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## Operators and Waves - Solutions

1. Using Eqs. (3.2), (3.3) and the wave function given in the problem

$$\hat{p}\psi(x) = -i\hbar \frac{d}{dx} A e^{i\alpha x} = -i^2 \alpha \hbar A e^{i\alpha x} = \alpha \hbar A e^{i\alpha x}$$

The wavefunction is an eigenfunction of the momentum operator with eigenvalue  $p = \alpha \hbar$ . The kinetic energy is given by Eq. (3.5) with  $V(x)=0$ :

$$KE = \frac{p^2}{2m} = \frac{\alpha^2 \hbar^2}{2m}$$

Alternatively, one can start with Eq. (3.6) with  $V(x) =$  and take the double derivative of the wave function. Of course, the same answer is obtained.

2. Using Eq. (3.2):

$$\begin{aligned}\hat{p}\phi_1(x) &= i\hbar k \cos kx \\ \hat{p}\phi_2(x) &= -i\hbar k \sin kx\end{aligned}$$

These wave functions are not eigenfunctions of the momentum operator. If they were eigenfunctions, then they would have the form  $\hat{p}\phi(x) = C\phi(x)$  for some constant  $C$ .

3. We want to find a linear combination  $\psi = A\phi_1(x) + B\phi_2(x)$  such that:

$$\hat{p}\psi = p\psi$$

for some constant  $p$ . Applying Eq. (3.3):

$$\hat{p}\psi = -i\hbar \frac{d\psi}{dx} = i\hbar k A \sin(kx) - i\hbar k B \cos(kx)$$

Since the constants  $A$  and  $B$  have switched places compared with  $\psi(x)$ , we see that an eigenvalue equation can only be formed with something like  $A=B$ . Looking more closely at the eigenvalue condition:

$$i\hbar k A \sin(kx) - i\hbar k B \cos(kx) = p(A \cos(kx) + B \sin(kx))$$

then setting the coefficients equal, a solution is found if  $B = iA$  and  $p = \hbar k$ . Hence,  $\psi$  is an eigenfunction of the momentum when

$$\psi(x) = A(\sin(kx) + i \cos(kx)) = Ae^{ikx}$$

where Euler's formula has been used. This  $\psi(x)$  has eigenvalue  $p = \hbar k$ .

**4. (a)** This one-dimensional lattice looks identical if the coordinate system is shifted by an integer multiple of the lattice spacing  $a$ :

$$\psi(x) = \psi(x + a)$$

The momentum eigenvalue equation then becomes

$$\hat{p}\psi(x) = p\psi(x) = p\psi(x + a)$$

**(b)** Using the  $\psi(x)$  from Problem 1, the general solution to this equation is:

$$\psi(x) = Ae^{ikx} = Ae^{ik(x+a)}$$

which has eigenvalue  $p = \hbar k$  (see Problem 1).

**(c)** Using the boundary condition given:

$$\psi(0) = A = \psi(a) = Ae^{ika}$$

we see that  $e^{ika} = 1$ . Using Euler's identity  $e^{i2\pi n} = 1$  gives  $ka = 2\pi n$  for integer  $n$ . Since the momentum eigenvalue is  $p = \hbar k$ :

$$p = \frac{2\pi\hbar n}{a} = \frac{nh}{a}$$

Comparing this with de Broglie's equation (1.26),  $p = h/\lambda$  we see that the electron takes on wavelengths  $\lambda$  equal to integer fractions of the lattice spacing  $a$ .

**5.** When  $E < V(x)$ , then  $V(x) - E$  is always positive. The Schrödinger equation then becomes:

$$\frac{d^2\psi}{dx^2} = \omega^2\psi$$

where  $\omega^2 = 2m(V - E)/\hbar^2$  is a positive constant. The general solution to this equation is:

$$\psi(x) = Ae^{\omega x} + Be^{-\omega x}$$

This wave function goes to infinity at either  $x = \infty$  or  $x = -\infty$  and so it cannot be normalized.

6. Note that the thickness  $L$  and the constant  $E_0$  are unchanged from MATLAB Program 3.2. The only change for this problem is that  $V_0 = 0.2 \text{ eV}$  whereas it was  $0.3 \text{ eV}$  in Program 3.2. We need only change line 9 of the MATLAB program to get:

```
xmax=20;
L=5;
n=5;
delta=xmax/n;
n1=fix(L/delta)+1;
n2=n-n1;
E0=1.759;
v=-ones(n-1,1);
d=[ 2*ones(n1,1); (2+0.2*E0*delta^2)*ones(n2,1) ];
A=diag(v,-1)+diag(v,1) + diag(d);
A(1,2)=-2;
A
[E V] = eig(A);
GroundState = V(1,1)/(E0*delta^2)
```

After running this program in MATLAB or Octave, the ground state eigenvalue for a five-point grid ( $n = 5$  above) returns a value of 0.0182 (in units of  $eV$ ). Increasing this to a ten-point grid (by changing line 3 of the above program to  $n = 10$ ) returns a more accurate value of 0.0284. Note that some larger values of  $n$  cause MATLAB to put the lowest eigenvalue at a location other than  $V(1,1)$  (see the last line in the MATLAB program above). This is not a problem, but requires more effort to find the lowest eigenvalue by printing out the full set of eigenvalues (remove the semicolon after `eig(A)`.)

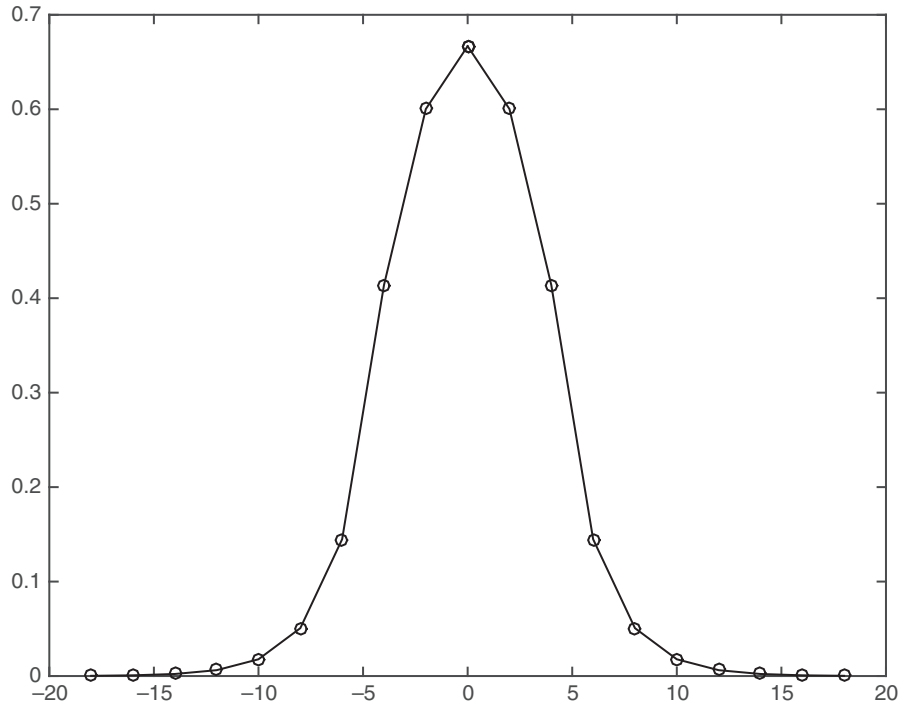
7. The eigenfunctions are calculated along with the eigenvalues in line 13 of MATLAB Program 3.2, where it has `[E V] = eig(A)`. The eigenvectors are stored in the array `E`. The wavefunction for the ground state is stored in the first eigenfunction. To access the first column of the array `E`, the following lines can be appended to Program 3.2:

```
y = E(:,1);
x = 0 : delta : (xmax-delta);
plot(x,y)
```

Note that the above plots only half of the wavefunction. Since the well is symmetric about the origin, the ground state wave function (an even solution) is also symmetric. To plot the full wave function, one can add the following lines:

```
xneg = -x;
plot( x,y, xneg,y)
```

The resulting plot is very similar to the wavefunction shown in Figure 3.2.



8. Figure 2.12 is for Problem 2.15, where only the odd solutions are allowed due to the boundary condition  $\psi(x = 0) = 0$  due to the infinite potential at  $x = 0$ . In the development of Section 3.2, Eq. (3.22) is only for the even solutions. This must be modified for the current problem to match the current boundary conditions. In particular:

$$u_1'' = \frac{u_2 - 2u_1 + 0}{\delta^2}$$

and all other derivatives are like Eq. (3.21). Hence, we only need to modify the first line of the matrix  $\mathbf{A}$  of Eq. (3.24), where the second entry changes from  $-2$  to  $-1$ . The MATLAB code becomes:

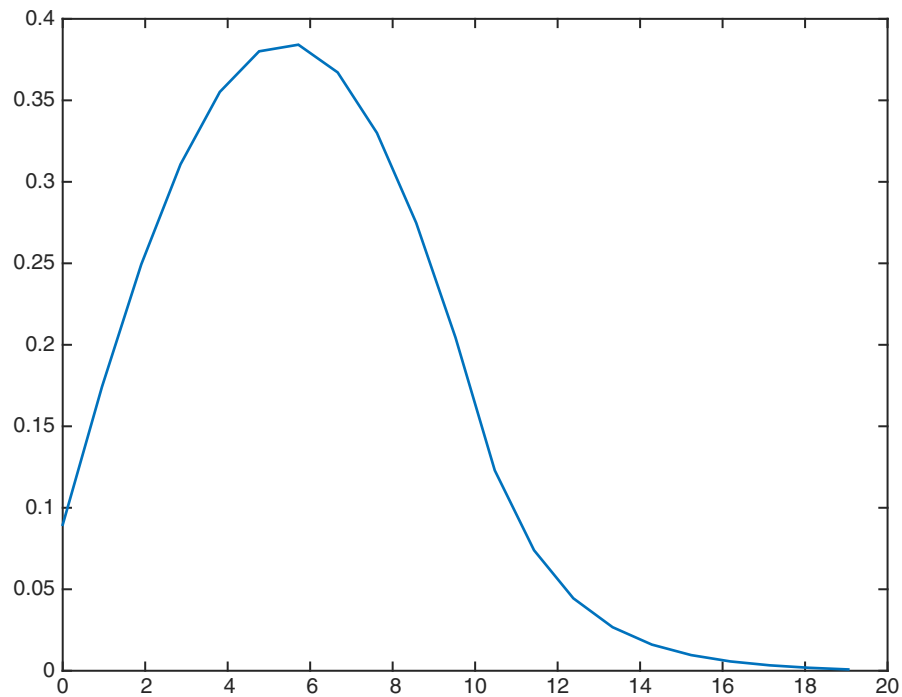
```
xmax=20;
L=10;
n=21;
delta=xmax/n;
n1=fix(L/delta)+1;
n2=n-n1;
E0=1.759;
v=-ones(n-1,1);
d=[ 2*ones(n1,1); (2+0.2*E0*delta^2)*ones(n2,1) ];
```

```

A=diag(v,-1)+diag(v,1) + diag(d);
A
[E V] = eig(A);
OddState = V(1,1)/(E0*delta^2)

```

Note that  $L$  has been changed from Problem 3.6, since the potential well goes from 0 to 10. One can confirm that the wave function looks reasonable by plotting the first eigenfunction as in the previous problem. (It may take more grid points than  $n = 21$  before one sees the boundary conditions properly satisfied at  $x = 0$ .) For the above case with  $n = 21$ , the energy of the lowest (odd) eigenstate is  $0.0344 \text{ eV}$ . For larger  $n$ , the approximation gets better and the eigenstate approaches an energy of  $0.04 \text{ eV}$ .



9. Following Section 3.3.1:

$$\frac{d^2\psi_1}{dx^2} + k_1^2\psi_1 = 0$$

and from Eq. (3.37):

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

giving the general solution for  $x < 0$ :

$$\psi_1 = Ae^{ik_1x} + Be^{-ik_1x}$$

For  $x > 0$ , using Eq. (3.34):

$$\frac{d^2\psi_2}{dx^2} - k_2^2\psi_2 = 0 \text{ where } k_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

gives the physically acceptable solution Eq. (3.35):

$$\psi_2(x) = De^{-k_2x}$$

Now, we impose continuity of the wave equation at  $x = 0$  and its first derivatives at  $x = 0$ :

$$\begin{aligned}\psi_1(0) &= \psi_2(0) \Rightarrow A + B = D \\ \psi_1'(0) &= \psi_2'(0) \Rightarrow ik_1(A - B) = -k_2D\end{aligned}$$

Divide both side of the second equation by  $ik_1$ :

$$A + B = D \tag{1}$$

$$A - B = -\frac{k_2}{ik_1}D = i\frac{k_2}{k_1}D \tag{2}$$

Adding these two equations, and solving for  $A$  in terms of  $D$ :

$$\begin{aligned}2A &= D\left(1 + i\frac{k_2}{k_1}\right) \\ A &= \frac{1}{2}D\left(1 + i\frac{k_2}{k_1}\right)\end{aligned} \tag{3}$$

Subtracting (1) from (2), and solving for  $B$  in terms of  $D$ :

$$\begin{aligned}2B &= D\left(1 - i\frac{k_2}{k_1}\right) \\ B &= \frac{1}{2}D\left(1 - i\frac{k_2}{k_1}\right)\end{aligned} \tag{4}$$

Dividing each of equations (3) and (4) by  $D$ :

$$\begin{aligned}\frac{A}{D} &= \frac{1}{2}\left(1 + i\frac{k_2}{k_1}\right) \\ \frac{B}{D} &= \frac{1}{2}\left(1 - i\frac{k_2}{k_1}\right)\end{aligned}$$

The reflection coefficient  $R$  is defined by Eq. (3.31) giving:

$$R = \frac{|B|^2 v_1}{|A|^2 v_1} = \frac{|B|^2}{|A|^2}$$

Using our ratios above:

$$R = \frac{\left(\frac{B}{D}\right)^* \left(\frac{B}{D}\right)}{\left(\frac{A}{D}\right)^* \left(\frac{A}{D}\right)} = \frac{\frac{1}{4}(1 - i\frac{k_2}{k_1})(1 + i\frac{k_2}{k_1})}{\frac{1}{4}(1 + i\frac{k_2}{k_1})(1 - i\frac{k_2}{k_1})} = 1$$

10. The probability that the particle is found in the region  $x > 0$  is given by:

$$P = \int_0^{\infty} |\psi(x)|^2 dx$$

Using Eq. (3.35):

$$P = \int_0^{\infty} D^2 e^{-2k_2 x} dx = \frac{D^2}{2k_2}$$

where  $k_2$  is given by Eq. (3.34). This probability is nonzero because of the uncertainty principle. Over a short period of time  $\Delta t$ , the energy is uncertain by  $\Delta E/\hbar$ , and the particle can exist in the region  $x > 0$  because the total energy is uncertain by this amount.

11. Using the equations just above Figure 3.6, the general solutions for each region are:

$$\begin{aligned} \psi_1(x) &= Ae^{ik_1 x} + Be^{-ik_1 x}, & x \leq 0 \\ \psi_2(x) &= Ce^{k_2 x} + De^{-k_2 x}, & 0 \leq x \leq L \\ \psi_3(x) &= Fe^{ik_1 x}, & x \geq 0 \end{aligned}$$

We impose the boundary conditions at  $x = 0$  and  $x = L$ :

$$\begin{aligned} \psi_1(0) &= \psi_2(0) \\ \psi_1'(0) &= \psi_2'(0) \\ \psi_2(L) &= \psi_3(L) \\ \psi_2'(L) &= \psi_3'(L) \end{aligned}$$

The first two yield the following system of equations:

$$\begin{aligned} A + B &= C + D \\ ik_1(A - B) &= k_2(C - D) \end{aligned}$$

We divide the second of these by  $ik_1$  and add the result to the first to obtain an expression for  $A$  in terms of  $C$  and  $D$ :

$$2A = C + D - i\frac{k_2}{k_1}(C - D) \quad (1)$$

Now, let's turn to the interface between regions 2 and 3. The boundary conditions produce the following system:

$$\begin{aligned} Ce^{k_2L} + De^{-k_2L} &= Fe^{k_1L} \\ k_2Ce^{k_2L} - k_2De^{-k_2L} &= ik_1Fe^{k_1L} \end{aligned}$$

Dividing the second of these equations by  $k_2$  reduces the system to:

$$\begin{aligned} Ce^{k_2L} + De^{-k_2L} &= Fe^{k_1L} \\ Ce^{k_2L} + De^{-k_2L} &= i\frac{k_1}{k_2}Fe^{k_1L} \end{aligned}$$

Add the two equations and we can solve for  $C$  in terms of  $F$ :

$$\begin{aligned} 2Ce^{k_2L} &= Fe^{k_1L} + i\frac{k_1}{k_2}Fe^{k_1L} \\ C &= \frac{F}{2}\left(1 + i\frac{k_1}{k_2}\right)e^{(ik_1-k_2)L} \end{aligned} \quad (2)$$

Subtract those same equations to solve for  $D$  in terms of  $F$ :

$$\begin{aligned} 2De^{-k_2L} &= Fe^{k_1L} - i\frac{k_1}{k_2}Fe^{k_1L} \\ D &= \frac{F}{2}\left(1 - i\frac{k_1}{k_2}\right)e^{(ik_1+k_2)L} \end{aligned} \quad (3)$$

Insert (2) and (3) into (1):

$$\begin{aligned} 2A &= \frac{F}{2}\left(1 + i\frac{k_1}{k_2}\right)e^{(ik_1-k_2)L} + \frac{F}{2}\left(1 - i\frac{k_1}{k_2}\right)e^{(ik_1+k_2)L} \\ &\quad - i\frac{k_2}{k_1}\frac{F}{2}\left[\left(1 + i\frac{k_1}{k_2}\right)e^{(ik_1-k_2)L} + \left(1 - i\frac{k_1}{k_2}\right)e^{(ik_1+k_2)L}\right] \end{aligned}$$

Divide both sides by  $A$  and simplify:

$$\begin{aligned} 4 &= \frac{F}{A}\left[\left(1 + i\frac{k_1}{k_2}\right) - \left(i\frac{k_1}{k_2} - 1\right)\right]e^{ik_1L-k_2L} + \frac{F}{A}\left[\left(1 - i\frac{k_1}{k_2}\right) + \left(i\frac{k_1}{k_2} + 1\right)\right]e^{ik_1L+k_2L} \\ &= \frac{F}{A}\left[\left(2 + i\frac{k_1^2 + k_2^2}{k_1k_2}\right)e^{ik_1L-k_2L} + \left(2 + i\frac{k_2^2 - k_1^2}{k_1k_2}\right)e^{ik_1L+k_2L}\right] \end{aligned}$$



Solve for  $F/A$ :

$$\frac{F}{A} = 4 \left[ \left( 2 + i \frac{k_1^2 + k_2^2}{k_1 k_2} \right) e^{ik_1 L - k_2 L} + \left( 2 + i \frac{k_2^2 - k_1^2}{k_1 k_2} \right) e^{ik_1 L + k_2 L} \right]^{-1}$$

**12.** The transmission probability is given by the equivalent of Eq. (3.31):

$$T = \frac{|F|^2 v_1}{|A|^2 v_1} = \left| \frac{F}{A} \right|^2$$

where the region after the barrier has the same momentum  $p = \hbar k$  as before the barrier, and hence the particle flux (given by the velocity  $v_1$ ) cancels out. Using the result from the previous problem:

$$4 = \frac{F}{A} \left[ \left( 2 + i \frac{k_1^2 + k_2^2}{k_1 k_2} \right) e^{ik_1 L - k_2 L} + \left( 2 + i \frac{k_2^2 - k_1^2}{k_1 k_2} \right) e^{ik_1 L + k_2 L} \right]$$

Using the given numerical values  $V_0 = 5.0 \text{ eV}$  and  $E = 4.0 \text{ eV}$ , along with the mass of the electron from Appendix A, gives:

$$k_1 = 10.25 \text{ nm}^{-1} \quad \text{and} \quad k_2 = 5.12 \text{ nm}^{-1}$$

with  $k_1/k_2 = 2$ . Using these values and the given value  $L = 0.1 \text{ nm}$ :

$$4 = \frac{F}{A} \left[ \left( 2 + i \frac{5}{2} \right) e^{0.512i} + \left( 2 + i \frac{3}{5} \right) e^{1.537i} \right]$$

Multiplying through by  $e^{-0.512i}$ :

$$4e^{-0.512i} = \frac{F}{A} \left[ \left( 2 + i \frac{5}{2} \right) + \left( 2 + i \frac{3}{5} \right) e^{1.025i} \right]$$

Now use the identity:

$$e^{1.025i} = \cos(1.025) + i \sin(1.025)$$

and multiplying through gives

$$4e^{-0.512i} = \frac{F}{A} \left[ (2 + 2.5i) + (2 + 1.5i)(0.519 + 0.855i) \right] = \frac{F}{A} \left[ (1.755 + 4.99i) \right]$$

It is now straight-forward to take the absolute square and substitute in  $T$ :

$$16 = T[3.08 + 24.9] = 28.0 T$$

Hence the transmission probability is  $T = 4/7$  or, in percentage, 57%.

**13.** Using the first equation from Section 3.4:

$$\Delta x \cdot \Delta p_x \geq \frac{\hbar}{2}$$

Taking the given values,  $\Delta x = 1.0 \text{ nm}$  and the value of  $\hbar$  from Appendix A:

$$p \sim \Delta p = \frac{1.055 \times 10^{-34} \text{ J} \cdot \text{s}}{2(1.0 \times 10^{-9} \text{ m})} = 5.28 \times 10^{-26} \text{ N} \cdot \text{s}$$

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14. Using the second equation from Section 3.4:

$$\Delta E \cdot \Delta t \geq \frac{\hbar}{2}$$

The natural line width is estimated as

$$\Delta E = \frac{1.055 \times 10^{-34} J \cdot s}{2(4.0 \times 10^{-10} s)} = 1.32 \times 10^{-25} J$$

Converting units:

$$\Delta E = 1.32 \times 10^{-25} J \cdot \frac{1 eV}{1.6 \times 10^{-19} J} = 8.24 \times 10^{-7} eV$$

15. Using the normalization condition, Eq. (2.18):

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

and inserting the given wave function and boundary conditions:

$$\int_0^1 B^2 e^{-2x} dx = 1$$

Doing the integral:

$$B^2 \left(-\frac{1}{2}\right) [e^{-2} - 1] = -0.5(0.1353 - 1) = 0.432$$

Taking the square root,  $B = 0.658$ .

16. Using Eq. (3.43) for the average value of an observable:

$$\langle Q \rangle = \int \psi^*(x) \hat{Q} \psi(x) dx$$

where  $\hat{Q}$  is the corresponding operator. In this case the kinetic energy is:

$$\frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$$

The integral becomes:

$$\begin{aligned} \langle KE \rangle &= \int_0^1 B e^{-x} \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2}\right) B e^{-x} dx \\ &= -\frac{\hbar^2}{2m} B^2 \int_0^1 e^{-2x} dx \\ &= \frac{\hbar^2}{4m} B^2 [e^{-2} - 1] \end{aligned}$$

where  $B$  is the normalization constant found in problem 15. Note that  $B$  must have the same units as momentum,  $m/s$ , to give  $KE$  in units of  $J$ .