SIMULATING THE SPECTRA OF LIGHT SOURCES

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The goal of the Visual Quantum Mechanics project[1] is to develop materials that help high school and undergraduate students to learn quantum physics without having a background in higher-level mathematics. To reach these students we are concentrating on activities that integrate hands-on experiments and multimedia materials with interactive software packages. One of the packages, Spectroscopy Lab Suite,[1] is designed to help students to learn how quantum-mechanical concepts such as energy levels and energy bands can explain the spectra of light emitted by different light sources. Spectroscopy Lab Suite is incorporated into the Learning Cycle[2] model of instruction, which makes extensive use of hands-on activities.

The opening screen of Spectroscopy Lab Suite shows the hierarchy of the various activities (see Fig. 1). This hierarchy is designed to reflect the pedagogical application of the package as envisaged as by us for use in our instructional units. Students first observe the spectra of gas lamps and construct an empirical model of discrete energy levels in an atom using the components of the Gas Lamps module. Students generally use the Emission module after observing the spectra emitted by gas-discharge tubes in the laboratory. We created the Absorption module because we believe that it is useful for students to see that light can be both emitted as well as absorbed by atoms when electrons make transitions from one energy level to another, even though they do not do an absorption experiment in our laboratory.

Having studied the spectra of atoms in a gas with discrete individual levels, students are ready to learn about atoms in various types of solids. Using the LEDs module, students can understand how energy bands may be used to predict the emission spectra of a light-emitting diode that they had earlier observed in the laboratory. In our instructional unit on luminescence, students observe the spectra of various luminescent sources using the Fluorescence and Phosphorescence modules. The IR Detector module helps students to construct a model of the infrared detector cards that are commonly used by TV-repair persons to check remote control devices. Finally, students study ruby, helium-neon, and diode lasers using the Lasers modules. We shall now describe the components of Spectroscopy Lab Suite in greater detail.

Gas Lamps

The screen for the Emission module shows an array of gas lamps on the left and a gas-lamp holder (see Fig. 2). Dragging one of the gas lamps into the gas-lamp holder causes it to light up and its spectrum to appear at the top of the screen. Five known gases (hydrogen, helium, neon, lithium, and mercury) and an unknown gas are available to students. Students draw horizontal lines to represent energy levels on a vertical energy scale and vertical arrows between the lines to indicate transitions. When students move the energy levels, they immediately see the corresponding changes in the energy of a spectral line that appears directly below the real spectrum of the gas. In the case of the unknown gas, students can alter the energies or wavelengths of the spectral lines to create any hypothetical spectrum.

Manipulating the energy-level diagram in this way, students compare the resulting trial spectrum with the real spectrum for the gas. In order to make a spectral line in the trial spectrum coincide with one in the real spectrum, students must create a transition between two energy levels whose difference in energies is equal to the energy of the emitted light,

$$E_{\text{upper}} - E_{\text{lower}} = E_{\text{light}} , \tag{1}$$

where E_{upper} is the energy of the upper energy-level in the transition, E_{lower} is the energy of the lower energy level in the transition, and E_{light} is the energy of the emitted light. By using this program students therefore learn that a spectral line represents a transition between energy levels, and that the

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set to 0.1 Ry, implying subspaces $\mathscr{V}_k$ of dimension 1 to 4. The linear systems (14) have been approximately solved by two multigrid V cycles. A discrete L^2 norm of the residuals $\mathbf{r}_k$ of the eigenvalue problem (see Box 1) is plotted against the number of BGII iterations.

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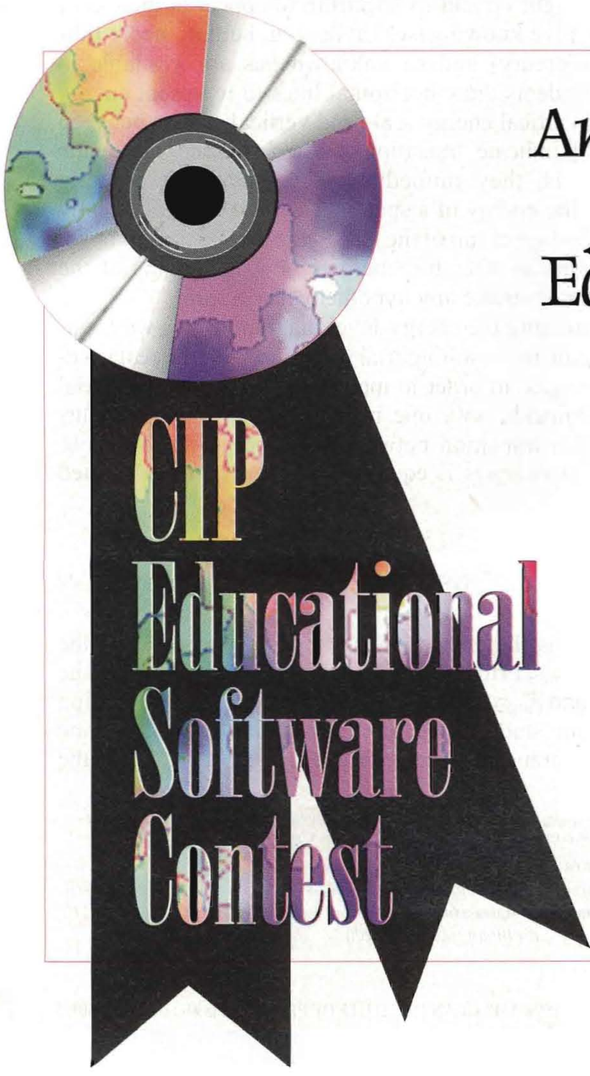

energy of the emitted light is equal to the difference between the energies of the energy levels.

The design of Gas Lamps in fact was motivated by our observation that students often wrongly believe that the spectral lines for a gas are discrete energy levels rather than transitions between energy levels. The Emission module corrects this misconception.

The Absorption module was developed to help students to learn that light can be absorbed by materials and that the process is the reverse of emission. This process is not easily studied in an introductory laboratory, and so students do not come to Absorption after direct observation of experimental results. The Absorption screen, however, is almost identical in appearance to the Emission screen, in order for students to realize that emission and absorption are related processes. To use the program, students drag one of the gas lamps and place it in the path of the white light source. Absorption lines corresponding to the source appear in the white-light spectrum. By a process similar to that of using the Emission module, students draw energy lines and indicate transitions on an energy-level diagram, in order to produce a trial spectrum that matches the given absorption spectrum.

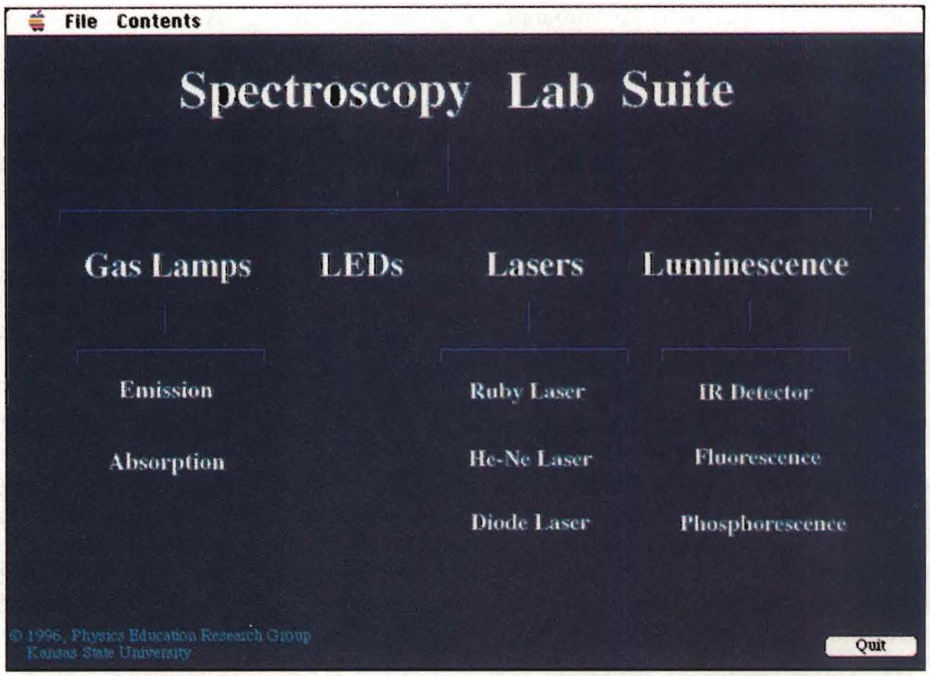

Figure 1. The hierarchy of the components in Spectroscopy Lab Suite reflects the pedagogical organization of the instructional units.

By using both the Emission and Absorption modules, students construct an empirical model of discrete energy levels in an atom. In our pedagogical approach, students do not yet understand why only certain energies are allowed in an atom. Instead, they concentrate on how a simple energy-level model can be used to explain spectra. Thus, they see that discrete energy levels are required by their observations.

When this component is used in a classroom with students working in small groups, different groups may arrive at different energy levels to explain the spectrum of the same gas. The teacher can take advantage of this discrepancy in order to explain that the energy levels chosen by students in this program are not unique. Given the information that the students possess, many different sets of levels are possible. Students therefore see that with limited information they cannot create a complete picture of energy levels in an atom.

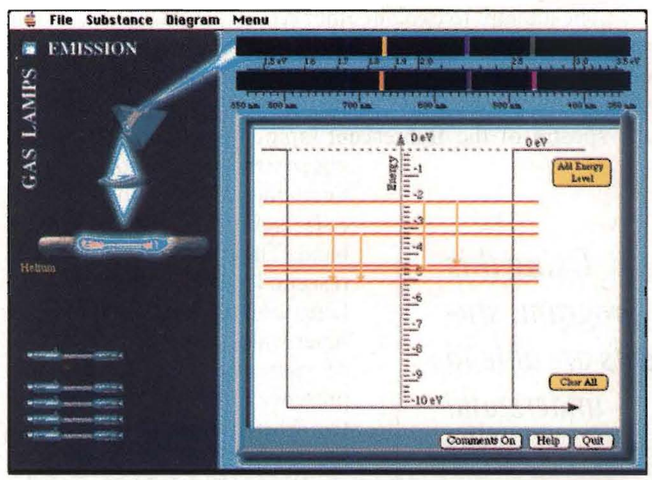

Figure 2. Energy levels and transitions drawn by students on the energy-level diagram produce a trial spectrum that matches the real spectrum of a gas.

LEDs

After constructing a model to explain the spectra of gases using Gas Lamps, students apply the model to light emitted by an LED. They observe that its spectrum is a broad band rather than a set of discrete lines. Based on this observation and the understanding that the discrete spectra of gas lamps are produced by discrete energy levels, students use the LEDs program to construct a model to explain the spectrum of an LED. In our instructional approach, hands-on experiments and simulations lead students from knowledge of discrete energies in atoms to an understanding of energy bands.

As shown in Fig. 3, the program screen of LEDs is similar to that of the Gas Lamps modules. An array of LEDs of different colors appears at the left side of the screen, along with an LED holder. Dragging an LED into the holder causes the spectrum of the LED to appear on the top right of the screen. Students then create the conduction band and valence band in the energy-level diagram that appears on the right. By adjusting the energy and widths of the energy bands, the student can change the trial spectrum that appears directly below the real spectrum. The program calculates the trial spectrum from the widths and positions of the energy band as follows:

$$E_{\text{midspectrum}} = \left(\frac{E_{\text{ctop}} + E_{\text{cbot}}}{2}\right) - \left(\frac{E_{\text{vtop}} + E_{\text{vbot}}}{2}\right) \quad (2)$$

$$\Delta E_{\text{spectrum}} = (E_{\text{ctop}} - E_{\text{vbot}}) - (E_{\text{cbot}} - E_{\text{vtop}}) \ , \quad (3)$$

where various terms are indicated in Fig. 4.

Although the LEDs module enables students to construct an empirical model of energy bands that explains the broad spectra of LEDs, it does not explain why energy bands should exist. Students are able to arrive at a model based on their observations that predicts the existence of energy bands without knowing the reason for their existence. In our course of instruction students use the programs in the Luminescence module to learn that discrete energy levels in an individual atom evolve into energy bands when two or more of these atoms are brought close together.

Luminescence

The attempt to explain other types of light sources using the energy-level model involves an increase in the complexity of energy bands and transitions. Students confront this complexity when they study luminescence. While investigating the spectra of the fluorescent lamp, for example, students observe the presence of both distinct lines (similar to the mercury spectrum) and a broad band. They know that the fluorescent lamp is a mercury gas lamp with a material coating the inner walls of the lamp. The use of mercury gas explains the presence of the mercury lines in the spectrum but not the broad band. When students construct a model for the broad band, they realize that its presence must be related to the material that coats the inner walls of the glass tube. But since no energy source is present in this material, it must be receiving its energy from the light emitted by the mercury inside the gas lamp. Students also realize that the energy of the light emitted by mercury and absorbed by the coating must be greater than the energy of the light emitted by the coating. When the light emitted by mercury is absorbed by the material, it causes a transition from the ground state to the excited state. Since the material re-emits the light with a lower energy, the light must be emitted by an intermediate state.

Using this program, students are able to understand the role of the metastable state and its relationship to fluorescent light.

A model consistent with these observations must therefore contain three sets of bands. In addition to the excited-state or conduction band and the ground-state or valence band, there must be a third, metastable-state band between these two.

The Fluorescence module enables students to construct the required model. Students begin by drawing the excited-state band and the metastable-state band. The program allows them to change the energies of either band. For the material to emit light, electrons must first be raised from the ground state to the excited state. On the left-hand side of the screen students can adjust the input energy from the internal source (see Fig. 5). For a transition to occur,

$$E_{\text{lamp}} \geq E_{\text{excited}} - E_{\text{ground}} \ , \quad (4)$$

where E_{lamp} is the input energy from the mercury source, E_{excited} is the excited-state band energy, and E_{ground} (= 0) is the ground-state energy.

As soon as the students choose an energy that is greater than the energy of the excited-state band and click the button

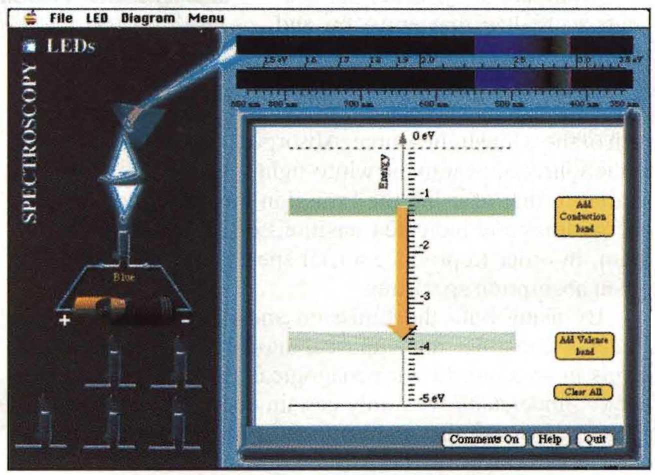

Figure 3. Students add conduction and valence bands to the energy-band diagram of an LED and match the resulting trial spectrum to the real spectrum for the LED.

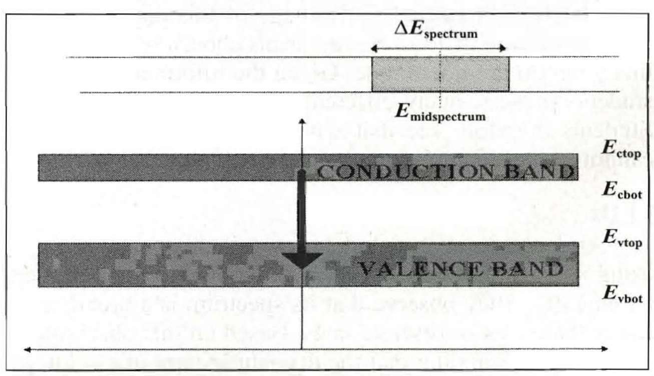

Figure 4. The energy and width of the conduction and valence bands are the key variables in the program's calculation of the trial spectrum for an LED.

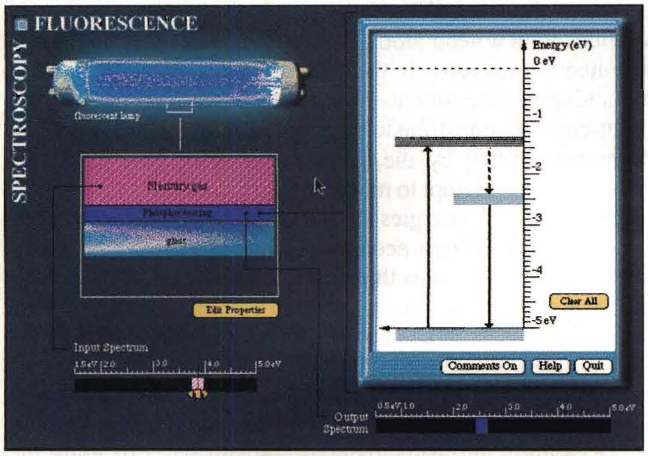

Figure 5. After adjusting the input energy and turning on the fluorescent lamp, students see transitions in the energy-level diagram and a corresponding output spectrum.

that turns on the source, they see a transition from the ground state to the excited state. The darkened ground state changes to a lighter shade, indicating a depopulation of ground-state energies. Simultaneously, the excited-state energy levels that were originally light turn darker, indicating that they are now populated with electrons. Next, a dashed transition line from the excited state to the metastable state appears, indicating a nonradiative transition. The metastable state turns darker, indicating that it is populated by electrons. Finally, a transition line from the metastable state to the ground state appears, representing the radiative transition that causes the material coating the inner surface of the tube to fluoresce. The corresponding spectrum appears directly below the energy-level diagram. The energy of the fluorescent output-spectrum is given by the equation

$$E_{\text{output}} = E_{\text{metastable}} - E_{\text{ground}} \,. \quad (5)$$

Using this program, students are able to understand the role of the metastable state and its relationship to fluorescent light. In our instructional model, students first observe the real spectrum of a fluorescent lamp through a spectroscope. Then by using the Fluorescence module they adjust the energy levels of the metastable and excited states to obtain a similar spectrum on the computer.

When students observe phosphorescent light sources such as a glow-in-the-dark toothbrush, they notice that these materials continue to glow even after the source of input energy is turned off. The Phosphorescence module enables students to understand this phenomenon on the basis of the energy levels and metastable states that they learned about in Fluorescence. The screen of the Phosphorescence module shows a glow-in-the-dark toothbrush (see Fig. 6). After creating excited and metastable states, students begin changing the energy of the light that irradiates the toothbrush. As soon as they choose an input energy that is greater than the energy of the excited-state band, a transition from the ground state to the excited state appears [Eq. (4)]. The darkened ground state changes to a lighter shade, indicating a depopulation of the ground state, while the excited state turns dark. Subsequently, a dashed transition line from the excited state to the metastable state appears, indicating a nonradiative transition, and the metastable state turns darker. Then the toothbrush on the screen is removed from liquid nitrogen and placed in front of a heat source. As the student increases the temperature of the heat source until it is greater than the energy difference between the excited state and the metastable state, the electrons in the metastable state go into the excited state,

$$E_{\text{heat source}} = \frac{k_B T}{q} \geq E_{\text{excited}} - E_{\text{metastable}} \,, \quad (6)$$

where $E_{\text{heat source}}$ is the energy of the heat source (measured in electron volts), T is the absolute temperature, and k_B is Boltzmann's constant. The shades of the corresponding levels change in the energy-level diagram. Finally a transition from the excited state to the ground state appears, along with emitted light and a spectrum with energy, as represented by Eq. (5).

Students apply the knowledge they have gained thus far in order to understand the infrared-detector cards that are commonly used by TV-repair technicians. The screen of the IR Detector module shows an image of a real detector card on the left of the screen. The various transitions are similar

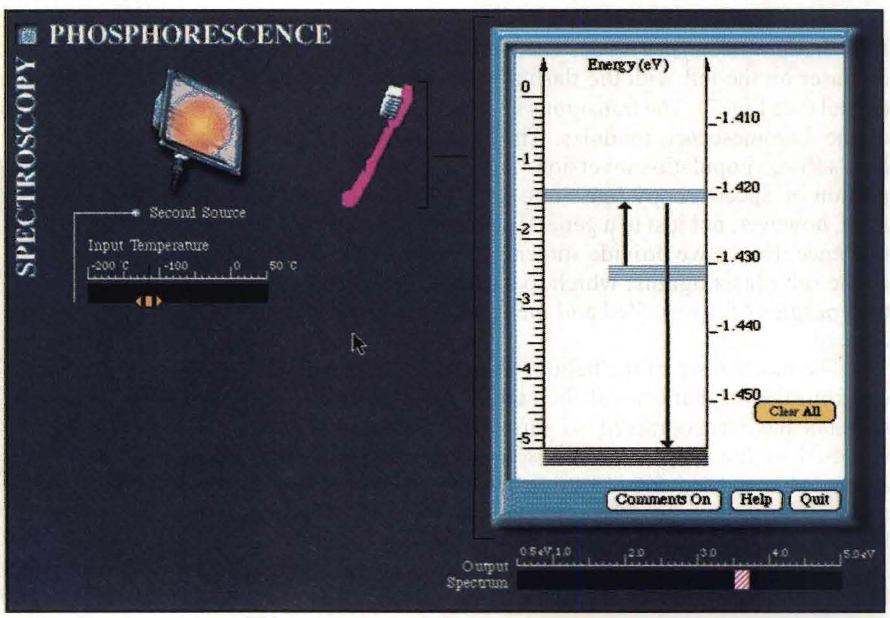

Figure 6. Increasing the temperature of the heat source elevates electrons to the excited state in the phosphorescent material of the toothbrush, producing the indicated transitions and spectrum of emitted light.

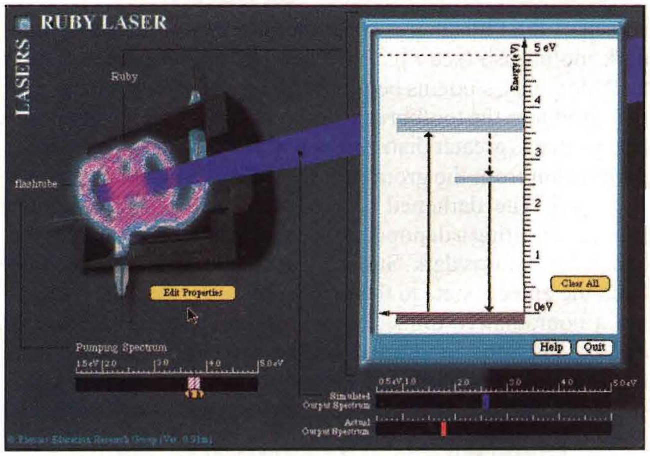

Figure 7. Trial-and-error selection of energy levels in the ruby produces the output spectrum of the emitted laser light, which students match to the actual spectrum of the laser.

to the ones in Phosphorescence. The card is placed in front of an infrared source that provides sufficient energy for electrons to make the transition from the metastable state to the excited state:

$$E_{\text{infrared source}} \geq E_{\text{excited}} - E_{\text{metastable}}. \quad (7)$$

Students perform several experiments on the card, including keeping it in the dark for several days in order to gauge its effectiveness as a temporary energy-storage device. Then they use the program to construct a model consistent with their observations.

Lasers

In the Lasers modules we focus on three types of lasers: ruby, helium-neon, and diode. The Ruby Laser screen shows the laser on the left with the flashtube surrounding the ruby crystal (see Fig. 7). The transitions shown are similar to those of the Luminescence modules. The shading of the energy levels shows population inversion. The modules in the Lasers portion of Spectroscopy Lab Suite refer to specific types of laser, however, not just to a general phenomenon as in Luminescence. Hence we provide students with the real spectrum of the ruby laser against which to check the correctness of the energies of the excited and metastable states they have created.

The mechanism of the helium-neon laser is quite different from the mechanisms of the other light sources that the students have encountered so far. Here the input energy supplied to the helium atoms is transferred to the neon atoms, while subsequent electronic transitions in neon cause the laser to emit light. The operation of the Helium-Neon Laser module is similar to that of the other Lasers modules, however. After creating excited and metastable states in helium and neon, students begin changing the input energies to the helium atoms. Input energy elevates the helium atoms to the excited state.

An animation shows the movement of helium and neon atoms in the laser. When a helium atom in the excited state collides with a neon atom, it transfers some of its energy to the neon. Electrons in the excited states of neon make a nonradiative transition to the metastable states, followed by a light-emitting transition to the ground state. Three energies of light are emitted by the helium-neon laser [see Eq. (5)].[3] Students then attempt to match the energy of the emitted laser light to the three energies shown in the program.

Ruby and helium-neon lasers have a primarily historical significance. The lasers that students will most often encounter in actual use are diode lasers. The Diode Laser module helps students to understand energy states in these ubiquitous devices. The opening screen has a typical diode laser connected in a circuit on the left, and a diagram of the internal structure of the laser. After creating the conduction and valence bands of the lasing material, students begin to adjust the band energies. The vertical line through the center of the energy-band diagram separates the p side and n side of the diode. The energy difference between the conduction and valence bands is the energy gap, E_g. This band structure is not realistic since the two bands on the p side and n side will not be aligned initially.[4] Students must drag the energy bands on the right (n side) downwards to represent the built-in voltage V_B of the diode.

For a p-n junction to work as a diode laser, the doping on either side must be degenerate, which means that

$$V_B \geq E_g \,. \quad (8)$$

When the criterion in Eq. (8) is satisfied, both the conduction and valence bands on the n side are darkened, indicating occupancy by electrons, while on the p side only the lower energy levels in the valence band are darkened. Increasing V_A causes the energy bands on the n side to rise, and students observe that the conduction band on the n side is occupied (darkened), while the upper energy levels in the valence band on the p side are unoccupied (not darkened). This situation corresponds to population inversion.

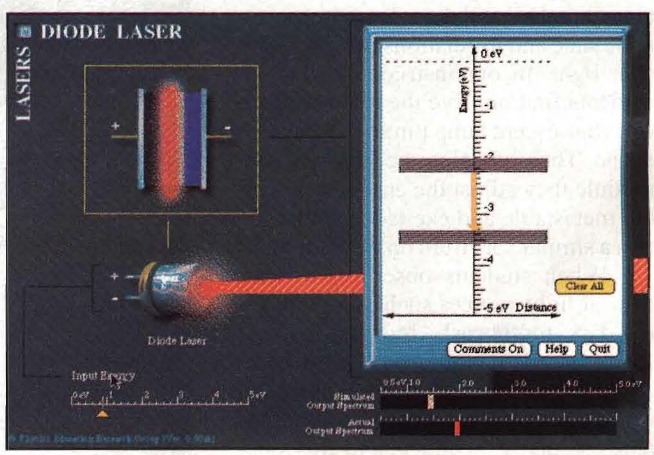

Figure 8. The energy gap of the semiconductor, which students select by trial and error, yields a spectrum that matches the actual spectrum for a typical AlGaAs diode laser.

When the applied voltage is increased so that

$$V_A \geq V_B \,, \tag{9}$$

the conduction bands on the p side also become dark, indicating that electrons have flowed from the conduction band on the n side to the conduction band on the p side. Subsequently, a transition from the conduction band to the valence band appears, indicating lasing. The corresponding energy-spectrum of the laser appears on a scale below the energy-level diagram. The energy of the emitted light is given by the equation

$$E_{laser} = E_g \,. \tag{10}$$

By a process similar to that of the other Lasers modules, students compare the spectrum of light emitted by the laser in the program to the typical spectrum of a red AlGaAs laser.[4]

With this combination of laboratory activities and computer modeling, students are able to understand some of the fundamentals of quantum science without recourse to higher-level mathematics.

Each module of the Spectroscopy Lab Suite was specifically designed for use in hands-on activities. With this combination of laboratory activities and computer modeling, students are able to understand some of the fundamentals of quantum science without recourse to higher-level mathematics.

Pedagogical implications

Although the various components of the Spectroscopy Lab Suite were created specifically for use with our Visual Quantum Mechanics[1] instructional units, we believe that the suite can be used in a variety of educational settings. The software is innovative technically and pedagogically in the following ways:

- Without requiring knowledge of higher-level mathematics, the single package of programs teaches exactly how energy levels and transitions are related to emitted light in solids and gases in a number of different situations. Hence it enables high-school and introductory undergraduate students to arrive at an understanding of the difference between solids and gases at the atomic level. By using the various programs students see that the main difference between gases and solids is that the energy levels in a gas are discrete, whereas those in a solid exist in bands, a difference that is reflected in the light emitted by each type of material. The Gas Lamps module is also particularly useful in conveying to students that a spectral line represents a transition between energy levels, not an energy level itself. The program thereby corrects the misconception common among students that energy levels correspond to lines in the spectrum.
- The interfaces of the modules are visually similar to the physical situations being explored. For instance, the Gas Lamps module shows various gas-discharge tubes that must be placed in the gas-lamp holder in order to emit light. The visual similarity between the students' laboratory observations and the program's screen display can be particularly useful in enhancing the students' understanding of the phenomena they have observed. Features such as this one also make the program easy to integrate with hands-on activities.
- The programs are both interactive and user-friendly. Users must determine the energy levels and the adjust them until the trial spectrum matches the real spectrum, so that the programs require students to be actively involved. In order to facilitate interactivity, we have designed the various buttons and other objects on the screen so that their functions are intuitively grasped by users. Hence the program is accessible to students who have limited computer experience. For these students a manual and online help are also available.
- Spectroscopy Lab Suite is the first pedagogical package, to the best of our knowledge, to be directly executable from the World Wide Web. Netscape 2.0 (or greater) and the Macromedia Shockwave Director plug-in are required.

Spectroscopy Lab Suite has been used in several instructional environments. At the time of writing, the package served in an introductory modern-physics course at Kansas State University taken primarily by secondary-education majors, and in high-school physics courses in several states. Students used the program with the accompanying hands-on activities, along with other programs and written materials. The results of these classroom field tests are encouraging, and we have incorporated the feedback that we received into the current version of the program. Both Windows and Macintosh versions can be downloaded from our World Wide Web site, http://www.phys.ksu.edu/perg/vqm. A Shockwave version of the program is also available at the Web site and can be run online.

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1. Supported by the National Science Foundation, under grant ESI 9452782. More information about Visual Quantum Mechanics may be obtained at our World Wide Web site, http://www.phys.ksu.edu/perg/vqm.
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