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String, Ring, Sphere: Visualizing Wavefunctions on Different Topologies

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QUANTUM PHENOMENA HAVE PENETRATED NEW SCIENTIFIC FIELDS AND EMERGING TECHNOLOGIES. THUS, THERE IS AN INCREASING DEMAND FOR FRESH APPROACHES TOWARD UNDERSTANDING QUANTUM THEORY FUNDAMENTALS IN scientific communities that previously have not been exposed to the subject. Traditional teaching methods have relied heavily on a profound knowledge of the mathematical structure; students are usually able to incorporate quantum mechanics principles only when they are at such an advanced stage of study that the mathematical basis makes sense to them. Unfortunately, many beneficiaries of quantum theory—such as chemists, engineers, biologists, and computer scientists, who traditionally lack a more rigorous mathematical foundation—have been left behind.

New Teaching Methods

The emerging challenge, then, is to develop new teaching methods for quantum mechanics that address its principles in students' early stages of study without compromising a more advanced approach at later stages. At present, it is natural to partially base such an approach on the use of computers because of their great ability to simulate and animate. This task seems straightforward because it relies on the fact that potential students have become accustomed to using advanced graphical and computational tools that apply to their field.

Simulations and visualization of microscopic encounters are commonly used in teaching molecular dynamics science. Because most people find the motion of solid bodies intuitive, they can follow complex chemical events by visually observing the atoms' classical motion. Examples of this approach range from simple inorganic gas phase reactions to complex systems such as enzymatic reactions. However, quantum mechanics lacks such an intuitive basis. Its basic entity—the wavefunction—is complex; therefore, it excludes even a direct connection to physical wave motion. Faced with these difficulties, we must devote considerable attention to developing and applying a visual language for teaching quantum mechanics. In this article, we address the design principles employed in the visualization of quantum wavefunctions, and their application in teaching the superposition principle.

The tools we describe here are only part of a larger set used to teach elementary quantum mechanics to chemistry and physics students for the last six years at the Hebrew University. Teaching experience supports the assumption that visualization enhances students' understanding of basic principles without compromising their mathematical rigor. Due to the tools' dynamical character, full appreciation of the methods requires online interaction. Readers should try these tools for themselves—students and interested parties can get free access through standard Web tools, such as those at www.fh.huji.ac.il/~guy/ChemBond/.

In this article, we will discuss the tools used to represent the quantum state of a single particle, which is described by a wavefunction. The wavefunction can be expressed as a sum of other wavefunctions (the superposition principle), each of which has a distinct property (such as a specific energy or momentum value). The composition of the quantum state determines the probability of measuring the specific value of the distinct property. The number and type of degrees of freedom a system possesses determines the topology on which the wavefunction is defined. For example, a wavefunction can describe a system in a one-dimensional (1D) open space, a system residing on a closed 1D ring, or a system on a 2D spherical surface.

Linear 1D Wavefunctions and Their Superposition

Let's start by visualizing a complex function of a single variable x, which represents a particle constrained to move in one dimension—a particle on a string, for instance. Popular examples using this topology are a particle in a 1D box, scattering by a step potential, and the harmonic oscillator. Think of a 1D complex function as a collection of vectors perpendicular to the x-axis, each one characterized by its length (magni-

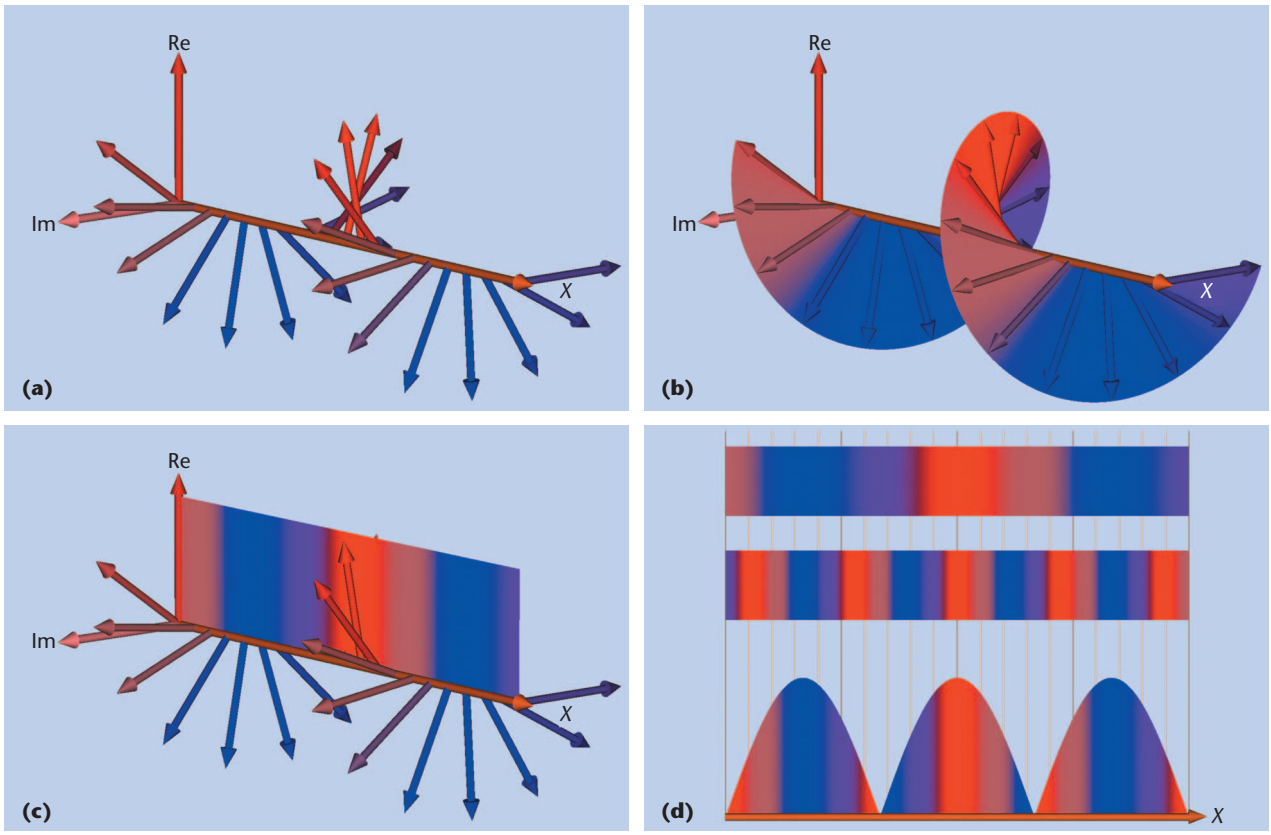

Figure 1. Coding phase by color. (a) A vector representation of complex numbers, (b) a 3D representation of a complex function, (c) reducing the representation to 2D, and (d) using the 2D representation to visualize wave superposition. Educational Java applets generated these graphical representations; they are available at www.fh.huji.ac.il/~guy/links/CISE2004.html.

tude) and by its angle in the complex plane (phase). This requires the ability to visualize a 3D representation, which is harder to interpret for people accustomed to working with 2D graphs. To reduce the representation's dimensionality, the angle of the vectors in the complex plane can be color-coded.

This approach is demonstrated for the plane wave $f(x) = A \cdot e^{ikx}$, an eigenfunction of the free particle in a 1D Hamiltonian. To simplify, the complex function is first reduced to a discrete matching rule between selected x values of the function's 1D domain and their complex $f(x)$ values (see Figure 1a). Arrows that originate from the appropriate x position represent the complex values; their length represents the complex value's magnitude. Because all the $f(x)$ values have the same magnitude (= A), all the arrows are the same length. The phase is represented in two ways: first, the arrows are rotated in the 2D plane perpendicular to the x-axis according to their phase value (zero phase is straight up, and positive phase change is counterclockwise); second, the arrows are color-coded (red denotes zero phase value, pink is $\pi/2$, blue is π, and violet is $-\pi/2$).

We chose these colors carefully to render this scheme more intuitive. Red and blue are primary colors widely associated with positive and negative (for example, colors on hot- and cold-water taps), so we chose them to represent the positive real and negative real phases. For the imaginary phases, we used less saturated (more "imaginary") colors, which are reminiscent of the primary colors: pink or "quasi-red" for the positive imaginary, and violet or "quasi-blue" for the negative imaginary. To keep the scale simple, other phase colors are generated by a continuous graduation between these four colors.

Because each value has a different phase (= kx), the arrows form a spiral with a wavelength of $2\pi/k$. The next step is to represent a continuous, rather than a discrete, function. This is achieved by connecting all the arrows to form a 3D spiraling band (see Figure 1b). The band's width at each x value equals $f(x)$'s magnitude, and $f(x)$'s phase value determines its direction and color. Because there is redundancy in having two kinds of phase representations, we can discard one without losing any information. By unfolding the spiraling band, the 3D representation is reduced to a 2D representation, but the phase information remains in the band's color (see Figure 1c). In the region where the band is colored red, the arrows point upward (zero phase), in the regions where it is pink, the arrows

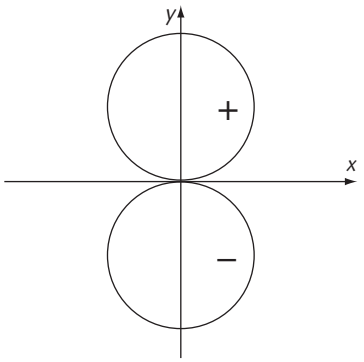

Figure 2. Polar diagram of the function $\sin(\varphi) = \frac{1}{2}i \cdot (e^{i\varphi} - e^{-i\varphi})$. φ is the angle with the positive x-axis; the – sign on the lower circle indicates that $\sin(\varphi)$ is negative for $\pi < \varphi < 2\pi$.

point perpendicular to the band ($\pi/2$ phase), and so on.

Another common method of color-coding uses the entire color-wheel spectrum and encodes the phase angle as the hue component.[1–3] We discovered that our four-color representation is easier to interpret than the full spectrum representation, especially when dealing with wavefunctions' superposition. Figure 1d illustrates the superposition of two plane waves with equal weights: $f(x) = A \cdot e^{ik_1 x} + A \cdot e^{ik_2 x}$. The two upper bands are the plane waves (as can be seen from their constant magnitude and periodically changing phase), and the lower band is the superposition. It is easy to identify the regions of constructive and destructive interference. At x values where the two phases match (red with red or blue with blue), the superposition exhibits constructive interference (the three maxima); where the phases oppose (pink with violet), the superposition exhibits destructive interference (the four nodes). The representation clearly shows the resulting beat-pattern in the envelope (the height of the band) and the harmonic carrier wave in the phase (the periodic change in color).

Angular Wavefunctions and Their Superposition

The wavefunction representation we introduced in the previous section is easily extended into more complicated topologies. A different possible topology is encountered in particles that are constrained to move in a circular orbit—a particle on a ring, for instance. The most notable example of this topology is the 2D rigid rotor. This system is represented as a function of a single angular variable, φ. The conventional representation of an angular function $f(\varphi)$ is by using polar diagrams, in which φ is the angle with the positive x-axis in the xy plane, and $|f(\varphi)|$ is the distance from the origin to the point on the graph. Figure 2 shows the polar diagram of the function $f(\varphi) = \sin(\varphi)$, which is the angular part of a "p-type" atomic orbital (p_y in this case). This type of representation is very misleading for many students, who misinterpret the diagram's shape as that of the orbital, and believe the electron is orbiting the nucleous in a figure-eight orbit or is confined in the area of the two lobes.[4] Both these misinterpretations include an additional dimension of motion (along the r polar coordinate) that the diagram does not represent. The polar diagram is also limited to representing only real functions and requires additional captioning in case the function has negative values (because it represents only the function's absolute value).

To emphasize the 1D topology of the wavefunction (a single variable φ), we propose an alternative representation. This representation is obtained from the linear color-coded representation by bending the x-axis in Figure 1c into a ring. The result is a colored band wrapped around a ring, whose width corresponds to the wavefunction's amplitude (its color corresponds to the phase).

This approach is demonstrated for the wavefunction family $f(\varphi) = e^{im\varphi}$, which are eigenfunctions of the free particle on a ring Hamiltonian. We can use these functions to study the reason for quantization in angular wavefunctions. Closing the string into a ring imposes a constraint on the wavefunction: because $\varphi = 0$ and $\varphi = 2\pi$ represent the same point on the ring, $f(0)$ must equal $f(2\pi)$. When $m = 1/2$ (see Figure 3a), the wavefunction has different phase values at $\varphi = 0$ and $\varphi = 2\pi$, as is apparent from the abrupt color change at $\varphi = 0$. To obtain a continuous function, m must have an integer value, as Figure 3b shows. Therefore, the quantization of the angular wavefunctions (and consequently that of angular momentum) is an outcome of the ring's topology.

When dealing with superposition of angular wavefunctions, color-coding helps distinguish between positive and negative m values. When m is positive (see Figure 3b), the order of the colors for increasing φ is red → *pink* → blue → *purple*. When m is negative (see Figure 3c), the order of the imaginary colors is reversed: red → *purple* → blue → *pink*. When superimposing the two wavefunctions by summing them together, the real parts interfere constructively, while the imaginary parts interfere destructively (see Figure 3d). This results in increasing amplitude along the x-axis and a node along the y-axis, which is the angular part of the p_x atomic orbital. Because the energy of free angular functions (with no angular dependence in the potential) depends only on $|m|$, p_x is also an eigenfunction of the Hamiltonian. In a similar way, the two eigenfunctions with $m = \pm 1$ can be subtracted, causing the real parts to interfere destructively and the imaginary parts to interfere constructively (see Figure 3e). The resulting wavefunction is pointing along the y-axis and resembles the p_y orbital, except that it is purely imaginary

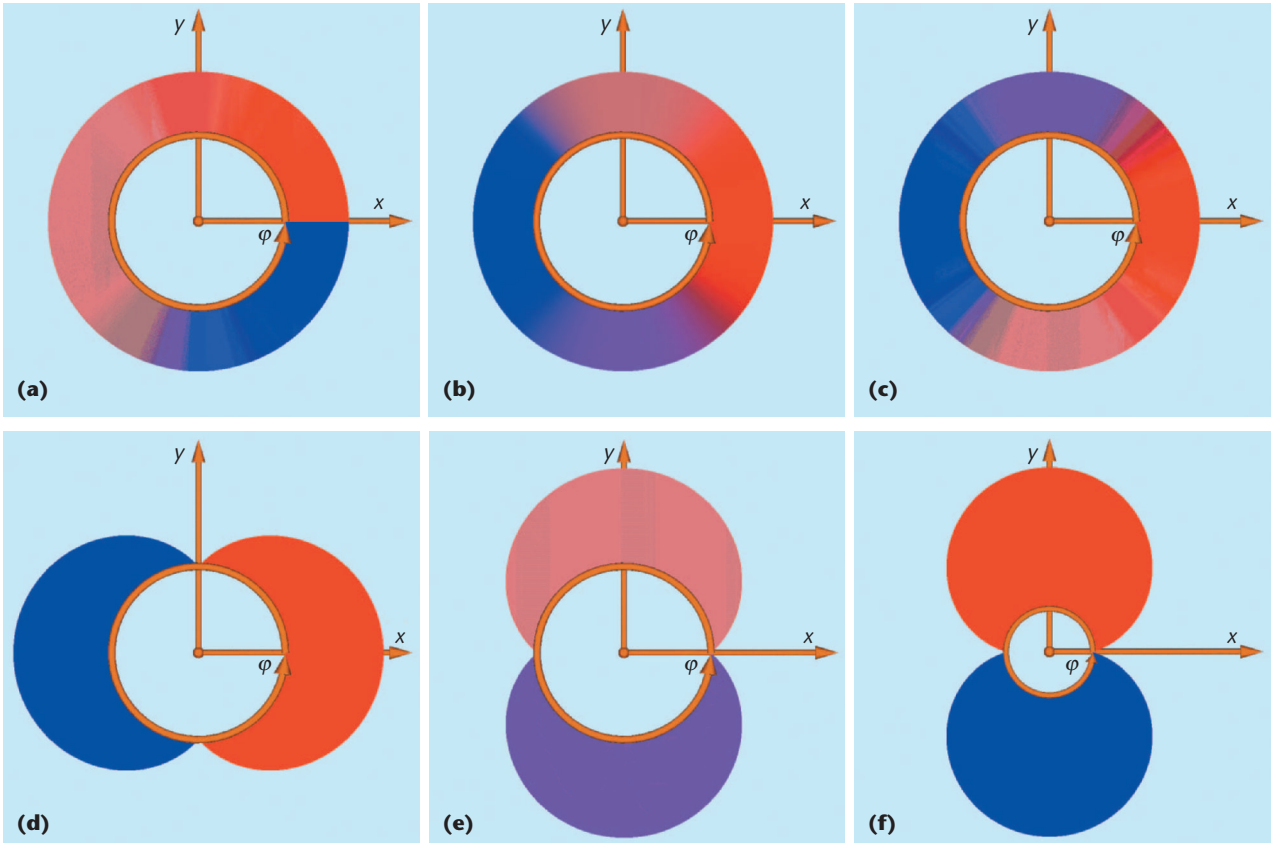

Figure 3. Wavefunctions on a ring. (a) $f(\varphi) = e^{i\varphi/2}$; (b) $f(\varphi) = e^{i\varphi}$; (c) $f(\varphi) = e^{-i\varphi}$; (d) $f(\varphi) = e^{i\varphi} + e^{-i\varphi}$; (e) $f(\varphi) = e^{i\varphi} - e^{-i\varphi}$; and (f) $f(\varphi) = (e^{i\varphi} - e^{-i\varphi})/i$.

rather than real. By multiplying the function by a constant phase of $e^{-i\pi/2}$ (see Figure 3f), we get the real function p_y. To show the similarity between this representation and the conventional polar diagram, we decreased the ring's radius in Figure 3f. As the ring's arbitrary radius approaches zero, the new representation reduces to a polar diagram with the added value of phase color, which allows the presentation of complex functions (compare Figure 3f to Figure 2).

Spherical Harmonics and Their Superposition

A closely related topology to the ring is the sphere, which adds a second angular variable, θ, the angle with the positive z-axis. The most notable example of this topology is the 3D rigid rotor, which is part of the solution of all central force systems, including the hydrogen atom. Again, to emphasize the system's 2D topology and avoid improper inclusion of distance from the origin as a variable (which often arises when using polar diagrams), the wavefunction is drawn on a sphere's surface. The wavefunction's phase is denoted by color, as before, but the amplitude is now encoded as opacity. The wavefunction is opaque at the maximum amplitude, partially transparent at medium amplitudes, and completely transparent at the nodes. The physical basis of this encoding comes from viewing opacity as a measure of probability density.

We demonstrate this approach for the three spherical harmonics with $l = 1$, $Y_1^m(\theta, \varphi)$, which are eigenfunctions of the free particle on a sphere Hamiltonian. The spherical topology imposes two constraints on the wavefunction. The first concerns φ, and is the same as in the case of the ring. The second constraint concerns the poles ($\theta = 0$ and 2π), in which the function's value must be the same for all φ values. This can be achieved either by setting $m = 0$ (see Figure 4a) or by having a node at the poles (Figures 4b and 4c). It is instructive to note the resemblance between Figures 3b and 3c and Figures 4b and 4c when viewed from the direction of the z-axis.

Encoding the amplitude with opacity does not provide a quantitative measure of it. However, the important features of the spherical wavefunctions—the direction of maximum amplitude and the existence of nodal planes—are easily observed. These features are also sufficient for determining the result of superposition of the spherical wavefunctions. Using similar arguments to those used in the previous section, it is easy to see that $p_x = Y_1^{+1} + Y_1^{-1}$ (see Figure 4d), and $p_y = (Y_1^{+1} - Y_1^{-1})/i$ (see Figures 4e and 4f). The third orbital in this set, p_z, is Y_1^0 (see Figure 4a). All three orbitals have

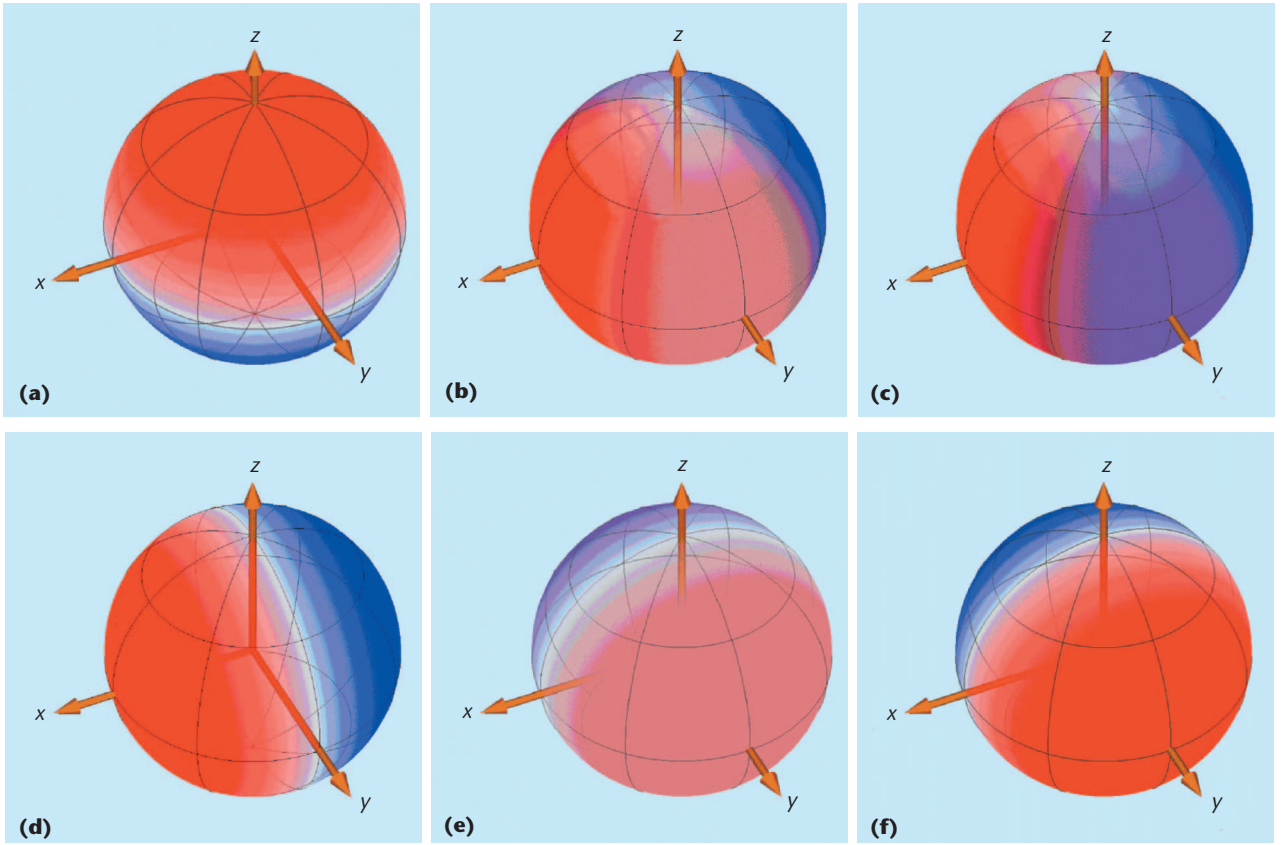

Figure 4. Wavefunctions on a sphere. (a) Y_1^0, (b) Y_1^{+1}, (c) Y_1^{-1}, (d) $Y_1^{+1} + Y_1^{-1}$, (e) $Y_1^{+1} - Y_1^{-1}$, and (f) $(Y_1^{+1} - Y_1^{-1})/i$. The latitude lines designate $\theta = \pi/4$, $\pi/2$, and $3\pi/4$; the longitude lines designate $\varphi = 0$ to $7\pi/4$ in $\pi/4$ increments.

maximum amplitude along the corresponding axis and a perpendicular nodal plane through the origin. These manipulations relate the three possible values for m (0 and ±1), when $l = 1$ in the hydrogen atom solution, to the three p orbitals used in chemistry in a simple, graphical way. Many students, who are never presented with images of Y_1^{+1} and Y_1^{-1}, fail to see the difference between the two sets.[4]

Using advanced computer graphics, we have demonstrated the ability of a graphical applet to illustrate the superposition principle in different topologies. The interactive ability to change parameters and follow their influence is a crucial aspect of the tool set we've described. Time evolution and its influence on the wavefunctions' superposition is an integral part of the proposed approach. As a result, the concept of unitary evolution becomes intuitive and is employed as a base for an axiomatic approach to quantum mechanics. Once the student masters the elementary steps, we can extend the wavefunction description to higher dimensions using the same principles and visual language. Thus, we have developed a tool for illustrating the superposition principle in the hydrogen atom and the hydrogen molecular ion in three dimensions as the natural next step. The insight gained by visualizing the same phenomena in different contexts contributes to the students' ability to abstract, which is key to understanding quantum phenomena in higher dimensions. CiSE

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