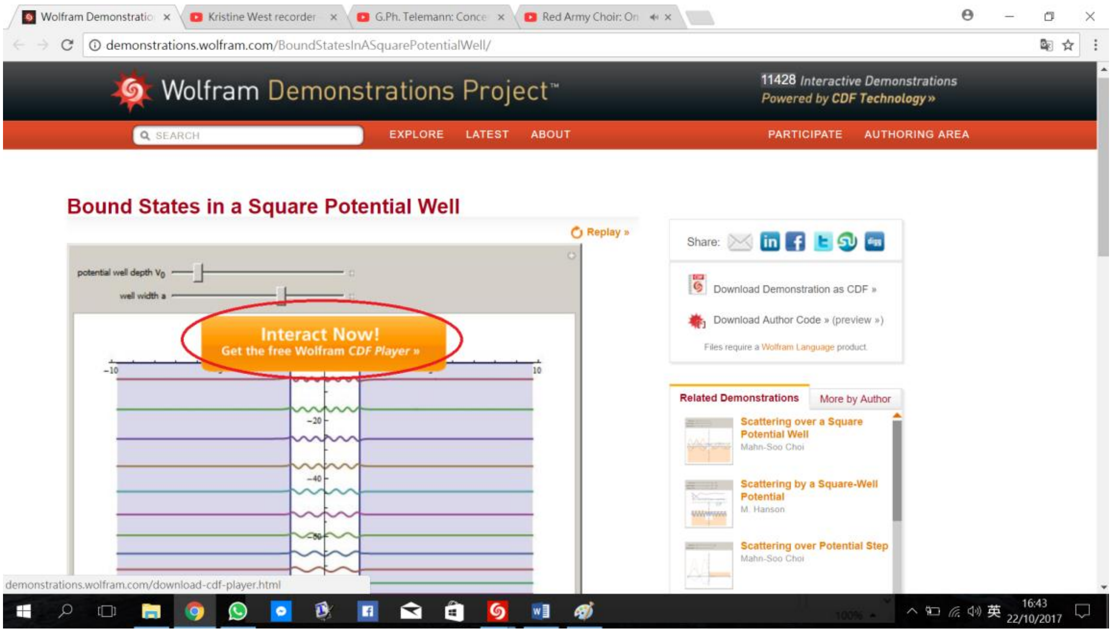
SQ.19

Aim: to study the effect of changing well width on energy of a bound state.

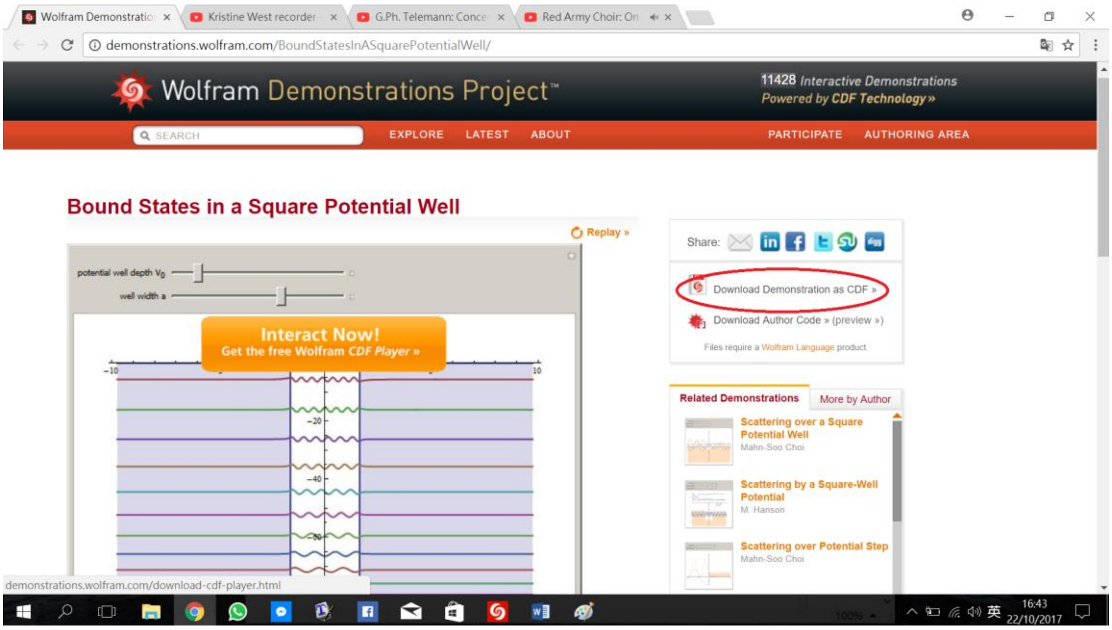
Follow the steps to download the free finite-well application.

(1) Go to http://demonstrations.wolfram.com/BoundStatesInASquarePotentialWell/ to download the Wolfram CDF Player

(2) Click the "Interact Now! Get the free Wolfram CDF Player" button to download the Wolfram CDF Player



(3) Click DoMonstration as CDF to download the cdf file.



(4) Open the cdf file, you can now use the application.

To investigate the effect of changing well width on energy of a bound state, V_0 = -8 was chosen. Besides, m and h-bar were chosen to be 1 automatically. Two values of a are shown below to let you see the effect.

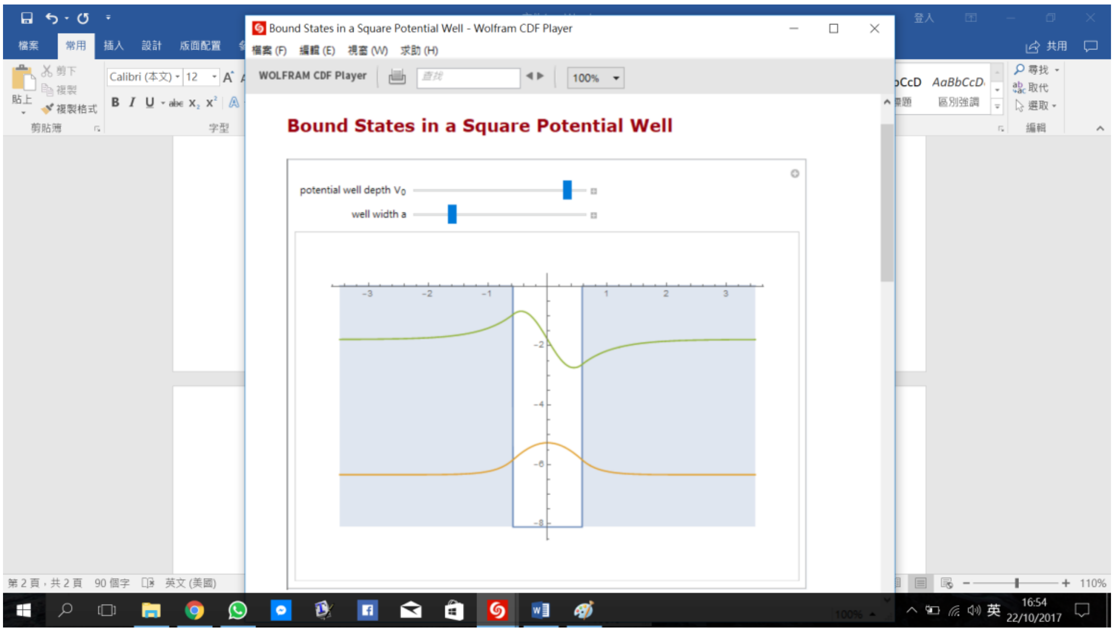


Fig.1 The energies of eigenfunctions when V_0 = -8 and a = 0.5. The energies of the ground state and the first excited state are about -6.5 and -2.

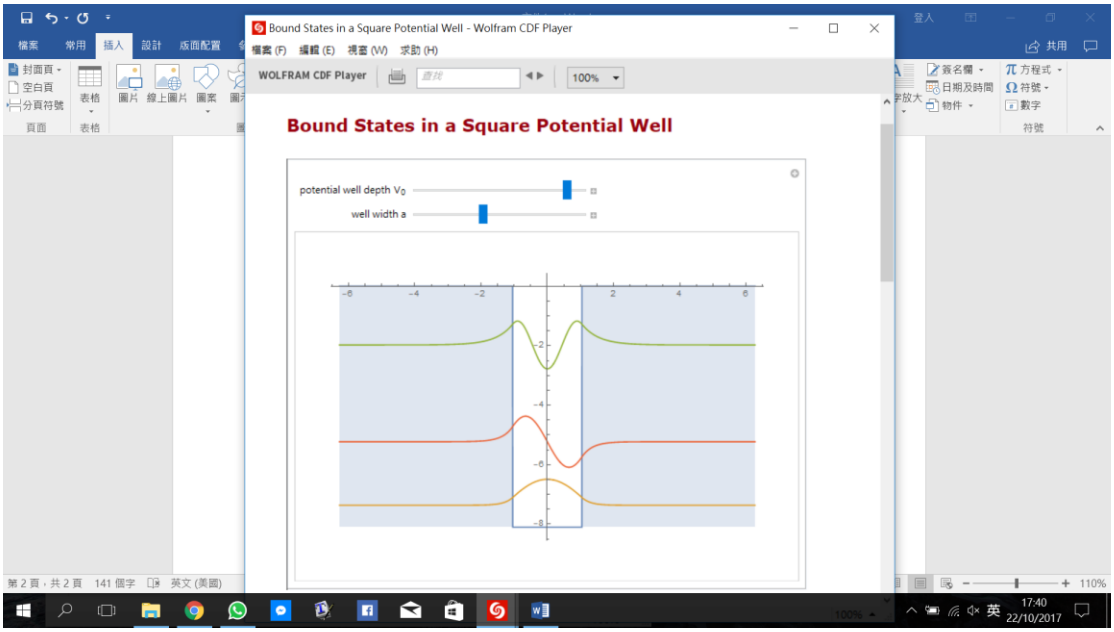


Fig.2 The energies of eigenfunctions when V_0 = -8 and a = 1. The energies of the ground state and the first excited state are about -7.5 and -5

When the width of the finite well (a) increases, the energies of the ground state and the first excited state decrease. Also, the second excited state appears.

Therefore, the energy of the states becomes smaller when the width becomes bigger.

You may also want to try to decrease the width to a very small number. Width a = 0.5, which is the smallest number you can set, was chosen.

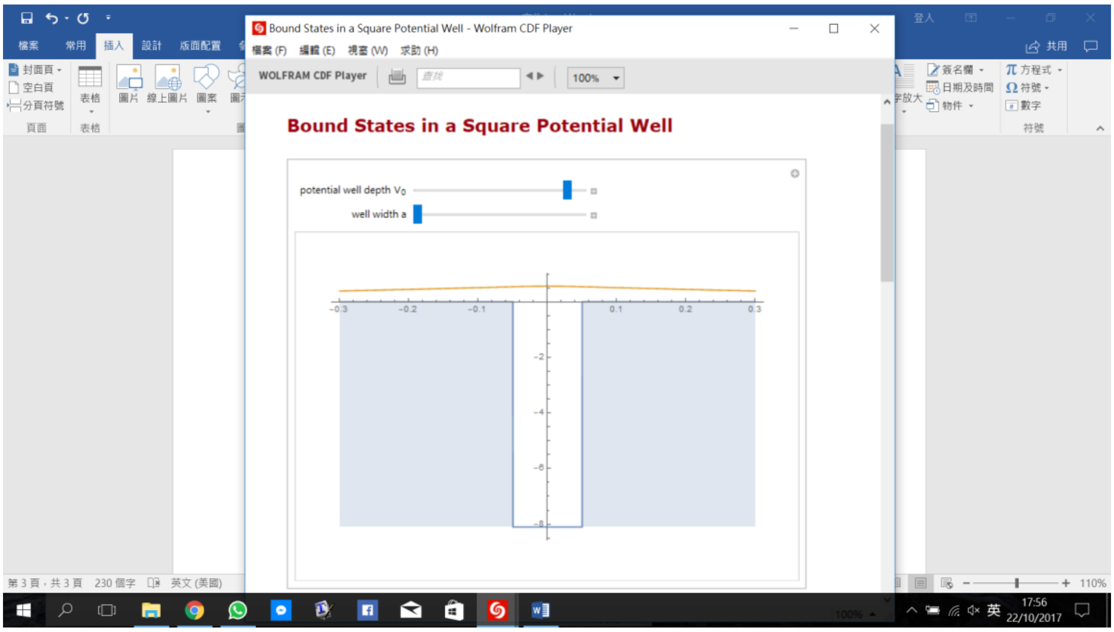


Fig.3 The energies of eigenfunctions when V_0 = -8 and a = 0.05.

You can still see that the is a ground state wavefunction, indicated by the yellow line. This shows that there is always a bound state no matter how shallow the well is.

SQ 20.

Aim: Study the odd-even parity of a wavefunction in an even-potential system

(a) In this question, we want to show if

$U(x) = U(-x)$ and $\psi_n(x)$ is a wavefunction with E_n, then $\psi_n(-x)$ is also a wavefunction with E_n.

First, we write down the TISE for $\psi_n(x)$

$$\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_n(x) + U(x)\psi_n(x) = E_n\psi_n(x). \quad (*)$$

We let $y = -x$, substitute into $(*)$.

$$\frac{\hbar^2}{2m}\frac{d^2}{d(-y)^2}\psi_n(-y) + U(-y)\psi_n(-y) = E_n\psi_n(-y)$$

Using the fact that $\frac{d}{d(-y)} = -\frac{d}{dy} \Rightarrow \frac{d^2}{d(-y)^2} = \frac{d^2}{dy^2}$

and $U(-y) = U(y)$

We have

$$\frac{\hbar^2}{2m}\frac{d^2}{dy^2}\psi_n(-y) + U(y)\psi_n(-y) = E_n\psi_n(-y).$$

Therefore $\psi_n(-x)$ is also a wavefunction with E_n.

In this question, we want to show that

$$\boxed{\text{if the energies are non-degenerate, the eigenfunctions are either even or odd about } x=0}$$

In (a), we show that $\psi_n(x)$ and $\psi_n(-x)$ are the solutions of the same TISE with energy E_n if $U(x) = U(-x)$.

Due to the non-degenerate property, $\psi_n(x)$ and $\psi_n(-x)$ must be the same solution, but different by a constant prefactor.

i.e. $\psi_n(x) = c\,\psi_n(-x)$ $(*)$.

We use $(*)$ twice:

$$\psi_n(x) = c\,\psi_n(-x) = c\left[c\,\psi_n(x)\right]$$
$$= c^2\,\psi_n(x).$$

Therefore c must either be 1 or -1.

Case 1: $c=1$.

Then $\psi_n(x) = \psi_n(-x)$.

The eigenfunction is even.

Case 2: $c=-1$

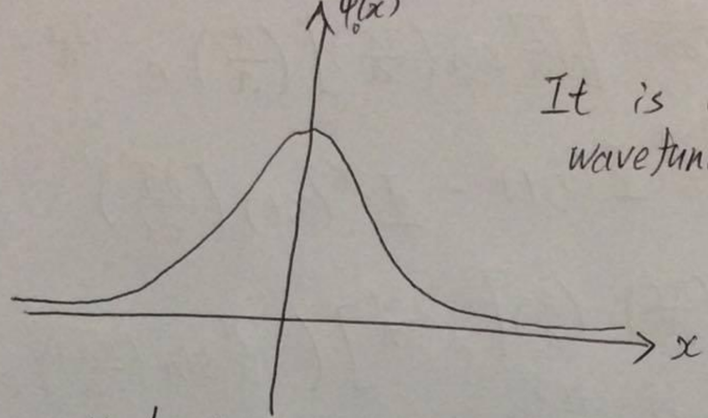
Then $\psi_n(x) = -\psi_n(-x)$

The eigenfunction is odd.

$\therefore$ We have proved the statement.

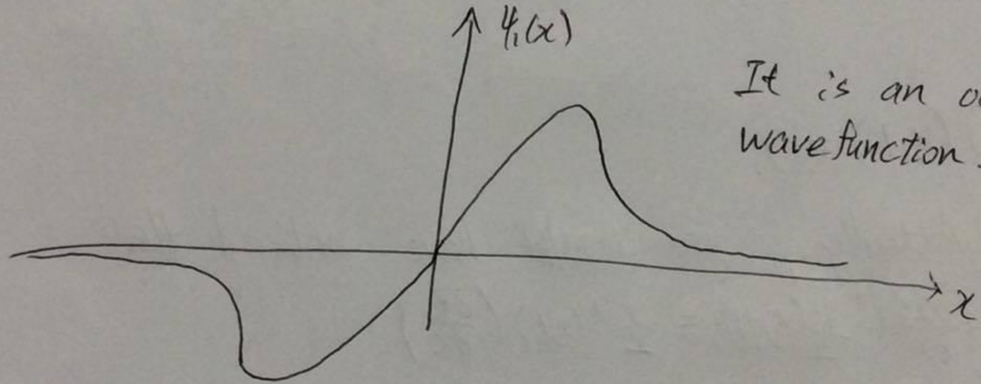
You can look at the simple harmonic oscillator as an example. $U(x) = U(-x) = \frac{1}{2} m\omega^2 x^2$ and the energies are non-degenerate.

Ground state: $E_0 = \frac{1}{2}\hbar\omega$.



It is an even wavefunction.

1st excited state: $E_1 = \frac{3}{2}\hbar\omega$.



It is an odd wavefunction.

SQ.21

$\boxed{\text{Aim: Find } J(x,t) \text{ in (1) 1D infinite well, (2) 1D. harmonic ground state and (3) free electron}}$

(a) We take $\psi(x) = \psi_1(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right)$ and $E_1 = \frac{\pi^2\hbar^2}{2ma^2}$ in a particle in a box system.

$$\Psi(x,t) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) e^{-\frac{iE_1 t}{\hbar}}$$

$J(x,t)$ is defined to be

$$J(x,t) = \frac{g}{2m}\frac{\hbar}{i}\left[\left(\frac{\partial \Psi(x,t)}{\partial x}\right)^* \Psi(x,t) - \Psi^*(x,t)\left(\frac{\partial \Psi}{\partial x}\right)\right].$$

$$\Psi(x,t) = \sqrt{\tfrac{2}{a}}\sin\left(\frac{\pi x}{a}\right) e^{-\frac{iE_1 t}{\hbar}}$$

$$\frac{\partial \Psi}{\partial x} = \left[\sqrt{\tfrac{2}{a}}\cos\left(\frac{\pi x}{a}\right)\right]\left(\frac{\pi}{a}\right) e^{-\frac{iE_1 t}{\hbar}}.$$

$$\left(\frac{\partial \Psi(x,t)}{\partial x}\right)^* \Psi(x,t) - \Psi^*(x,t)\left(\frac{\partial \Psi}{\partial x}\right)$$

$$= \left[\sqrt{\tfrac{2}{a}}\cos\left(\frac{\pi x}{a}\right)\left(\frac{\pi}{a}\right) e^{\frac{iE_1 t}{\hbar}}\right]\left(\sqrt{\tfrac{2}{a}}\sin\left(\frac{\pi x}{a}\right) e^{-\frac{iE_1 t}{\hbar}}\right)$$

$$- \left(\sqrt{\tfrac{2}{a}}\sin\left(\frac{\pi x}{a}\right) e^{-\frac{iE_1 t}{\hbar}}\right)\left(\sqrt{\tfrac{2}{a}}\cos\left(\frac{\pi x}{a}\right)\left(\frac{\pi}{a}\right) e^{-\frac{iE_1 t}{\hbar}}\right)$$

$$= 0$$

$$\therefore J(x,t) = 0.$$

Actually, you might have noticed that

(☆☆) $\left(\frac{\partial \Psi}{\partial x}\right)^* \Psi(x,t) - \Psi^*(x,t)\left(\frac{\partial \Psi}{\partial x}\right)$

$$= \left(\frac{d\psi_1(x)}{dx} e^{+\frac{iE_1 t}{\hbar}}\right)\left(\psi_1(x) e^{-\frac{iE_1 t}{\hbar}}\right) - \left(\psi_1(x) e^{\frac{iE_1 t}{\hbar}}\right)\left(\frac{d\psi_1(x)}{dx} e^{-\frac{iE_1 t}{\hbar}}\right) = 0$$ in this case.

(b) $\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$, $E_0 = \frac{1}{2}\hbar\omega$.

$\Psi(x,t) = \psi_0(x)\, e^{-\frac{iE_0 t}{\hbar}}$

Using method (☆☆) again

$\left(\frac{\partial \Psi}{\partial x}\right)^* \Psi(x,t) - \Psi^*(x,t)\left(\frac{\partial \Psi}{\partial x}\right)$.

$$= \left(\frac{d\psi_0}{dx} e^{\frac{iE_0 t}{\hbar}}\right)\left(\psi_0 e^{-\frac{iE_0 t}{\hbar}}\right) - \left(\psi_0 e^{\frac{iE_0 t}{\hbar}}\right)\left(\frac{d\psi_0}{dx} e^{-\frac{iE_0 t}{\hbar}}\right)$$

$$= 0.$$

$$\therefore J(x,t) = 0.$$

(c) $\psi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$, $E_k = \frac{\hbar^2 k^2}{2m}$

and $\omega_k = \frac{E_k}{\hbar}$.

$$\therefore \Psi(x,t) = \psi_k(x)\, e^{-\frac{iE_k t}{\hbar}} = \frac{1}{\sqrt{2\pi}} e^{i(kx-\omega_k t)}$$

$$\frac{\partial \Psi}{\partial x} = ik\,\Psi(x,t).$$

$$\left(\frac{\partial \Psi}{\partial x}\right)^* \Psi(x,t) - \Psi^*(x,t)\left(\frac{\partial \Psi}{\partial x}\right)$$

$$= \left[(-ik)\Psi^*(x,t)\right]\Psi(x,t) - \Psi^*(x,t)\left[ik\,\Psi(x,t)\right].$$

$$= -2ik\,|\Psi(x,t)|^2 = -2ik\left(\frac{1}{2\pi}\right)$$

$$= -\frac{ik}{\pi}.$$

$$J(x,t) = \frac{g}{2m}\frac{\hbar}{i}\left(-\frac{ik}{\pi}\right) = -\frac{g}{2m}\frac{\hbar k}{\pi}$$