1 Wavefunctions, wavevectors, and state vectors: What's the difference?

There is none. The three words are usually used synonymously. Sometimes one also hears "ket vector" or "ket".

Associated with each isolated quantum system is a Hilbert space. Each member of the Hilbert space is a wavefunction, or a wavevector, or a state vector. Each represents a possible state of the isolated system. (This is sometimes called the first postulate of quantum mechanics.)

If the Hilbert space is infinite-dimensional, the wavefunction (or wavevector or state vector) is often represented as a function of a continuous variable, or as an infinite-dimensional vector. If the Hilbert space is finite-dimensional, the wavefunction is a finite vector.

Examples of a system with infinite-dimensional Hilbert space:
(1) particle on line; (2) particle in space; (3) two particles in space.

Example of system wth finite-dimensional Hilbert space:
(1) A single spin-$\frac{1}{2}$ object.

2 Single particle on a line: Representing $\psi(x)$ as a vector

The state vector or wavefunction of a single particle on a line is a function of a single variable, $\psi(x)$, where x is the position. How does it make sense to think of this as a vector?

A related question is: in what basis is this expressed?

The difficulty here is that x is a continuous variable, while we usually think of a vector as having a discrete index. As an approximate (physicist's) visualization technique, we could discretize space, i.e., approximate the line as a discrete set of closely spaced points

$$\ldots - 3\epsilon, -2\epsilon, -\epsilon, 0, \epsilon, 2\epsilon, 3\epsilon, \ldots$$

Then any function of x is approximated as an infinite vector of discrete points, e.g.,

$$\psi(x) \approx \begin{pmatrix} \vdots \\ \psi(-3\epsilon) \\ \psi(-2\epsilon) \\ \psi(-\epsilon) \\ \psi(0) \\ \psi(\epsilon) \\ \psi(2\epsilon) \\ \psi(3\epsilon) \\ \vdots \end{pmatrix}$$

In the limit $\epsilon \to 0$ this becomes more and more accurate. This is one way to think of a function as being like a vector.

2.1 Set of basis states

When we write a vector as a column of coefficients, we have chosen a basis. In the above representation, the basis states are those where the particle is located at a particular position, $x = n\epsilon$ ($n \in \mathbb{Z}$). In the limit $\epsilon \to 0$ all points on the line are allowed. Thus the basis states are Dirac delta functions, $\delta(x - x_0)$. There are an infinite number of them, one corresponding to each point x_0 on the line.

For a finite Hilbert space, any state vector can be expressed by expanding in a set of orthonormal basis states $\{|\phi_m\rangle\}$:

$$|\psi\rangle = \sum_m c_m |\phi_m\rangle \tag{1}$$

where c_m are the coefficients. The vector representation of $|\psi\rangle$ contains these coefficents, $|\psi\rangle = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix}$, by using the identification

$$|\phi_1\rangle \equiv \begin{pmatrix} 1 \\ 0 \\ \vdots \end{pmatrix}, \quad |\phi_2\rangle \equiv \begin{pmatrix} 0 \\ 1 \\ \vdots \end{pmatrix}, \ldots$$

What is the analog for the infinite-dimensional case of a single particle on a line?

$$\psi(x) = \int dy \psi(y) \delta(y - x) \tag{2}$$

This is a bit confusing because the same symbol $\psi(.)$ is used to represent the wavefunction and it's coefficients in the expansion; it is a tautology based on the definition of the delta function. However, comparing the two equations (1) and (2) shows that $\psi(x)$ is the analog of a vector of coefficients in the finite-dimensional case.

2.2 Approximate representations for operators

In our visualization exercise above (using a discretization at intervals ϵ), we have managed to pretend to write the wavefunction as a discrete-index vector. Continuing with this approximate representation, we could write operators as matrices as well. The position operator is

$$\hat{x} = x\hat{I}$$

which turns (in the discrete approximation) into the diagonal matrix

$$\hat{x} \approx \begin{pmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & -3\epsilon & 0 & 0 & 0 & 0 & 0 & 0 & \dots \\ \dots & 0 & -2\epsilon & 0 & 0 & 0 & 0 & 0 & \dots \\ \dots & 0 & 0 & -\epsilon & 0 & 0 & 0 & 0 & \dots \\ \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots \\ \dots & 0 & 0 & 0 & 0 & +\epsilon & 0 & 0 & \dots \\ \dots & 0 & 0 & 0 & 0 & 0 & +2\epsilon & 0 & \dots \\ \dots & 0 & 0 & 0 & 0 & 0 & 0 & +3\epsilon & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}.$$

How about the momentum operator? Recall that

$$\hat{p} \equiv -i\hbar\partial_x.$$

This operator computes the derivative of the function $f(x)$ it is acting on, i.e., to find $\hat{p}f(x)$ at point x one needs the value of the function f not only at x but in a region neighboring x. This suggests that the matrix is not diagonal. In the discretized description, at the point $x = n\epsilon$ a reasonable approximation for $f'(x)$ is

$$f'(n\epsilon) = \frac{f\big((n+1)\epsilon\big) - f\big((n-1)\epsilon\big)}{2\epsilon}$$

Thus the approximate representation for the momentum operator would be

$$\hat{p} \;\approx\; \frac{-i\hbar}{2\epsilon}\begin{pmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & 0 & -1 & 0 & 0 & 0 & 0 & 0 & \dots \\ \dots & 1 & 0 & -1 & 0 & 0 & 0 & 0 & \dots \\ \dots & 0 & 1 & 0 & -1 & 0 & 0 & 0 & \dots \\ \dots & 0 & 0 & 1 & 0 & 0 & 0 & 0 & \dots \\ \dots & 0 & 0 & 0 & 1 & 0 & -1 & 0 & \dots \\ \dots & 0 & 0 & 0 & 0 & 1 & 0 & -1 & \dots \\ \dots & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}.$$

Exercise: represent the operators $\hat{x}^2$ and $[\hat{x}, \hat{p}]$ as approximate matrices.

Reminder: these are approximate representations which are developed here to help visualization, and to help accept the idea that functions are just vectors of infinite dimension. However, these approximate representations are actually useful if we want to represent wavefunctions and operators on a computer. In actual modern-day use of quantum mechanics, we need computer representations all the time.