Answers to Physics 176 One-Minute Questionnaires March 29, 2011

Can you have a probability density that is a function of vectors instead of the components of a vector?

The answer is yes because there is no practical difference between defining a probability density (or any function) in terms of the components of a vector versus the vector itself. For example, a molecule can be described by two 3-vectors $\mathbf{x} = (x_1, x_2, x_3)$ and $\mathbf{v} = (v_1, v_2, v_3)$ or, completely equivalently, by the six vector components $(x_1, x_2, x_3, v_1, v_2, v_3)$, so we could write the probability density as a function of vectors like this, $\mathcal{D}(\mathbf{x}, \mathbf{v})$, or write it equivalently as $\mathcal{D}(x_1, x_2, x_3, v_1, v_2, v_3)$.

A way to see that these are equivalent is that vector components like x_i and v_i can be obtained by operations carried out on the vectors \mathbf{x} and \mathbf{v} themselves, for example

$$x_1 = \mathbf{x} \cdot \hat{x}, \qquad v_2 = \mathbf{v} \cdot \hat{y}, \tag{1}$$

where \hat{x} is a unit vector along the positive x-axis and \hat{y} is a unit vector along the positive y-axis. So any expression involving the components of the vectors can be alternatively interpreted as some operation involving the vectors themselves and vice versa.

Are continuous energies (like $(1/2)PV^2$, mgh), actually continuous or are they discretized in units of Planck's constant?

That's a tricky question. If the universe is finite in size (it is not known one way or the other but most scientists believe it is), then all energy levels must be quantized because of the properties of the Schrodinger equation in a finite region of space. But if you calculate the order of magnitude of the energy difference ΔE between two energy levels of an electron (the lightest mass stable particle produces the largest energy difference) in a box of size L(see Eq. (A.14) on page 369 of Schroeder) where L is of order 10 billion light years, one gets

$$\Delta E \approx \frac{h^2}{8mL^2} \tag{2}$$

$$\approx \frac{(7 \times 10^{-34} \,\mathrm{J \cdot s})^2}{(7 \times 10^{-34} \,\mathrm{J \cdot s})^2} \tag{3}$$

$$8 \times (9 \times 10^{-31} \,\text{kg}) \times ((10 \times 10^9 \,\text{ly}) \times 10^{16} \,\text{m/ly})^2$$

$$\approx 10^{-71} \,\text{eV},$$
(4)

which is far far tinier than any experimental device can detect. Even for a one centimeter cube of some metal like copper, the energy spacings between the electron energy levels are too small to be measureable.

So the answer to your question is that, for a finite universe, the energy spacings are in principle always discrete but in practice the energy levels of free particles are spaced so closely that no experiment can prove they do not vary continuously. So it is fine to assume that classical energies are perfectly continuous.

Can you explain why the proof of the equipartition theorem does not carry over to quantum systems?

One reason is that energy levels of a bound quantum system like a hydrogen atom are discrete (not continuous) and so there is no chance of describing the energy of the system as a quadratic expression cq^2 of some continuously varying variable q.

Why energy levels of bound states are discrete is in turn explained in many introductory books on quantum physics as a basic consequence of having a wave function $\Psi(t, \mathbf{x})$ that decays to infinity sufficiently rapidly (so that the integral of $|\Psi|^2$ over all of space is finite, a necessary requirement for the quantity $|\Psi|^2$ to have the meaning of a probability density) while simultaneously satisfying the Schrodinger equation. A clear discussion of how discrete states arise is given in the book "An Introduction to Quantum Mechanics" by Taylor and French, which is roughly at the Physics 143 level.

In your example of a dielectric material, what is the physical meaning of $\langle p_z \rangle$ and where does $d\Omega = \sin(\theta) d\theta d\phi$ in Z come from?

The physical meaning of $\langle p_z \rangle$ is the extent to which a small vector electric dipole $\mathbf{p} = p\hat{\mathbf{n}} = (Qd)\hat{\mathbf{n}}$ is able to align along some fixed external electric field, say $\boldsymbol{\mathcal{E}} = \boldsymbol{\mathcal{E}}\hat{\mathbf{z}}$, when the dipole is being shaken about by molecular collisions with a surrounding reservoir. The maximum alignment occurs when \mathbf{p} is parallel to $\boldsymbol{\mathcal{E}}$ in which case $\langle p_z \rangle = p$ and this is what would occur at absolute zero. For sufficiently high temperatures, $\langle p_z \rangle = 0$, the dipole is fluctuating so much that it has no net alignment with the electric field on average so its component along the electric field has an average of zero.

The reason why $\langle p_z \rangle$ is an important quantity scientifically or for engineers is that it can be related to the dielectric constant ϵ of a dielectric medium that consists of polar molecules (like a water molecule) whose electric dipole strength is approximately independent of the strength of the external electric field $\boldsymbol{\mathcal{E}}$.

Dielectrics can also consist of non-polar molecules that do not have an electric dipole in the absence of an electric field, but instead develop a small dipole (whose strength is now proportional to, rather than independent, \mathcal{E}) because an external electric field polarizes the electron cloud surrounding the nuclei of the molecule. This is a more complicated case than the case of fixed dipoles but is discussed in many undergraduate textbooks on electrodynamics, e.g., the excellent book "Electricity and Magnetism" by Edward Purcell.

The solid angle $d\Omega = \sin(\theta) \, d\theta \, d\phi$ arises in the partition function:

$$Z = \int_0^{2\pi} \int_0^{\pi} e^{\beta p \mathcal{E} \cos(\theta)} \sin(\theta) \, d\theta \, d\phi = 4\pi \frac{\sinh(\beta p \mathcal{E})}{\beta p \mathcal{E}},\tag{5}$$

because, if the angles θ and ϕ are allowed to vary over an infinitesimal range

$$0 \le \phi \le 2\pi, \qquad 0 \le \theta \le \pi,\tag{6}$$

then all vectors (θ, ϕ) that lie within the infinitesimal solid angle $d\Omega = \sin(\theta) d\theta d\phi$ are basically pointing in the same direction and so should be treated as equivalent. The quantity $d\Omega$ is thus the effective degeneracy of electric dipoles **p**

$$\mathbf{p} = p\left(\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta)\right),\tag{7}$$

that point along the direction (θ, ϕ) .

Perhaps another way to see this, is that the state of an electric dipole of fixed magnitude p is given by the values of the two angles θ and ϕ . Thus the partition function looks like this:

$$Z = \sum_{s} e^{-\beta E_s} \tag{8}$$

$$= \sum_{n} d_n e^{-\beta E_n} \tag{9}$$

$$= \sum_{\theta} \sum_{\phi} d(\theta, \phi) e^{-\beta E(\phi, \theta)}$$
(10)

$$= \int_0^{\pi} \int_0^{2\pi} d\Omega \, e^{\beta p \mathcal{E} \cos(\theta)}. \tag{11}$$

More generally, if one has some object whose state is defined by some continuous variables such as (q_1, q_2, q_3) and each variable is allowed to vary over some infinitesimal range $q_i, q_i + dq_i$ positioned at q_i , then the degeneracy $d(q_1, q_2, q_3)$ of that state is the Jacobian or phase space volume. In Cartesian coordinates, d(x, y, z) = 1, in spherical coordinates, $d(r, \theta, \phi) = r^2 d\Omega = r^2 \sin(\theta) \, d\theta \, d\phi$, in cylindrical coordinates $d(r, \theta, z) = r \, d\theta \, dz$, and so on. These are the only cases encountered in practice.

Why do we use momentum rather than velocity in quantum physics?

One reason is that quantum theory (as confirmed by experiments) says that the fundamental quantity that characterizes a quantum system, the wave function $\Psi(t, \mathbf{x})$ (here written for a single particle), is a spatially extended object and so it is not meaningful to assign a velocity vector $\mathbf{v} = d\mathbf{x}/dt$ to such an object. For example, the wave function $\Psi(t, x)$ of a free "particle" moving along the real line is given by

$$\Psi(t,x) = e^{kx - \omega t}.$$
(12)

This wave has a well-defined momentum k but not a well defined velocity since this function has a finite value throughout all of space.

The second reason is that the velocity of a quantum mechanical object is not well defined scientifically because the position \mathbf{x} is a discontinuous function of time. By definition, \mathbf{v} is the change in position $\mathbf{x}_2 - \mathbf{x}_1$ of some object over a brief time interval Δt , from an initial starting point \mathbf{x}_1 to a final point \mathbf{x}_2 , in the limit that Δt becomes small. But locating a quantum object at the initial position \mathbf{x}_1 requires carrying out some measurement on the object, and the uncertainty principle $\Delta x \Delta p \geq \hbar$ implies that the measurement, while localizing the object to a small region of space, simultaneously will induce a large change in the momentum of the particle in which case it is not possible to talk about the velocity of the particle a short time Δt later.

I have heard the word "countably infinite". Does this word refer to the first infinity you mentioned, the set of integers?

Yes. A set is called "countably infinite" if there is a bijective mapping (oneto-one and onto) of the set with the integers, i.e., you can pair each member of one set with a unique member of the other set. Thus all the integers, the positive integers, the even integers, the infinitely many prime numbers, and the rational numbers are all countably infinite. The mathematical symbol for this infinity is \aleph_0 where \aleph is the first letter of the Hebrew alphabet.

The next infinity, denoted by \aleph_1 , is the infinity of real numbers, which is also the infinity of irrational numbers, of the complex numbers, and of the

transcendental numbers (numbers that are not the root of any polynomial with integer coefficients).

Check out the Wikipedia article "Continuum hypothesis" where you can learn a bit more about cardinality of infinite sets and some of the profound mathematical questions raised by trying to understand the different kinds of infinities.