes the interaction at quantum level, will ultimately depend on scale, rather than only distance [5]; this is exactly the case for $W(a, b)$.

Near the central point $\frac{x-b}{a} \approx \bar{x}$, i.e. close to the "actual" position of the particle, we have

$$\imath\hbar \frac{\partial}{\partial t}\langle v; a, b|\psi\rangle \approx \left[\frac{p^2}{2ma^2} + \frac{\hbar^2}{4ma^2(\Delta x)^2} + W(a,b)\right]\langle v; a, b|\psi\rangle \tag{11}$$

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