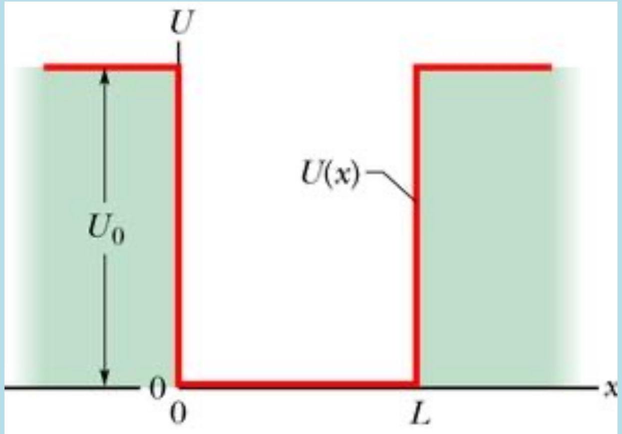
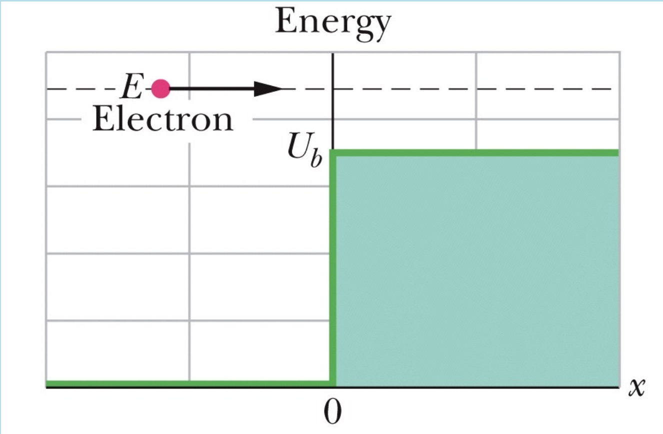
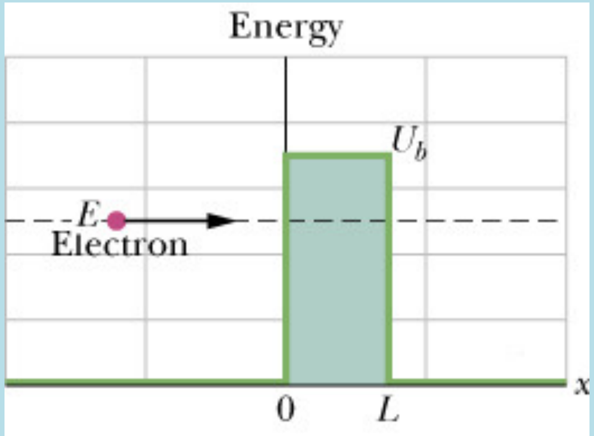
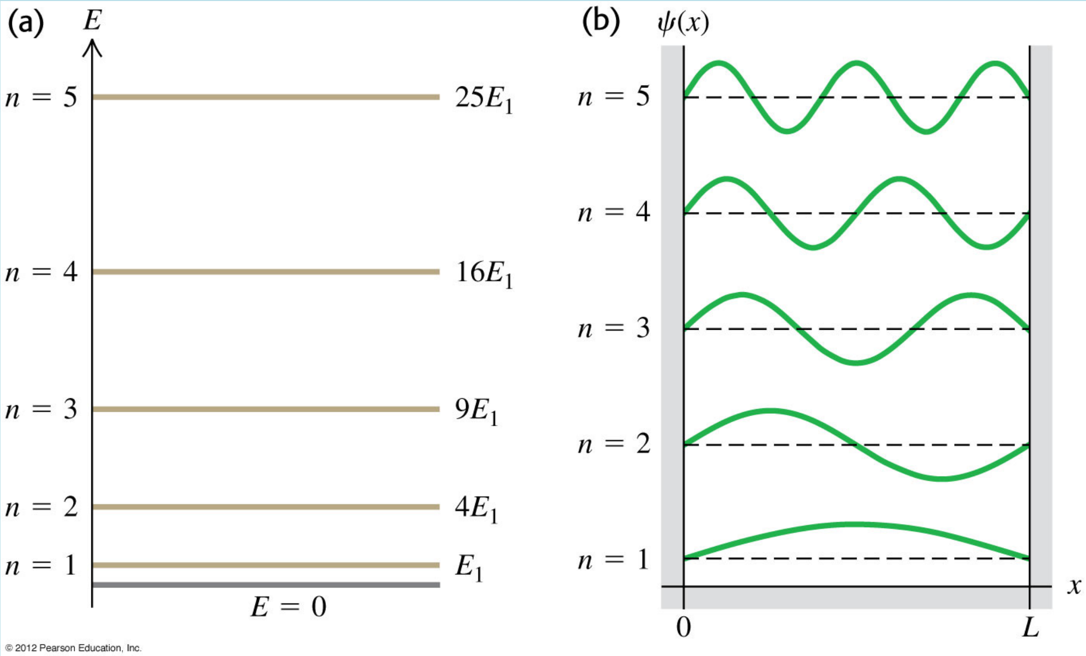
一維階梯狀位能下的定態





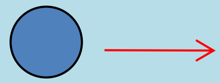


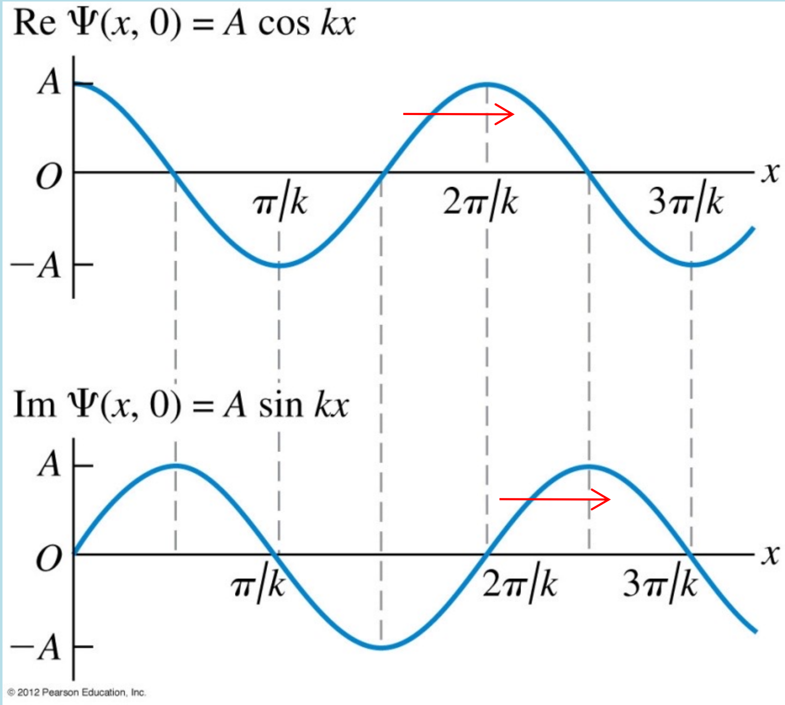


當波被限制於一個範圍內時，

被限制的波的狀態如駐波般，

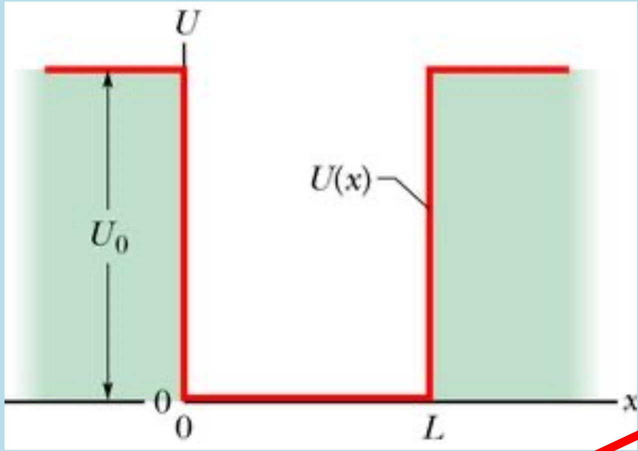
能量只有在某些值，定態薛丁格方程式才有解！

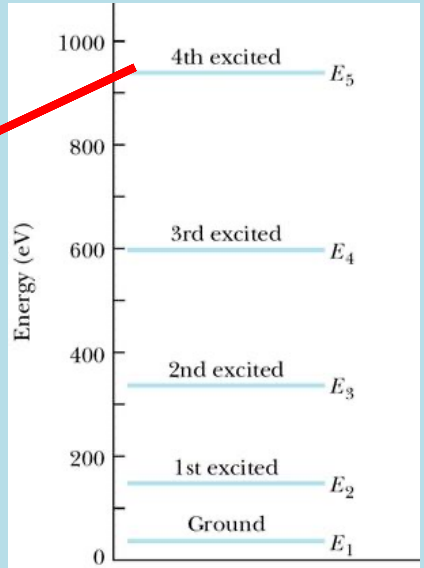


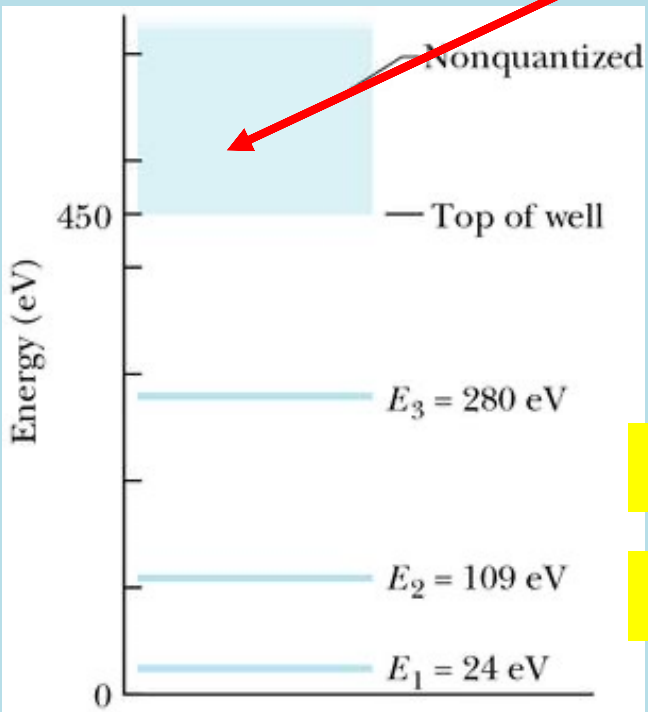


$$\Psi(x,t) = \psi_E(x) \cdot e^{-i\frac{E}{\hbar}t} = Ae^{i\left(kx-\frac{E}{\hbar}t\right)} + Be^{-i\left(kx+\frac{E}{\hbar}t\right)}$$

若波未被限制，如自由電子波：任意的E數值，定態方程式都有解！







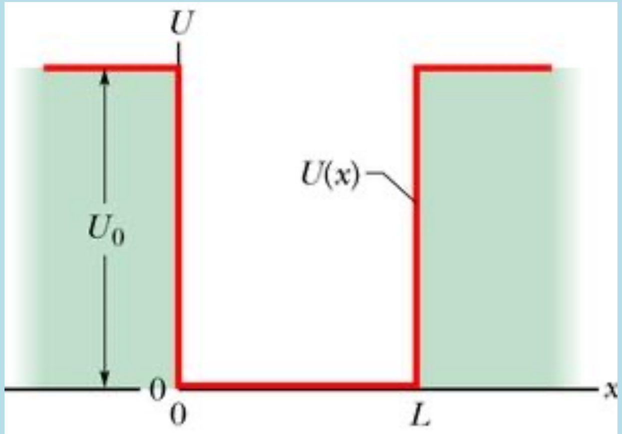
電子被拘限於一定區域時，能量為離散的能階

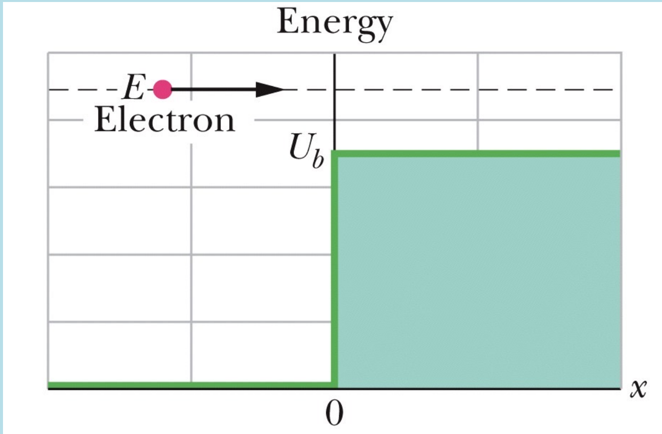
電子不被拘限於一定區域時，能量為連續

如果是有限大位能井，能量就會同時有連續與離散的部分！

因為能階高到一定值後，就不再被束縛了

一維階梯狀位能下的定態





束縛的定態將展現能量量子化！

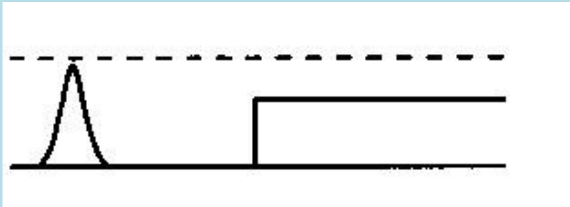
在非束縛的情況中，定態能組成入射波包，可以描述散射問題！

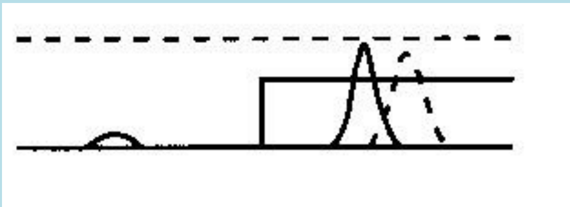
這些問題的物理意義差別很大：但在數學解法上卻非常類似！

這些問題都可以分解為一段段常數位能的區域，分開求解。

然後在邊界處，以連續條件將得到的各個解聯(match)起來。

階梯狀位能，散射



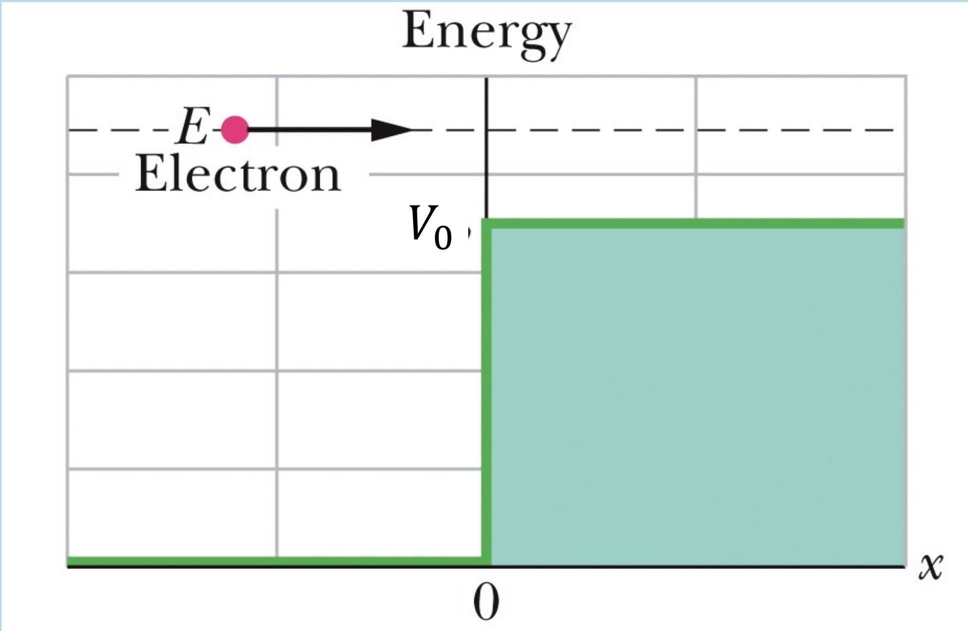


階梯狀位能散射

$V = 0, \quad x < 0$

$V = V_0, \quad x > 0$

$E > V_0$



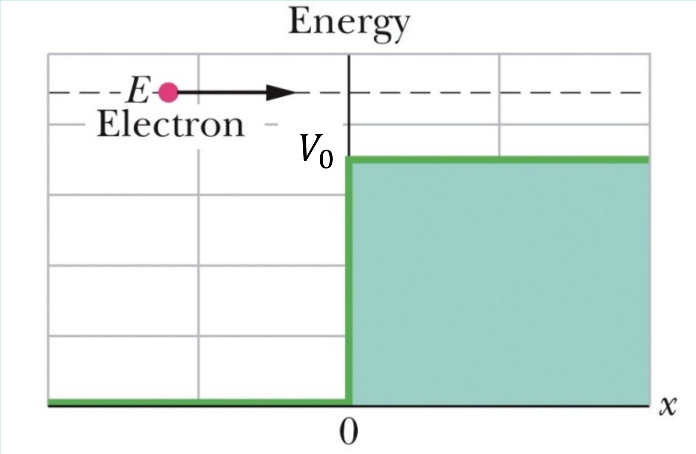
解這個位能下的定態，即能量的本徵函數。

也就是解與時間無關的薛丁格方程式。

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_E(x)}{dx^2} + V(x)\cdot\psi_E(x) = E\cdot\psi_E(x)$$

反射與透射

在兩個區域內分別都是自由粒子，自由電子波定態解可以適用：



$x < 0$ $\quad \psi_E = Ae^{ikx} + Re^{-ikx}$

$$k \equiv \sqrt{\frac{2mE}{\hbar^2}}$$

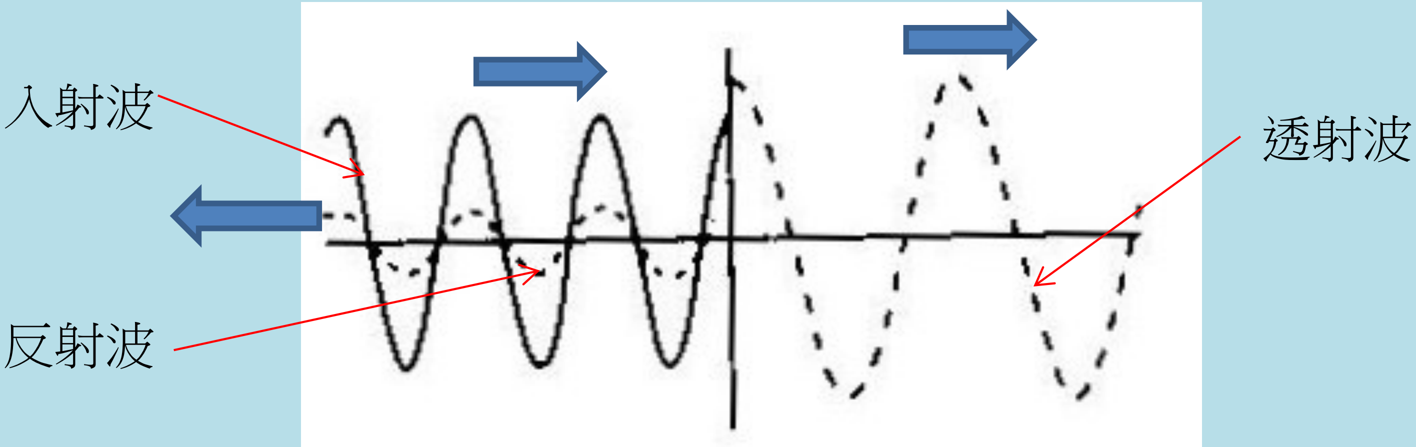
$x > 0$ $\quad \psi_E = Te^{iqx}$

若只考慮由左入射的波，e^{-iqx}的部分可忽略。

$$q \equiv \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$$

$k > q$ $\quad \lambda_1 < \lambda_2$

由左向右入射的正弦波，在邊境產生向右的透射波，及向左的反射波。



由左向右入射的波，嚴格應該用波包處理，

但我們先以自由電子波e^{ikx}近似，所以就取$A = 1$。

之後可將此定態解乘高斯分布的k進行疊加，那入射部分就真的是波包了。

$x < 0$ $\psi_E = e^{ikx} + Re^{-ikx}$ $\psi' = ike^{ikx} - ikRe^{-ikx}$

$x > 0$ $\psi_E = Te^{iqx}$ $\psi' = iqTe^{iqx}$

ψ及ψ'在邊界原點連續，可以得到兩個連續條件，正好求解得R, T。

$1 + R = T$

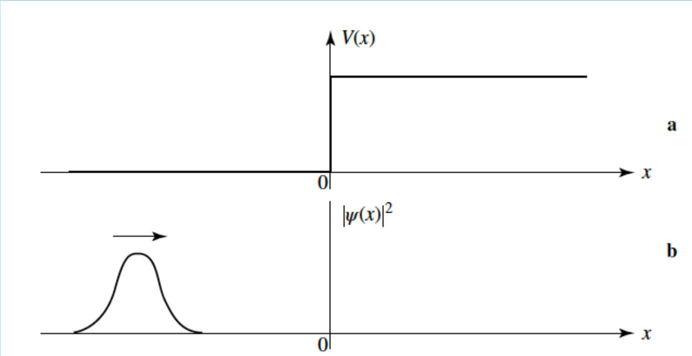
$k - kR = qT$

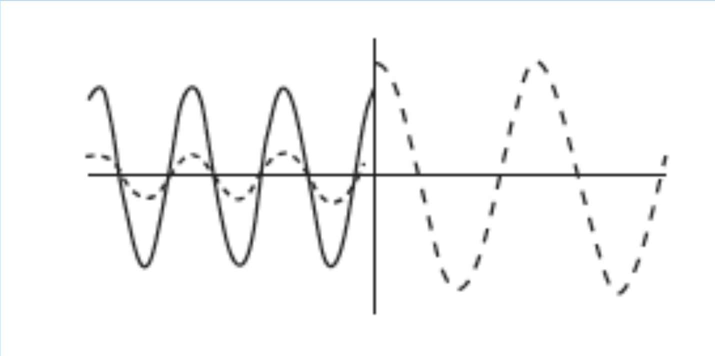
$$R = \frac{k - q}{k + q}$$

$$T = \frac{2k}{k + q}$$

$k > q, T > 1$

R決定了反射波強度，T決定了透射波強度。





$\psi(x)$的微分也必須連續！

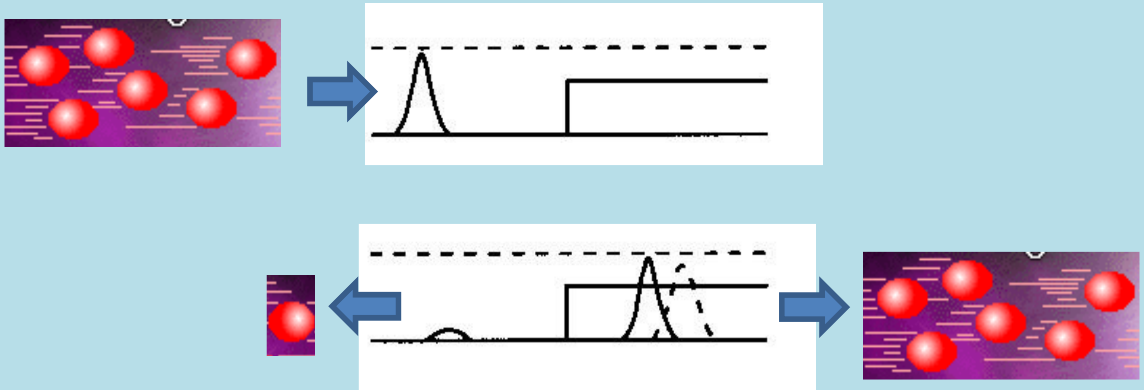
$$\left(\frac{d\psi}{dx}\right)_{a+\varepsilon}-\left(\frac{d\psi}{dx}\right)_{a-\varepsilon}=\int_{a-\varepsilon}^{a+\varepsilon}dx\frac{d}{dx}\frac{d\psi}{dx}=\int_{a-\varepsilon}^{a+\varepsilon}dx\frac{2m}{\hbar^2}[V(x)-E]\psi\xrightarrow[\varepsilon\to 0]{}0$$

$V(x)$在$a-\varepsilon$與$a+\varepsilon$間都是有限值！

若位能與波函數都是有限值，波函數與微分都要連續。

波恩發現，這兩個往相反方向移動的波包，是有觀測上的意義的。

實驗發現，將一束電子入射，散射後電子的分布，的確等於散射波的波強度！

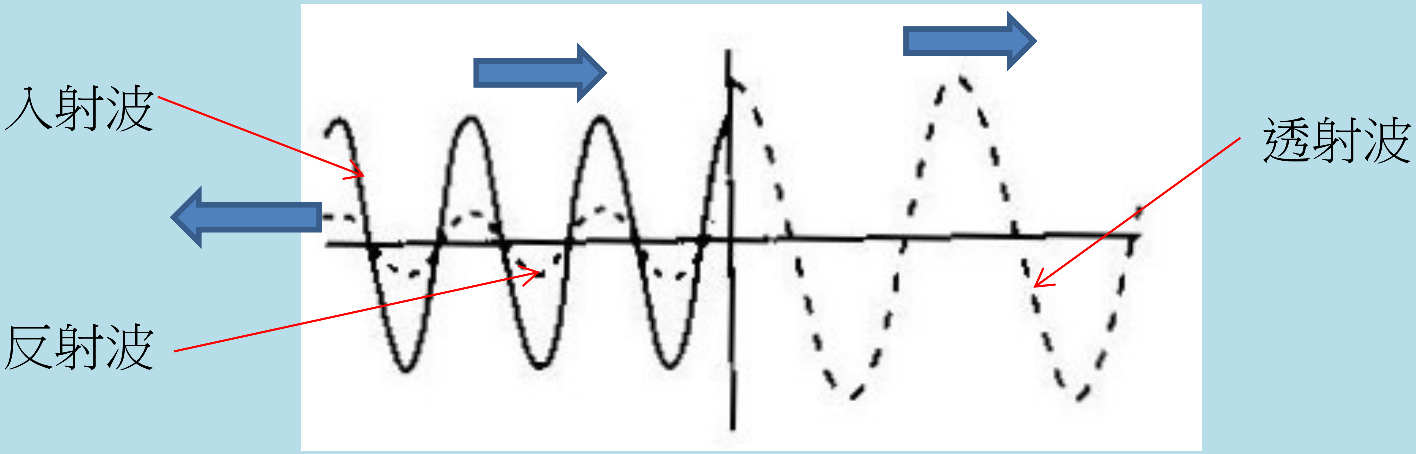


以上圖為例，向右運動的波包總強度，大約是向左運動的波包總強度的九倍！

實驗上看到：大概十個電子入射，散射後就是會有九個向右，一個向左運動！

電子束散射後，各處電子的分佈≈散射後，各處電子波的強度

R, T就是反射波與透射波強度。

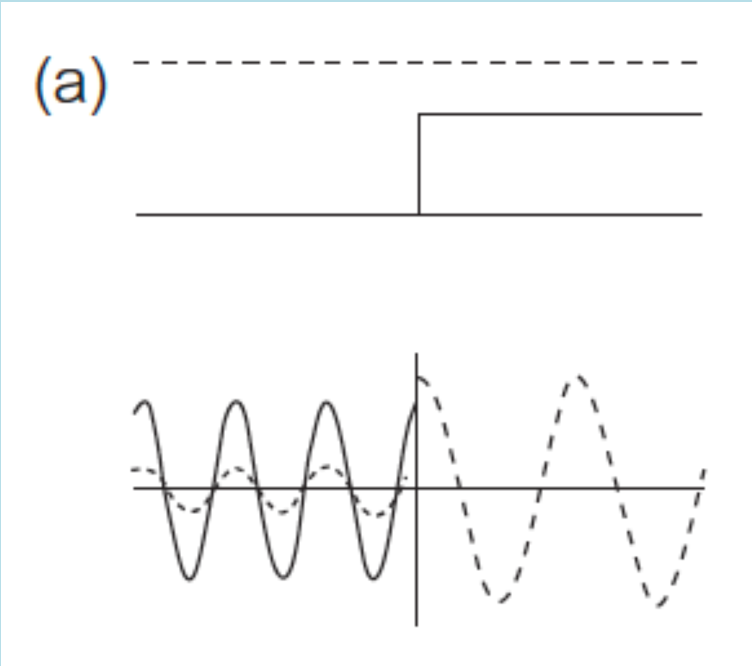


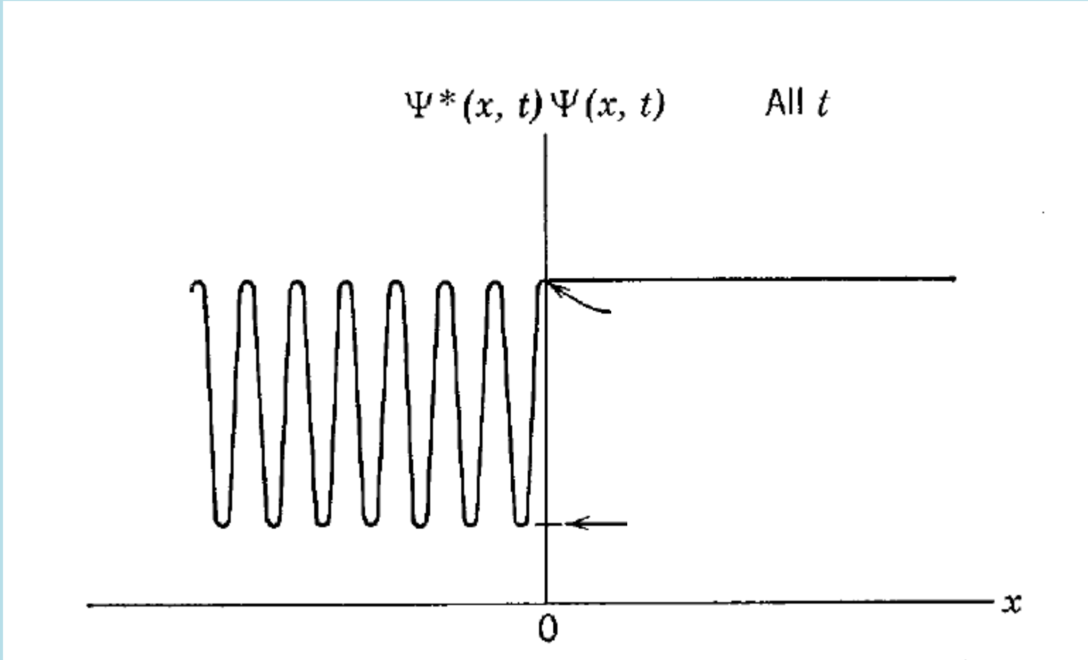
我們得到的定態解，乘上時間演化就是完整的波函數：

$$\Psi_k(x,t) = \begin{cases} e^{i(kx-Et/\hbar)} + Re^{-i(kx+Et/\hbar)} & x < 0 \\ Te^{i(qx-Et/\hbar)} & x > 0 \end{cases}$$

入射波的相位會向右傳播，透射波也向右，反射波的相位向左傳播。

機率分布





反射的波與入射波疊加干涉！機率分布與位置有關。

但機率總和是無限大，以上的解並不能歸一化。

我們可以利用之前定義的機率的流 Probability Current來觀察反射與透射。

機率流是局部的物理量，不涉及積分，而且可以適用於一束電子。

計算機率密度的時變率：

$$\frac{\partial}{\partial t}|\Psi(x,t)|^2 = \frac{\partial}{\partial t}[\Psi^*(x,t)\cdot\Psi(x,t)] = \frac{\partial\Psi^*}{\partial t}\cdot\Psi + \Psi^*\cdot\frac{\partial\Psi}{\partial t}$$

$$= -i\frac{\hbar}{2m}\left(\frac{\partial^2\Psi^*}{\partial x^2}\cdot\Psi - \Psi^*\cdot\frac{\partial^2\Psi}{\partial x^2}\right) =$$

$$= -i\frac{\hbar}{2m}\frac{\partial}{\partial x}\left(\frac{\partial\Psi^*}{\partial x}\cdot\Psi - \Psi^*\cdot\frac{\partial\Psi}{\partial x}\right) \equiv \frac{\partial}{\partial x}j(x,t)$$

機率密度的時變率等於一個量的空間微分，這與電荷守恆式一樣。

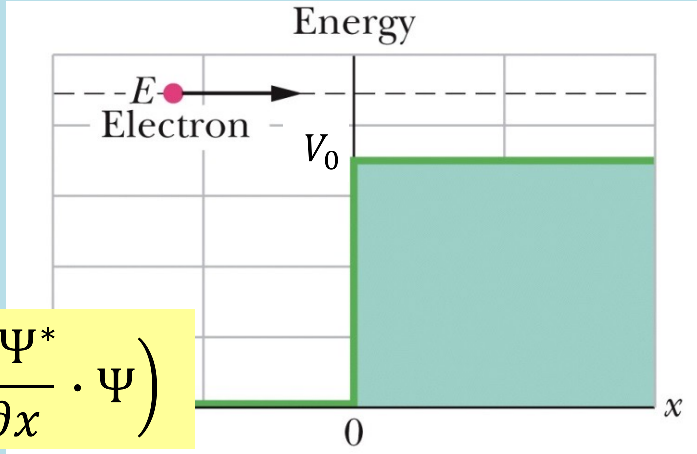
$$\frac{\partial}{\partial t}P(x,t) = \frac{\partial}{\partial x}j(x,t)$$

$$\frac{\partial}{\partial t}Q + \vec{\nabla}\cdot\vec{j} = 0$$

$$j(x,t) = -i\frac{\hbar}{2m}\left(\frac{\partial\Psi^*}{\partial x}\cdot\Psi - \Psi^*\cdot\frac{\partial\Psi}{\partial x}\right)$$

Probability Current

現在可以計算各處的機率流 Probability Current



$$\psi_E = e^{ikx} + Re^{-ikx} \qquad x < 0$$

$$j = -i\frac{\hbar}{2m}\left(\frac{\partial \Psi^*}{\partial x}\cdot\Psi - \Psi^*\cdot\frac{\partial \Psi}{\partial x}\right) = -i\frac{\hbar}{2m}\,\mathrm{Im}\left(\frac{\partial \Psi^*}{\partial x}\cdot\Psi\right)$$

$$= -\frac{\hbar}{2im}\mathrm{Im}\left[\left(-ike^{-ikx} + ikR^*e^{ikx}\right)\left(e^{ikx} + Re^{-ikx}\right)\right]$$

交叉項的虛數部會抵消。

$$j_I - j_R = \frac{\hbar k}{m}\left(1 - |R|^2\right) \qquad \sim v\cdot 1 - v|R|^2$$ 這分別是入射流與反射流。

若是一束電子的話，反射電流就等於乘電子密度： $j_R \sim \rho v|R|^2$

相對於入射電流ρv：$|R|^2$可解讀是反射率， $\rho|R|^2$看成是反射電子密度。

$$\psi_E = Te^{iqx} \qquad x > 0$$ 代入以上機率流公式。

$$j_T = \frac{\hbar q}{m}|T|^2 \sim v'|T|^2$$ 這是透射流，$|T|^2$是透射率。

現在代入實際的透射率及反射率：

$x < 0$

$$j = \frac{\hbar k}{m}(1 - |R|^2)$$

$$R = \frac{k - q}{k + q}$$

反射流等於

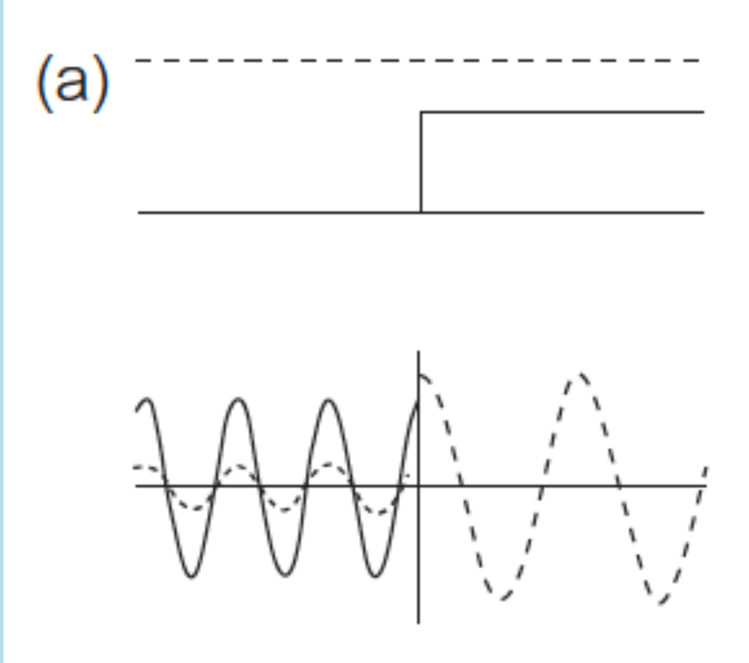
$$j_R = \frac{\hbar k}{m}|R|^2 = \frac{\hbar k}{m}\left(\frac{k - q}{k + q}\right)^2$$

$x > 0$

$$T = \frac{2k}{k + q}$$

透射流

$$j_T = \frac{\hbar q}{m}|T|^2 = \frac{\hbar k}{m}\frac{4kq}{(k + q)^2}$$



可以驗證入射流等於反射流加透射流。

$$\frac{\hbar k}{m} = \frac{\hbar k}{m}|R|^2 + \frac{\hbar q}{m}|T|^2 \qquad j_I = j_R + j_T$$

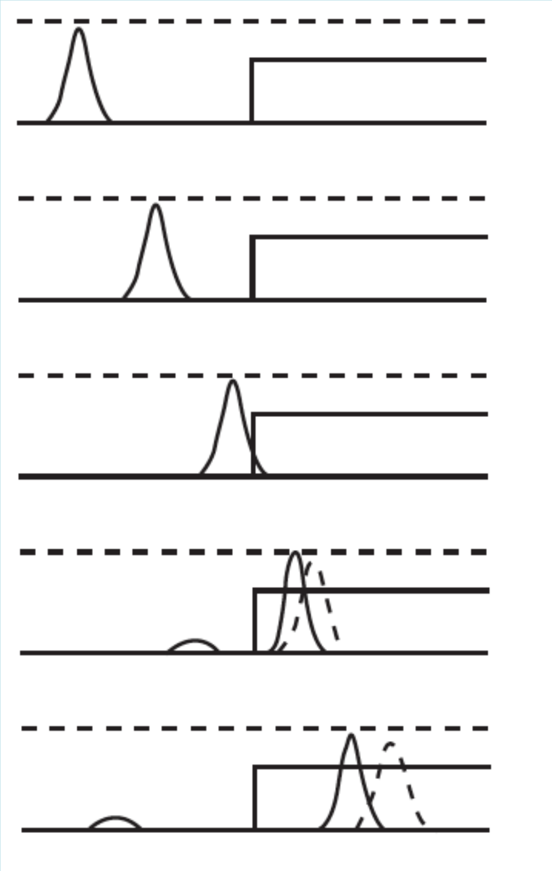
T雖然大於1，透射流小於入射流，因為在$x > 0$電子速度較慢。 $k > q$

$v' < v$

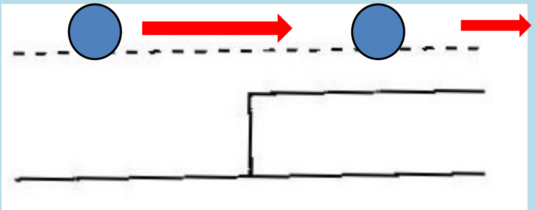
這個定態解本身無法滿足歸一律，nonnormalizable，不是一個實際可行的解。

但它們可以被用來疊加出由左向右入射的波包！

我們就能以波包來描述電子的散射現象！



古典粒子會直接穿越，只是速度變慢。



我們得到的定態解，乘上時間演化就是完整的波函數：

$$\Psi_k(x,t) = \begin{cases} \left(e^{ikx} + Re^{-ikx}\right)e^{-iE(k)t/\hbar}, & x < 0 \\ Te^{iqx}e^{-iE(k)t/\hbar} & x > 0 \end{cases}$$

注意兩個式子有各自適用範圍

由左向右入射的波包本身不是定態，但它們是以上定態的疊加！

注意入射波e^{ikx}是平面自由波，用它可以疊加出入射波包。

$$\Psi(x,t) = \int_{\bar{k}}^{\infty} dk\, A(k)\, \Psi_k(x,t)$$

選擇$A(k)$是高斯分佈函數。

$$A(k) = e^{-\frac{\alpha(k-k_0)^2}{2}}$$

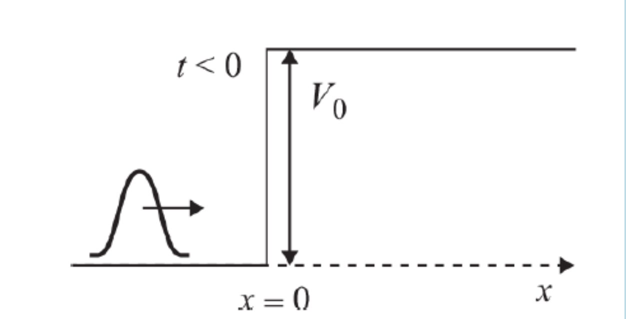
$$\Psi(x,t) = \begin{cases} \displaystyle\int_{\bar{k}}^{\infty} dk\, A(k)\left(e^{ikx} + Re^{-ikx}\right)e^{-iE(k)t/\hbar}, & x < 0 \\ \displaystyle\int_{\bar{k}}^{\infty} dk\, A(k)\, Te^{iqx}e^{-iE(k)t/\hbar} & x > 0 \end{cases}$$

$$\bar{k} \equiv \sqrt{\frac{2mV_0}{\hbar^2}}$$

We can split the solution $\Psi(x, t)$ into incident, reflected, and transmitted waves as follows:

$$\Psi(x,t) = \begin{cases} \Psi_{\text{inc}}(x,t) + \Psi_{\text{ref}}(x,t), & x < 0 \\ \Psi_{\text{tr}}(x,t) & x > 0 \end{cases}$$

$$\Psi_{\text{inc}}(x,t) = \int_{\bar{k}}^{\infty} dk\, A(k)\, e^{ikx} e^{-iE(k)t/\hbar} \qquad x < 0$$



入射波即是過去我們計算過的波包。

$$\Psi_{\text{ref}}(x,t) = \int_{\bar{k}}^{\infty} dk\, A(k)\, R(k) e^{-ikx} e^{-iE(k)t/\hbar} \qquad x < 0$$

$$R = \frac{k-q}{k+q}$$

$$\Psi_{\text{tr}}(x,t)(x,t) = \int_{\bar{k}}^{\infty} dk\, A(k)\, T(k) e^{iqx} e^{-iE(k)t/\hbar} \qquad x > 0$$

$$T = \frac{2k}{k+q}$$

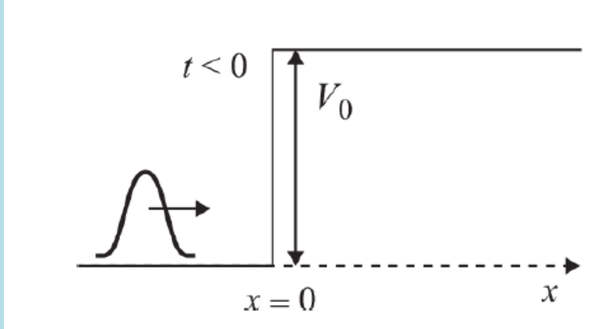
T, R都與k有關，但若波包的振幅$A(k)$集中在一中間值k_0附近，

T, R可以以k_0代入所得的 T, R 來近似，於是這兩個係數即為常數，可從積分提出。

$$R \sim \frac{k_0 - q_0}{k_0 + q_0} \qquad T \sim \frac{2k_0}{k_0 + q_0}$$

意思是可以以自由電子正弦波e^{ik_0x}來近似入射的波包，以計算係數T, R 。

$$\Psi_{\text{inc}}(x,t) = \int_{\bar{k}}^{\infty} dk \cdot A(k) e^{ikx} e^{-i\frac{\hbar^2 k^2 t}{2m\ \hbar}} \qquad x < 0$$

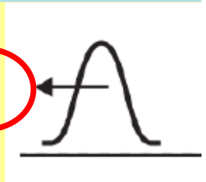


入射波為以速度$\hbar k/m$向右移的波包，

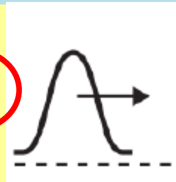
$t = 0$ 時，中心在原點。 因此$t < 0$由左方移入。

$t > 0$ 後，此波包向右移出$x < 0$的適用範圍，於是不再成立而消失。

反射波及透射波也是 $t = 0$ 時，中心在 $x = 0$ ，但分別向左及向右移的兩個波包。

$\Psi_{\text{ref}}(x,t) = R$  $\qquad x < 0$

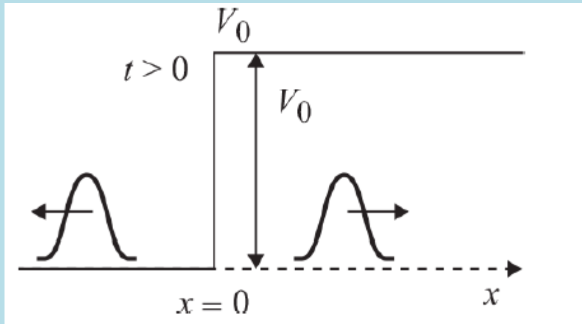
$t < 0$ 時，中心在右邊 $x > 0$ 不在適用範圍內。

$\Psi_{\text{tr}}(x,t) = T$  $\qquad x > 0$

$t < 0$ 時，中心在左邊 $x < 0$ 也不在適用範圍內。

透射與反射波包，要在 $t > 0$ 後才會出現在各自的適用範圍內。

R即是反射波包的振幅，T即是透射波包的振幅。



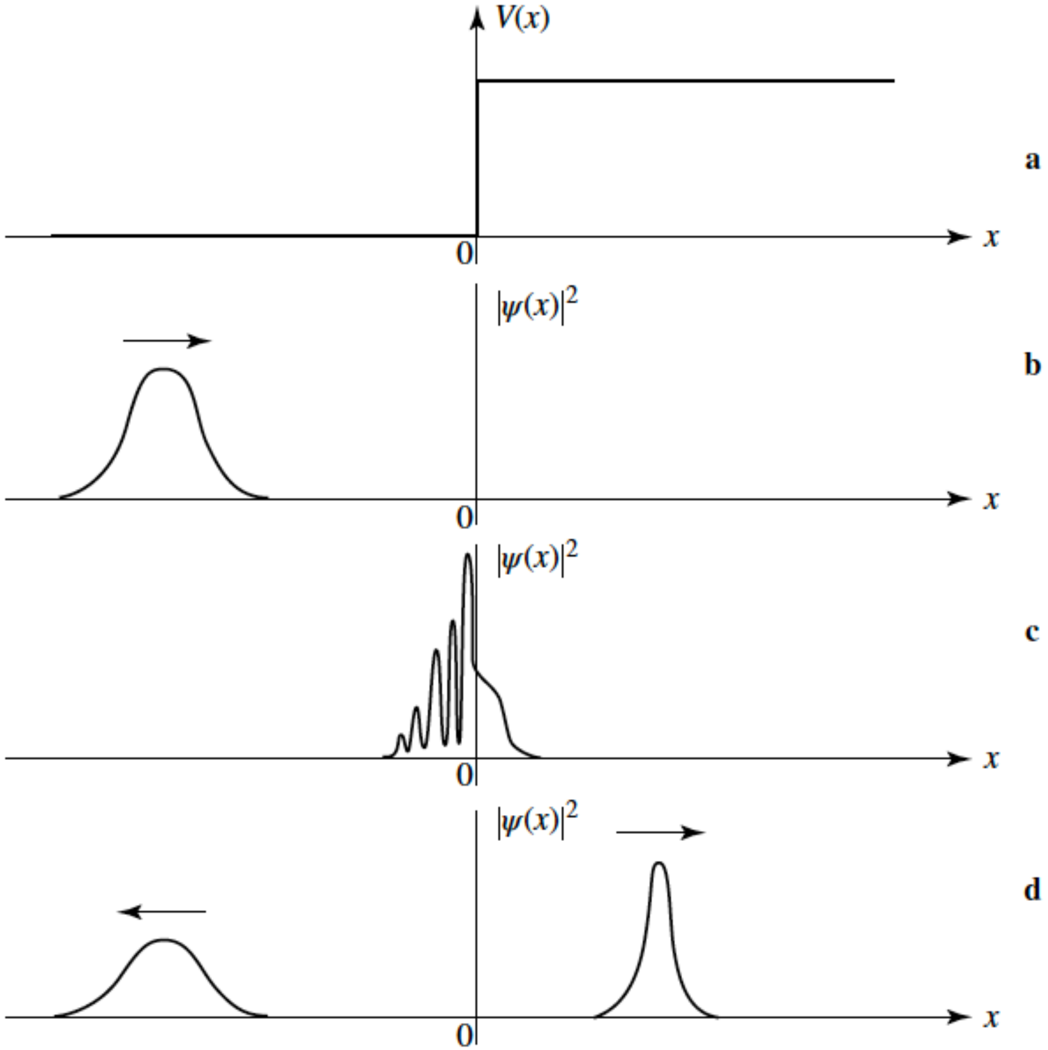


*Figure 1: Behavior of a wave packet at a potential step, in the case $E > V_0$. The potential is shown in figure **a**. In figure **b**, the wave packet is moving towards the step. Figure **c** shows the wave packet during the transitory period in which it splits in two. Interference between the incident and reflected waves are responsible for the oscillations of the wave packet in the $x < 0$ region. After a certain time (fig. **d**), we find two wave packets. The first one (the reflected wave packet) is returning towards the left; its amplitude is smaller than that of the incident wave packet, and its width is the same. The second one (the transmitted wave packet) propagates towards the right; its amplitude is slightly greater than that of the incident wave packet, but it is narrower.*

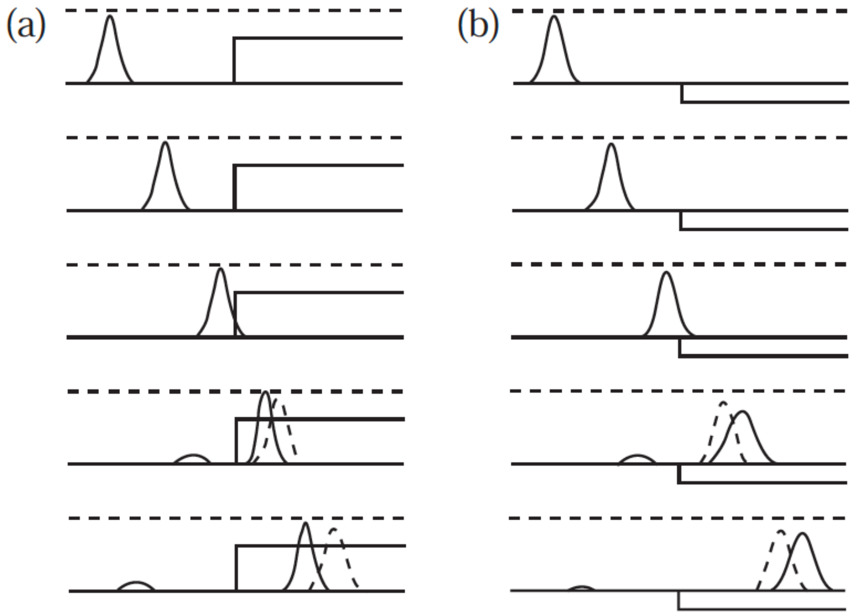


Figure 11.5. Gaussian wavepacket scattering (solid curves) from a discontinuous step potential for (a) $E > V_0 > 0$ and (b) $E > 0 > V_0$. The dashed curves show an unscattered Gaussian (no step potential) for comparison. For example, in (a), the transmitted "lump" of probability lags behind the "free Gaussian" as it slows down over the potential barrier, while for (b) it speeds up over the potential well and

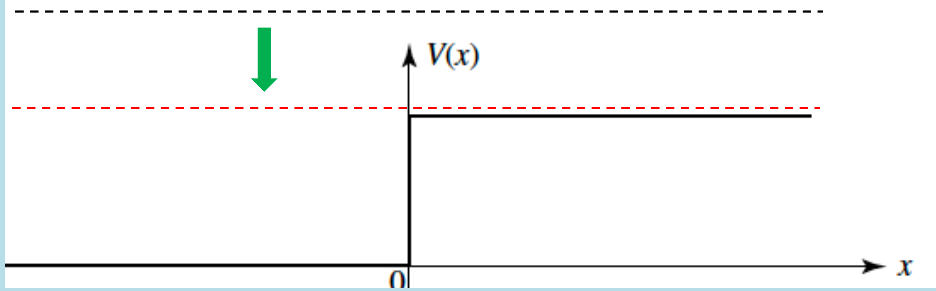
R反射率，T透射率。

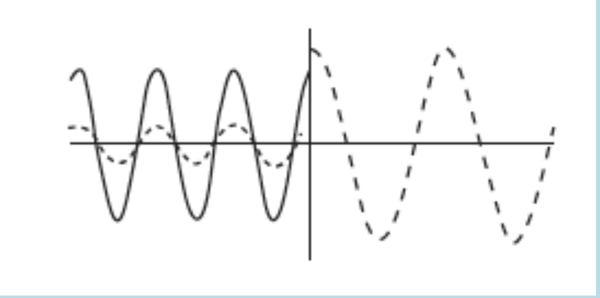
$$R=\frac{k-q}{k+q}$$ $$T=\frac{2k}{k+q}$$ $$k\equiv\sqrt{\frac{2mE}{\hbar^2}}$$ $$q\equiv\sqrt{\frac{2m}{\hbar^2}(E-V_0)}$$ $$k>q, T>1$$

$E\gg V_0$ $k\approx q, R\to 0, T\to 1$ 階梯位能如同不存在一樣！

$E\downarrow$,則 $R\uparrow, T\downarrow$ 在$x>0$透射率漸漸下降！

$E\to V_0$ $q\to 0, Te^{iqx}\to T, R\to 1, T\to 0$ 波在$x>0$波函數不是零，但不傳播！





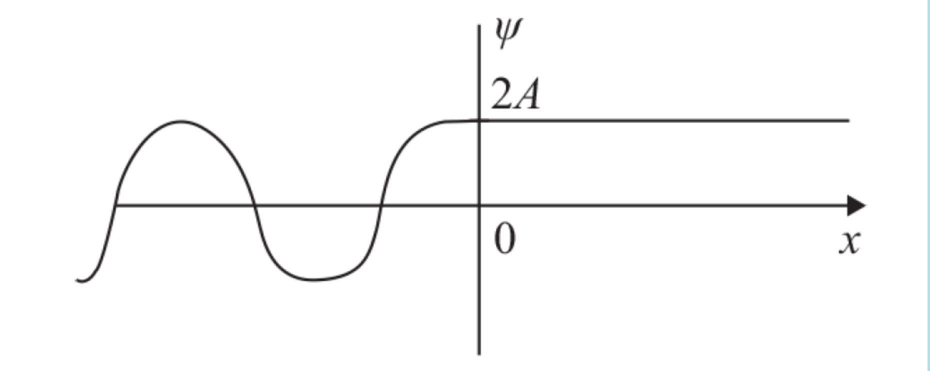


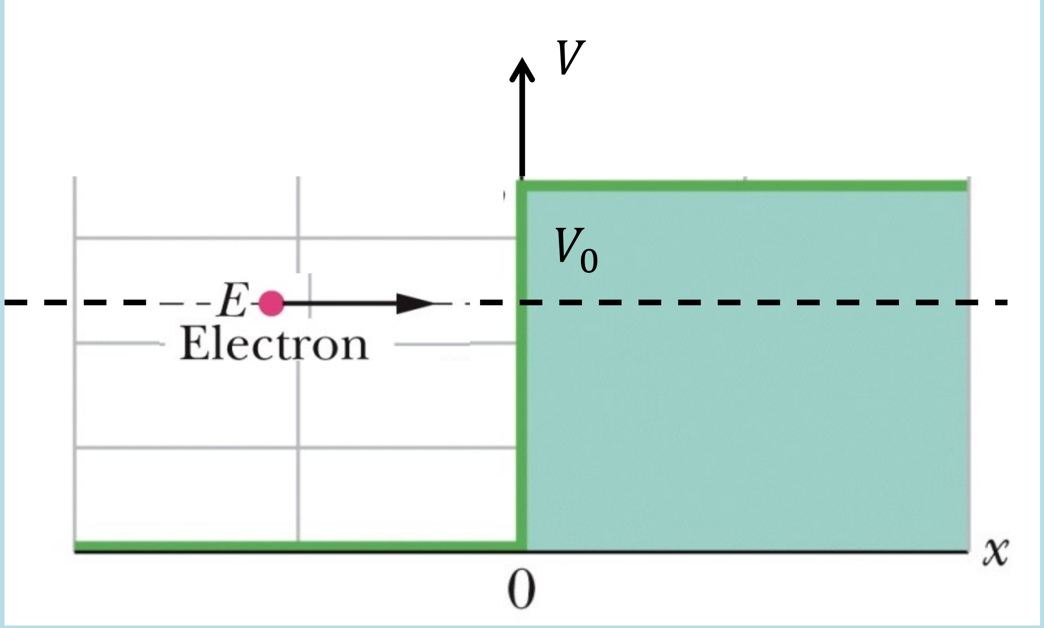
Figure 8.3
Energy eigenstate of the step potential for $E = V_0$.

階梯狀位能全反射

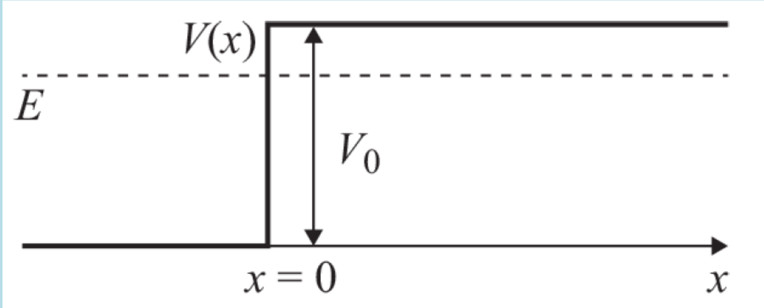
$$V = 0, \qquad x < 0$$

$$V = V_0, \qquad x > 0$$

如果 $E < V_0$



$x < 0$ $\psi_E = e^{ikx} + Re^{-ikx}$ $k \equiv \sqrt{\frac{2mE}{\hbar^2}}$



$x > 0$ $E < V_0$ 古典粒子不能存在這樣的區域

但與時間無關的薛丁格方程式依舊有解：

$$\frac{d^2\psi_E}{dx^2} = \kappa^2\psi_E \text{ ，} - E]\psi_E \equiv \kappa^2\psi_E \qquad \kappa \equiv \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

$$\psi_E = Ce^{-\kappa x} + De^{\kappa x}$$

在量子力學中，波函數還是有解，只是不再是正弦波，而是指數函數。

波函數若向右隨x增加，則在無限遠處波函數發散，不可能，因此$D = 0$。

$\psi_E = Te^{-\kappa x}$ 進入折返點內禁止區後，振幅會指數遞減！

$$\psi_E = e^{ikx} + Re^{-ikx} \qquad x < 0$$

$$\psi_E = Te^{-\kappa x} \qquad x > 0$$

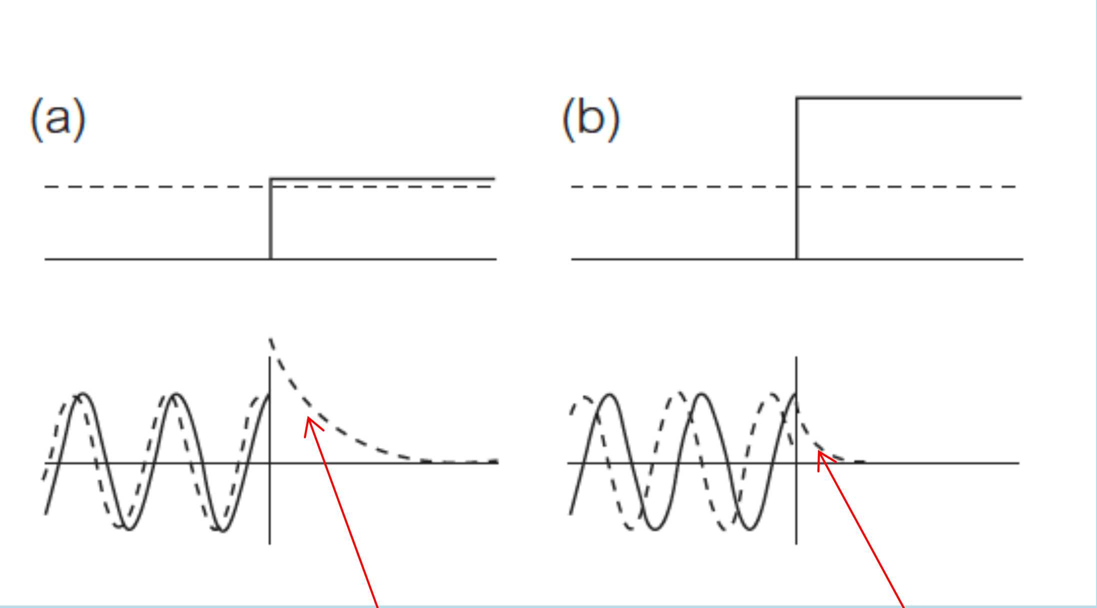
同樣要求ψ及ψ'在邊界原點連續，

$$1 + R = T \qquad k - kR = i\kappa T$$

與之前式子相同，只要以$i\kappa$替代q即可！

$$R = \frac{k - i\kappa}{k + i\kappa}$$

$$T = \frac{2k}{k + i\kappa}$$



$$P = |\Psi|^2 = \left|\psi_E(x)\cdot e^{-i\frac{E}{\hbar}t}\right|^2 = |\psi_E(x)|^2\left|e^{-i\frac{E}{\hbar}t}\right|^2 = |\psi_E(x)|^2 = |T|^2 e^{-2\kappa x}$$

在禁止區，機率密度不再是常數，而是隨滲透距離x指數遞減了！

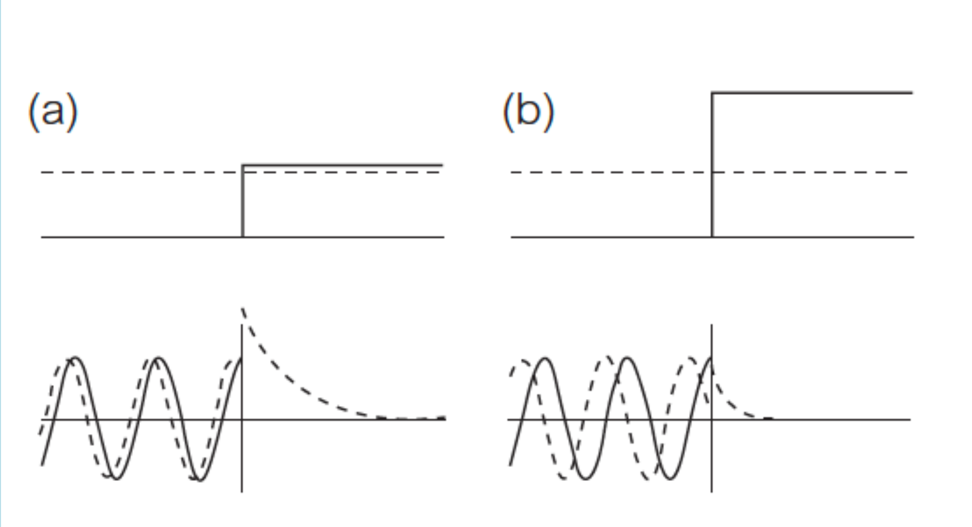


Figure 11.4. Same as for Fig. 11.3, but for two cases where $V_0 > E > 0$.

$$k - i\kappa \equiv |k - i\kappa| e^{-i\delta}$$

$$\frac{\kappa}{k} = \tan\delta$$

$$k + i\kappa = |k + i\kappa| e^{i\delta}$$

$$R = \frac{k - i\kappa}{k + i\kappa} = \left|\frac{k - i\kappa}{k + i\kappa}\right| e^{-2i\delta} = e^{-2i\delta}$$

反射波與入射波振幅相同，但相差一個相角2δ！δ由E決定。

$$\psi_E = e^{ikx} + Re^{-ikx} = e^{ikx} + e^{-i(kx+2\delta)}$$

$$|R|^2 = \left|e^{-2i\delta}\right|^2 = 1$$

反射率為1，完全反射。透射率是零。

在禁止區，雖然有滲透機率，可算出機率流為零，並沒有機率流進去！

$$j = -i\frac{\hbar}{2m}\left(\frac{\partial\psi^*}{\partial x}\cdot\psi - \psi^*\cdot\frac{\partial\psi}{\partial x}\right)$$

對實數的ψ，兩項抵消， $j = 0$。

$E = 0.5V_0$ $\delta = \frac{\pi}{4}$

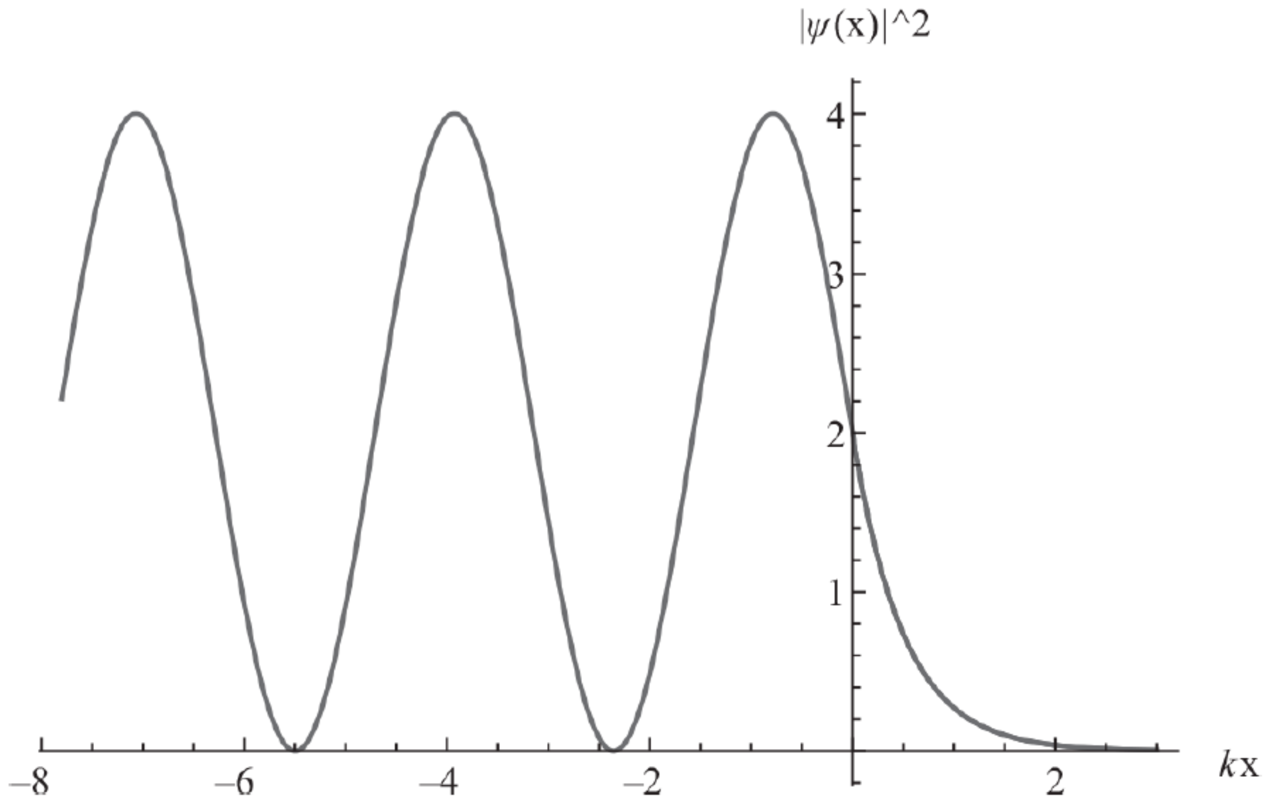


Figure 8.6

Probability density $|\psi(x)|^2$ as a function of position for an energy eigenstate with $E = \frac{1}{2}V_0$, giving $\delta(E) = \frac{\pi}{4}$ and $k = \kappa$, and setting $A = 1$ in (8.1.32). The value of $|\psi(0)|$ (equal to $\sqrt{2}$ here) is nonzero for arbitrary phase shift $\delta(E)$. The probability density decays exponentially for $x > 0$.

We conclude this section with some observations about particles in the forbidden region. For energy eigenstates with $E < V_0$ and for the wave packets built as a superposition of such eigenstates, there is some nonvanishing probability density in the forbidden region $x > 0$. Such nontrivial probability density implies some likelihood of detecting the particle in the forbidden region. If so, it would seem that such a particle would have an unphysical negative kinetic energy. This conclusion does not follow in quantum mechanics, however. Once we measure the particle position, the wave function collapses to become narrowly localized within the forbidden region, in a region the size of the detector resolution. This means that the collapsed wave function is *no longer* an energy eigenstate. The measured value of the energy becomes ambiguous. For any localized wave function, moreover, the expected value $\langle \frac{\hat{p}^2}{2m} \rangle$ of the kinetic energy is always positive.

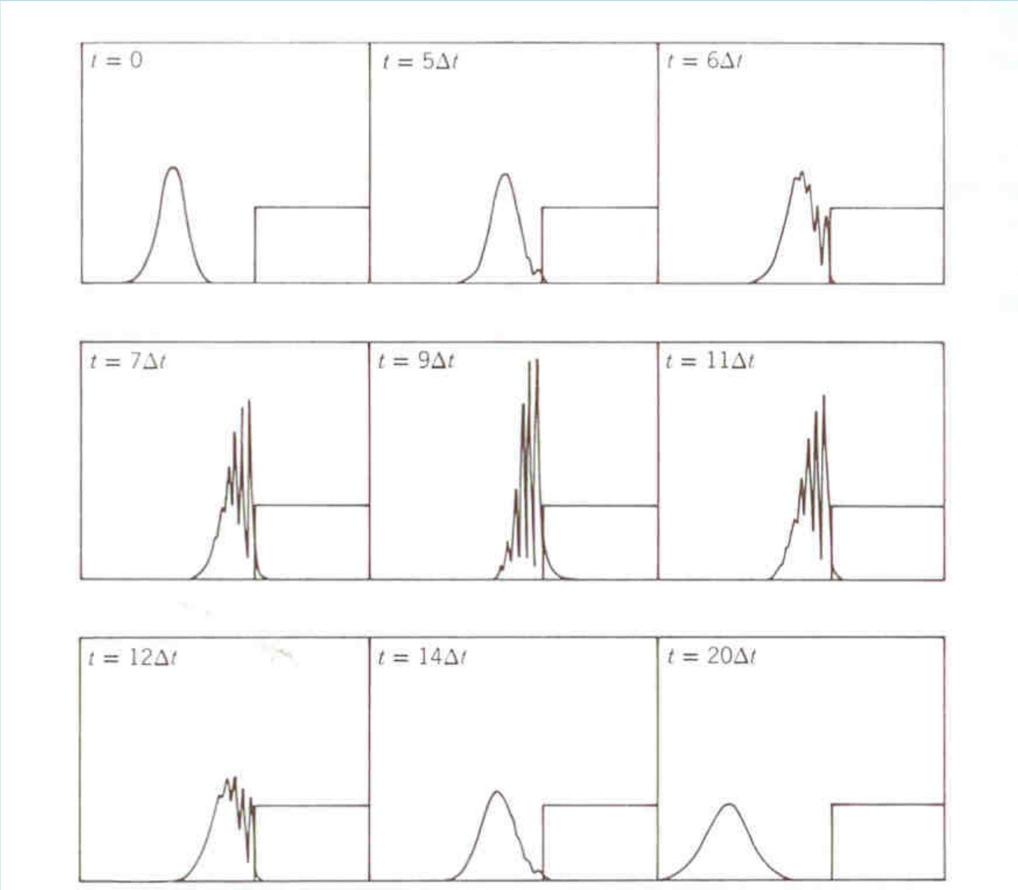
這個波的散射可以用波包處理。

波包撞擊位階時，波會滲入禁止區，

但在碰撞過後而言，滲入的部分就會消失，

反射波包的行為幾乎如同一個古典的反彈粒子。

但反射波與入射波的相角差2δ，會造成入射波包與反射波包的時間延遲！

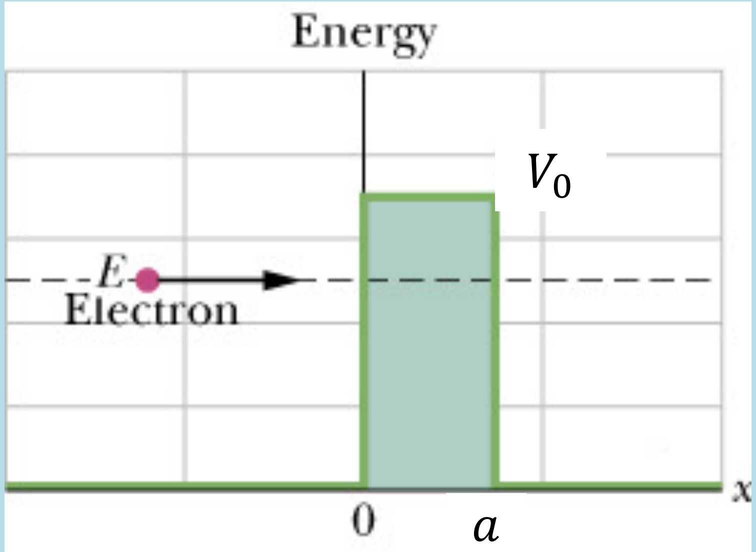


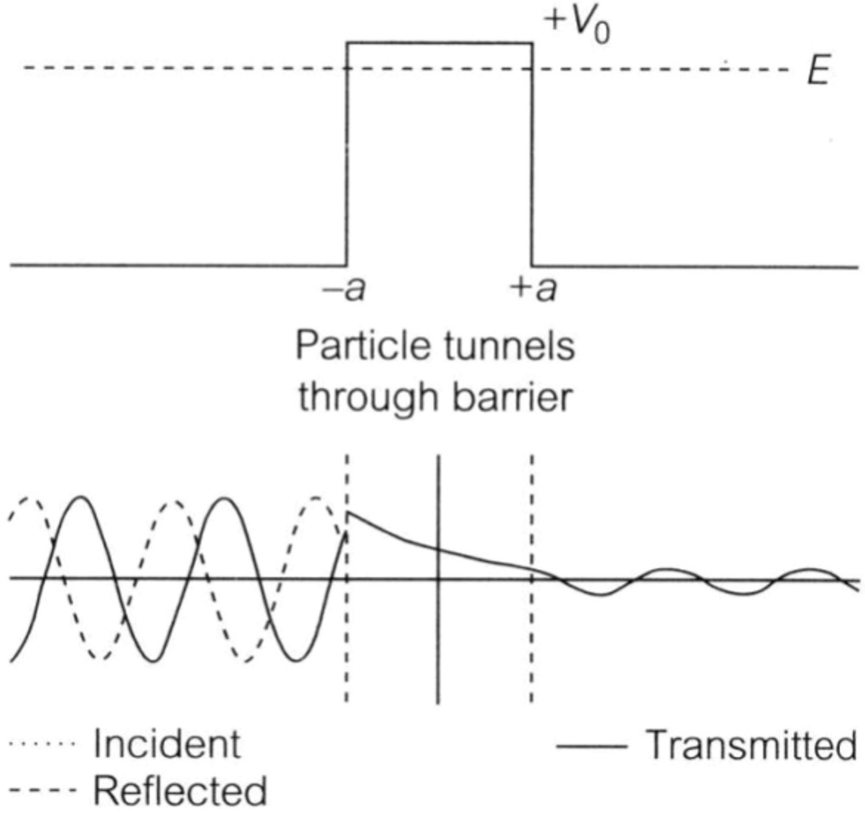
穿隧效應 Tunneling Effect

在禁止區，雖然有滲透機率，可算出機率流為零，並沒有機率流進去！

但如果這位能只持續很小一個範圍，位能很薄，粒子便能滲透過去，

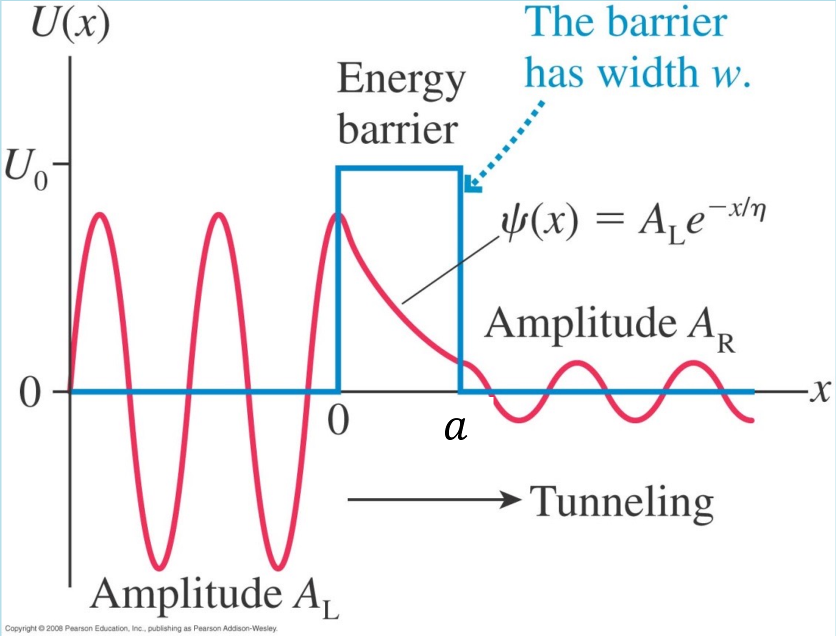
在位能壘後方形成一個自由粒子波！

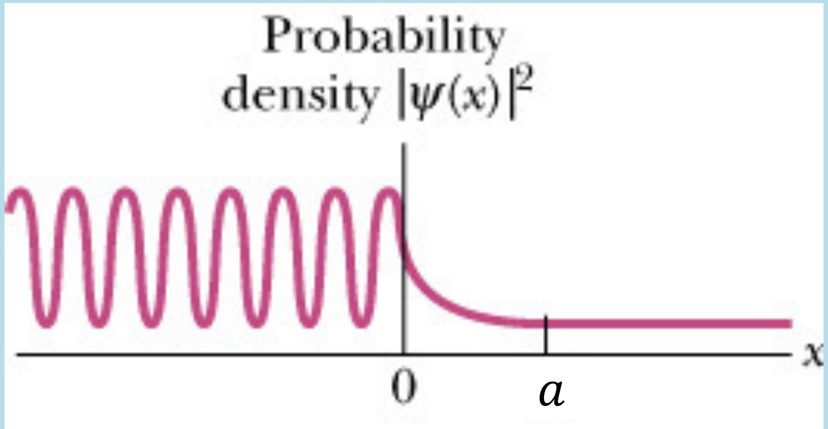



+V_0
E
$-a$
$+a$
Particle tunnels through barrier
Incident
Reflected
Transmitted

穿牆人 Le Passe-MurailleMarcel Aymé, 1943

Tunneling effect 穿隧效應





在位壘中 $\psi_E(x) \sim Ae^{-\kappa x}$

機率密度 $P = |\psi_E|^2 = |A|^2 e^{-2\kappa x}$

隨距離而指數遞減。在$x = a$，ψ_E要連續。

穿透後$x > a$機率 $\sim |\psi_E(a)|^2 \propto e^{-2\kappa a}$

一個電子有這麼多的機率會穿透，其餘的機率則反彈回來！

$$\kappa \equiv \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

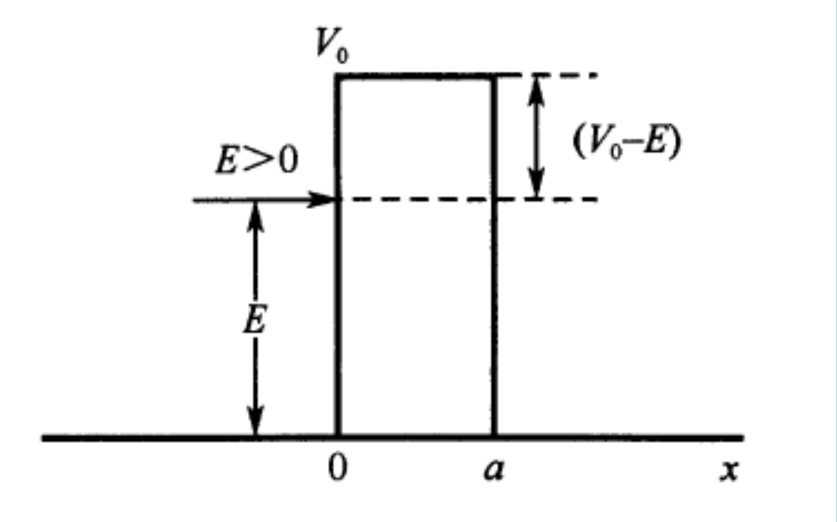
能量差距越小，κ越小，穿透率越大！

比較嚴格的計算

$x < 0$

$$\psi_E = e^{ikx} + Re^{-ikx}$$

$$k \equiv \sqrt{\frac{2m}{\hbar^2} E}$$



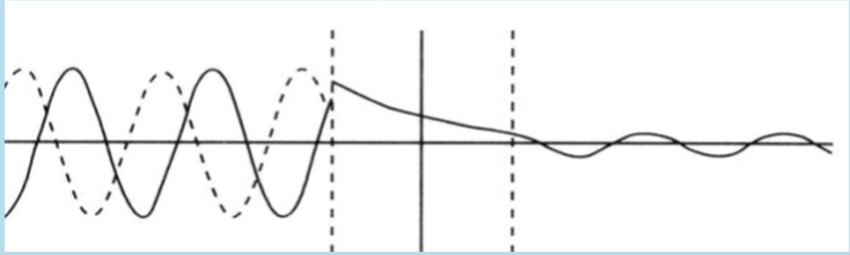
$0 < x < a$ 在位壘中，指數遞增也要列入

$$\psi_E = Ae^{-\kappa x} + Be^{\kappa x}$$

$$\kappa \equiv \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

$x > a$

$$\psi_E = Se^{ikx}$$



ψ與ψ'在兩邊界都要連續，

$$1 + R = A + B \qquad \frac{ik}{-\kappa}(1 - R) = A - B \qquad x = 0$$

$$Se^{ika} = Ae^{-\kappa a} + Be^{\kappa a} \qquad \frac{ik}{-\kappa}\left(Se^{ika}\right) = Ae^{-\kappa a} - Be^{\kappa a} \qquad x = a$$

$$1+R=A+B$$
$$\frac{\mathrm{i}k}{\kappa}(1-R)=A-B$$

两式相加、减，得

$$A=\frac{1}{2}\left[\left(1+\frac{\mathrm{i}k}{\kappa}\right)+R\left(1-\frac{\mathrm{i}k}{\kappa}\right)\right] \tag{3.3.11a}$$

$$B=\frac{1}{2}\left[\left(1-\frac{\mathrm{i}k}{\kappa}\right)+R\left(1+\frac{\mathrm{i}k}{\kappa}\right)\right] \tag{3.3.11b}$$

在点 $x=a$，ψ 及 ψ' 的连续条件导致

$$Ae^{\kappa a}+Be^{-\kappa a}=Se^{\mathrm{i}ka}$$
$$Ae^{\kappa a}-Be^{-\kappa a}=\frac{\mathrm{i}k}{\kappa}Se^{\mathrm{i}ka}$$

两式分别相加、减，得

$$A=\frac{S}{2}\left(1+\frac{\mathrm{i}k}{\kappa}\right)e^{\mathrm{i}ka-\kappa a} \tag{3.3.12a}$$

$$B=\frac{S}{2}\left(1-\frac{\mathrm{i}k}{\kappa}\right)e^{\mathrm{i}ka+\kappa a} \tag{3.3.12b}$$

比较式(3.3.11)和(3.3.12)，消去 A、B，得

$$\begin{aligned}\left(1+\frac{\mathrm{i}k}{\kappa}\right)+R\left(1-\frac{\mathrm{i}k}{\kappa}\right)&=S\left(1+\frac{\mathrm{i}k}{\kappa}\right)e^{\mathrm{i}ka-\kappa a}\\ \left(1-\frac{\mathrm{i}k}{\kappa}\right)+R\left(1+\frac{\mathrm{i}k}{\kappa}\right)&=S\left(1-\frac{\mathrm{i}k}{\kappa}\right)e^{\mathrm{i}ka+\kappa a}\end{aligned} \tag{3.3.13}$$

再从上式消去 R，得

$$\frac{Se^{\mathrm{i}ka-\kappa a}-1}{Se^{\mathrm{i}ka+\kappa a}-1}=\left(\frac{1-\mathrm{i}k/\kappa}{1+\mathrm{i}k/\kappa}\right)^2 \tag{3.3.14}$$

不难解出

$$Se^{\mathrm{i}ka}=\frac{-2\mathrm{i}k/\kappa}{[1-(k/\kappa)^2]\operatorname{sh}\kappa a-2\mathrm{i}\frac{k}{\kappa}\operatorname{ch}\kappa a} \tag{3.3.15}$$

不难解出

$$Se^{ika} = \frac{-2ik/\kappa}{[1-(k/\kappa)^2]\text{sh}\kappa a - 2i\frac{k}{\kappa}\text{ch}\kappa a} \tag{3.3.15}$$

因此，透射系数为

$$|S|^2 = \frac{4k^2\kappa^2}{(k^2-\kappa^2)^2\text{sh}^2\kappa a + 4k^2\kappa^2\text{ch}^2\kappa a} = \frac{4k^2\kappa^2}{(k^2+\kappa^2)^2\text{sh}^2\kappa a + 4k^2\kappa^2}$$

$$= \left[1+\frac{(k^2+\kappa^2)^2}{4k^2\kappa^2}\text{sh}^2\kappa a\right]^{-1} = \left[1+\frac{1}{\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)}\text{sh}^2\kappa a\right]^{-1} \tag{3.3.16}$$

估算．设 $\kappa a \gg 1$，此时 $\text{sh}\kappa a \approx \frac{1}{2}e^{\kappa a} \gg 1$，式(3.3.16)可近似表示成

$$|S|^2 \approx \frac{16k^2\kappa^2}{(k^2+\kappa^2)^2}e^{-2\kappa a}$$

$$= \frac{16E(V_0-E)}{V_0}\exp\left[-\frac{2a}{\hbar}\sqrt{2m(V_0-E)}\right] \tag{3.3.19}$$

现代物理学丛书

量子力学

卷 I

（第四版）

曾谨言 著

3.3.1 方势垒的穿透

先考虑最简单的方势垒穿透问题. 设具有一定能量 E 的粒子,沿 x 轴正方向射向方势垒(图 3.11),

$$V(x) = \begin{cases} V_0, & 0 < x < a \\ 0, & x > a, \quad x < 0 \end{cases} \tag{3.3.1}$$

按照经典力学观点,若 $E<V_0$,则粒子不能进入势垒,将被弹回去. 若 $E>V_0$,则粒子将穿过势垒. 但从量子力学观点来看,考虑到粒子的波动性,此问题与波透过一层介质(厚度为 a)相似,有一部分波穿过,一部分波被反射回去. 因此,按波函数的统计诠释,粒子有一部分概率穿过势垒,并有一定的概率被反射回去.

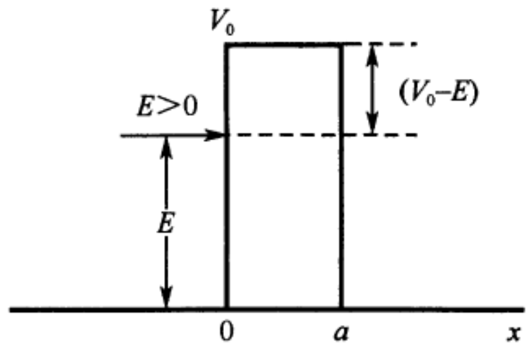


图 3.11 方势垒的穿透

先考虑 $E<V_0$ 情况.

在势垒之外($x<0, x>a$,经典允许区),Schrödinger 方程为

$$\frac{d^2}{dx^2}\psi = -k^2\psi, \qquad k = \sqrt{2mE}/\hbar \tag{3.3.2}$$

它的两个线性无关解可取为

$$\psi \propto e^{\pm ikx} \tag{3.3.3}$$

按假设,粒子是从左入射. 由于势垒的存在,在 $x<0$ 区域中,既有入射波,也有反射波. 但在 $x>a$ 区域中,只有透射波,所以

$$\psi(x)=\begin{cases} e^{ikx}+Re^{-ikx} & (x<0) \quad (3.3.4a)\\ Se^{ikx} & (x>a) \quad (3.3.4b)\end{cases}$$

式(3.3.4a)右边第一项为入射波，其波幅(任意地)取为 1，只是为了方便，对于粒子进入势垒和反射的几率没有影响. 按概率流密度公式

$$j_x=\frac{\hbar}{2mi}\left(\psi^*\ \frac{\partial}{\partial x}\psi-\psi\frac{\partial}{\partial x}\psi^*\right)$$

取入射波 $\psi_i=e^{ikx}$ 就相当于粒子入射流密度取为

$$j_i=\frac{\hbar}{2mi}\left(e^{-ikx}\ \frac{\partial}{\partial x}e^{ikx}-\text{c. c.}\right)=\frac{\hbar k}{m}=v \tag{3.3.5}$$

式(3.3.4a)右边第二项 Re^{-ikx} 为反射波，相应的反射流密度为

$$|j_r|=|R|^2v \tag{3.3.6}$$

式(3.3.4b)代表透射波，透射流密度为

$$j_t=|S|^2v \tag{3.3.7}$$

所以

$$\text{反射系数}=|j_r/j_i|=|R|^2 \tag{3.3.8}$$

$$\text{透射系数}=j_t/j_i=|S|^2 \tag{3.3.9}$$

以下将根据方势垒边界上波函数及其导数的连续条件来确定 R 与 S，从而求出反射系数与透射系数.

在势垒内部（$0<x<a$，经典禁区），Schrödinger 方程为

$$\frac{d^2}{dx^2}\psi=\kappa^2\psi,\quad \kappa=\sqrt{2m(V_0-E)}/\hbar$$

其通解可表示为

$$\psi=Ae^{\kappa x}+Be^{-\kappa x} \tag{3.3.10}$$

在 $x=0$ 点，ψ 及 ψ' 的连续条件导致

$$1+R=A+B$$

$$\frac{ik}{\kappa}(1-R)=A-B$$

两式相加、减，得

$$A=\frac{1}{2}\left[\left(1+\frac{ik}{\kappa}\right)+R\left(1-\frac{ik}{\kappa}\right)\right] \tag{3.3.11a}$$

$$B=\frac{1}{2}\left[\left(1-\frac{ik}{\kappa}\right)+R\left(1+\frac{ik}{\kappa}\right)\right] \tag{3.3.11b}$$

在点 $x=a$，ψ 及 ψ' 的连续条件导致

$$Ae^{\kappa a}+Be^{-\kappa a}=Se^{ika}$$

$$Ae^{\kappa a}-Be^{-\kappa a}=\frac{ik}{\kappa}Se^{ika}$$

两式分别相加、减，得

$$A=\frac{S}{2}\left(1+\frac{ik}{\kappa}\right)e^{ika-\kappa a} \tag{3.3.12a}$$

$$B=\frac{S}{2}\left(1-\frac{ik}{\kappa}\right)e^{ika+\kappa a} \tag{3.3.12b}$$

比较式(3.3.11)和(3.3.12)，消去 A、B，得

$$\begin{aligned}\left(1+\frac{ik}{\kappa}\right)+R\left(1-\frac{ik}{\kappa}\right)&=S\left(1+\frac{ik}{\kappa}\right)e^{ika-\kappa a}\\ \left(1-\frac{ik}{\kappa}\right)+R\left(1+\frac{ik}{\kappa}\right)&=S\left(1-\frac{ik}{\kappa}\right)e^{ika+\kappa a}\end{aligned} \tag{3.3.13}$$

再从上式消去 R，得

$$\frac{Se^{ika-\kappa a}-1}{Se^{ika+\kappa a}-1}=\left(\frac{1-ik/\kappa}{1+ik/\kappa}\right)^2 \tag{3.3.14}$$

再从上式消去 R，得

$$\frac{Se^{ika-\kappa a}-1}{Se^{ika+\kappa a}-1}=\left(\frac{1-ik/\kappa}{1+ik/\kappa}\right)^2 \tag{3.3.14}$$

不难解出

$$Se^{ika}=\frac{-2ik/\kappa}{[1-(k/\kappa)^2]\mathrm{sh}\kappa a-2i\dfrac{k}{\kappa}\mathrm{ch}\kappa a} \tag{3.3.15}$$

因此，透射系数为

$$\begin{aligned}|S|^2&=\frac{4k^2\kappa^2}{(k^2-\kappa^2)^2\mathrm{sh}^2\kappa a+4k^2\kappa^2\mathrm{ch}^2\kappa a}=\frac{4k^2\kappa^2}{(k^2+\kappa^2)^2\mathrm{sh}^2\kappa a+4k^2\kappa^2}\\&=\left[1+\frac{(k^2+\kappa^2)^2}{4k^2\kappa^2}\mathrm{sh}^2\kappa a\right]^{-1}=\left[1+\frac{1}{\dfrac{E}{V_0}\left(1-\dfrac{E}{V_0}\right)}\mathrm{sh}^2\kappa a\right]^{-1}\end{aligned} \tag{3.3.16}$$

类似地从式(3.3.13)消去 S，得出反射系数

$$|R|^2=\frac{(k^2+\kappa^2)^2\mathrm{sh}^2\kappa a}{(k^2+\kappa^2)^2\mathrm{sh}^2\kappa a+4k^2\kappa^2} \tag{3.3.17}$$

可以看出

$$|R|^2+|S|^2=1 \tag{3.3.18}$$

$|R|^2$ 代表粒子被势垒反射回去的概率，$|S|^2$ 代表粒子穿透势垒的概率. 式(3.3.18)正是概率守恒(即粒子数守恒)的表现.

按照经典力学来看，在 $E<V_0$ 情况下，粒子根本不能穿过势垒，将完全被弹回. 而按照量子力学计算，在一般情况下，透射系数 $T\neq0$. 这种现象——粒子能穿过比它动能更高的势垒，称为隧道效应(tunnel effect)，它是粒子波动性的反映. 但只在一定条件下，这种效应才显著. 在图 3.12 中，给出了势垒穿透的波动图像.

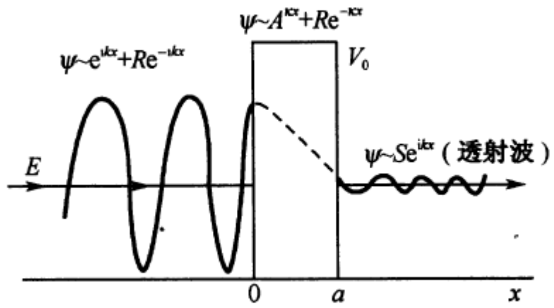


图 3.12

我们现在对透射系数作一个简单

估算. 设 $\kappa a \gg 1$,此时 $\mathrm{sh}\kappa a \approx \frac{1}{2}e^{\kappa a} \gg 1$,式(3.3.16)可近似表示成

$$|S|^2 \sim \left(\frac{4\kappa k}{k^2+\kappa^2}\right)^2 e^{-2\kappa a}$$

$$|S|^2 \approx \frac{16k^2\kappa^2}{(k^2+\kappa^2)^2}e^{-2\kappa a} = \frac{16E(V_0-E)}{V_0}\exp\left[-\frac{2a}{\hbar}\sqrt{2m(V_0-E)}\right] \qquad (3.3.19)$$

可以看出 T 与势垒宽度 a,(V_0-E),以及粒子质量 m 的依赖关系都很敏感. 随势垒宽度 a 和粒子质量 m 增大,T 将指数衰减,$T \propto e^{-a\sqrt{m}}$. 所以,在宏观实验中,不容易观测到粒子穿透势垒的现象.

例如,对于电子,设 $E=1\mathrm{eV}, V_0=2\mathrm{eV}, a=2\times10^{-8}\mathrm{cm}$,可以估算出 $T\approx0.51$. 若 $a=5\times10^{-8}\mathrm{cm}$,则 $T\sim0.024$,迅速变小. 若电子换成质子,因为 $m_p/m_e\approx1840$,$a=2\times10^{-8}\mathrm{cm}$,可估算出 $T\approx2.6\times10^{-38}$.

对于 $E>V_0$ 情况(图 3.13),只需在式(3.3.16)中,把 $\kappa\to ik'$,k'为实数

$$k' = \sqrt{2m(E-V_0)/\hbar^2} \qquad (3.3.20)$$

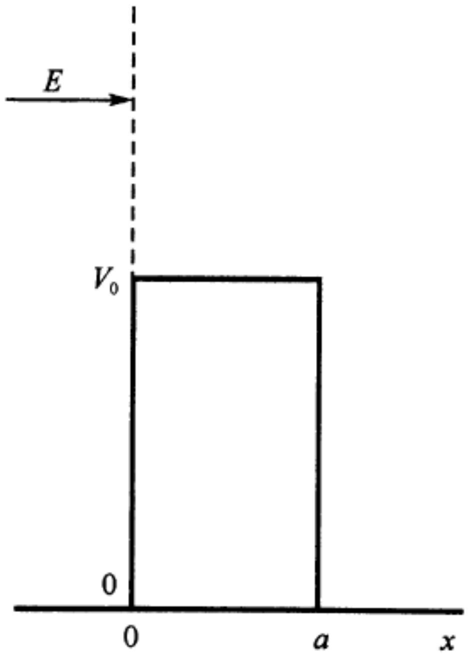


图 3.13

再利用 $\mathrm{sh}(ik'a)=i\sin k'a$,可得

$$|S|^2 = \frac{4k^2k'^2}{(k^2-k'^2)^2\sin^2 k'a+4k^2k'^2} = \frac{1}{1+\frac{1}{4}\left(\frac{k}{k'}-\frac{k'}{k}\right)^2\sin^2 k'a} \quad (k'\leqslant k) \qquad (3.3.21)$$

更厲害：方程式是線性，若位能壘不是方形，可用方形位能壘來組合近似！

$$P_T = |S|^2 \sim \left(\frac{4\kappa k}{k^2+\kappa^2}\right)^2 e^{-2\kappa a}$$

The approximate expression for the ratio of transmitted flux to incident flux, $|T|^2$, is an extremely sensitive function of the width of the barrier, and of the amount by which the barrier exceeds the incident energy, since

$$\kappa a = \left[\frac{2ma^2}{\hbar^2}(V_0 - E)\right]^{1/2} \qquad (4\text{-}41)$$

In general, the barriers that occur in physical phenomena are not square, and to discuss some applications, we must first obtain an approximate expression for the transmission coefficient $|T|^2$ through an irregularly shaped barrier. The proper way to do this, given the fact that there is no exact solution available for most potentials, is through the Wentzel–Kramers–Brillouin (WKB) approximation technique.[1] Our discussion will be less mathematical.

We observe that (4-36) consists of a product of a *pre-factor* and a much more rapidly varying exponential factor. Thus we may isolate this behavior by writing, again approximately

$$\ln|T|^2 = (\text{const}) - (2\kappa)(2a)$$

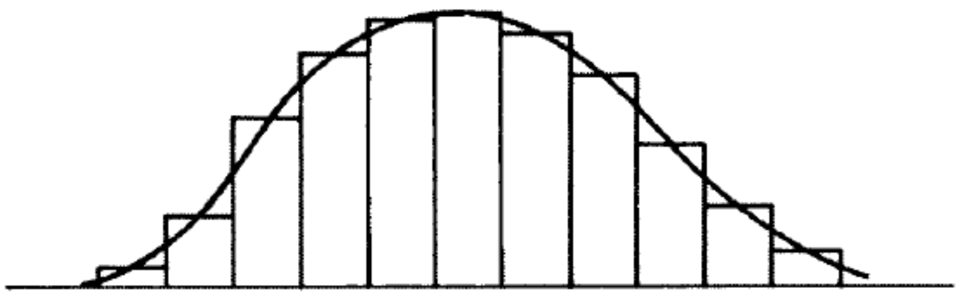
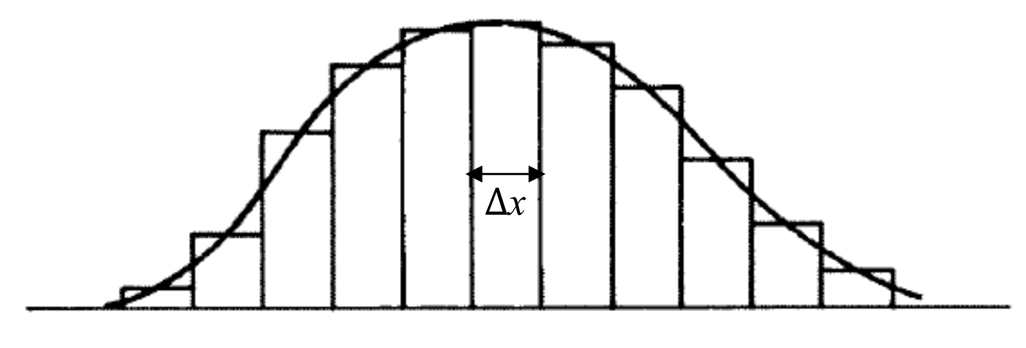


Figure 4-4 Approximation of a smooth barrier by a juxtaposition of square potential barriers.

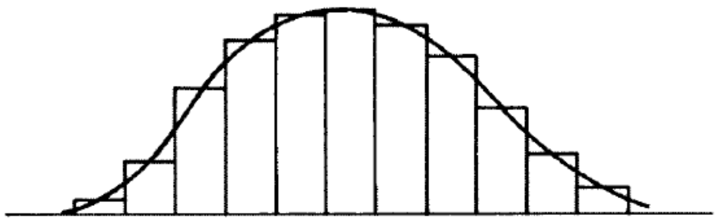


總透射率等於個別透射率的乘積：

$$
\begin{aligned}
P_T &= \prod_i P_i(x_i) \\
&\approx \prod_i e^{-2\kappa(x_i)\Delta x} \quad (\text{where} \quad \kappa(x) \equiv \sqrt{2m(V(x)-E)/\hbar^2}) \\
&= e^{-2\sum_i \kappa(x_i)\Delta x} \\
&\approx e^{-2\int_a^b \kappa(x)\,dx}
\end{aligned}
$$

$$
P_T = \exp\left(-2\sqrt{\frac{2m}{\hbar^2}}\int_a^b \sqrt{V(x)-E}\,dx\right) \qquad (11.49)
$$

in which the energy dependent factor 2κ multiplies the *width* of the barrier $2a$. The procedure we adopt is to treat a smooth curved barrier as a juxtaposition of square barriers, as shown in Fig. 4-4. If the transmission probability for each barrier is small, the overall probability is the product of the individual ones. Equivalently the overall transmission coefficient is a product of the transmission coefficients of the individual barriers. In effect, when most of the flux is reflected by a single barrier, the transmission through each "slice" is an independent, improbable event. We may therefore write, approximately



$$\begin{aligned} \ln|T|^2 &= \sum_{\text{slices}} \ln|T_{\text{slice}}|^2 = -2\sum_n \Delta x_n \langle\kappa\rangle_n \\ &= -2\int_{\text{barrier}} dx\sqrt{2m(V(x)-E)/\hbar^2} \end{aligned} \tag{4-42}$$

In the "slices" Δx_n is the width and $\langle\kappa\rangle$ is the average value of κ for that slice of the barrier. In the last step, a limit of infinitely narrow barriers was taken. It is clear from the expression that the approximation is least accurate near the *turning points*, where the energy and potential are nearly equal, since there (4-36) is not a good approximation to (4-35). It is also important that $V(x)$ be a slowly varying function of x, since otherwise the approximation of a smooth barrier by a stack of square ones is only possible if the latter are narrow. However, there (4-36) is again a poor approximation. A proper treatment using the WKB approximation includes a discussion of the behavior near the turning points. For our purposes it is a fair approximation to write

$$|T|^2 = Ce^{-2\int dx\sqrt{2m(V(x)-E)/\hbar^2}} \tag{4-43}$$

where the integration is over the region in which the square root is real.

A subject which is often discussed in modern physics courses is the *photoelectric effect* in which electrons are emitted from a metal by the absorption of sufficiently energetic photons. The effect is illustrated in Fig. 11.10(a) where the Fermi energy of the filled electron sea is still an energy W below the threshold for a free particle; W is often called the *work function* of the metal. A photon of energy E_γ can extract an electron from the sea provided that $E_\gamma \geq W$, with any remaining energy transferred to the electron as kinetic energy. Such experiments provide

場放射：加上電場，可以使電子穿隧離開固體。

$V(x) \sim W - e\mathcal{E}x$

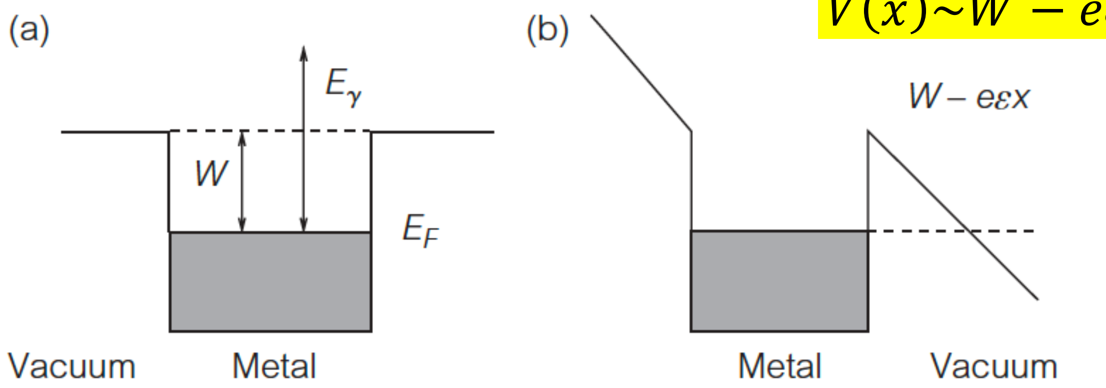


Figure 11.10. (a) Allowed electron states for a metal showing the filled Fermi sea and the photoelectric effect; (b) An external electric field is applied illustrating the triangular barrier giving rise to field emission.

A completely different form of electron emission which relies instead on a purely classical electric field, but which makes use of quantum tunneling, is *field emission*. In this case, shown in Fig. 11.10(b), an external electric field $\mathcal{E}$ is applied to the sample; electrons at the top of the sea can now tunnel through the triangular-shaped potential barrier. In this simple approximation, the probability of tunneling corresponding to Eqn. (11.49) is (P11.8) external electric field $\mathscr{E}$. This phenomenon is described as *cold emission*. It occurs because the external field changes the potential seen by the electron from a macroscopically wide barrier of height W to one described by $W - e\mathscr{E}x$, where x is the distance from the wall of the box (Fig. 4-5b). The change creates a barrier of finite width, and electrons can tunnel through it. We define the most easily removed electrons as having energy $E = 0$. This then gives the transmission coefficient as

$$P_T \sim C e^{-2\int_0^a dx\sqrt{2m(W - e\mathcal{E}x)/\hbar^2}} \tag{4-44}$$

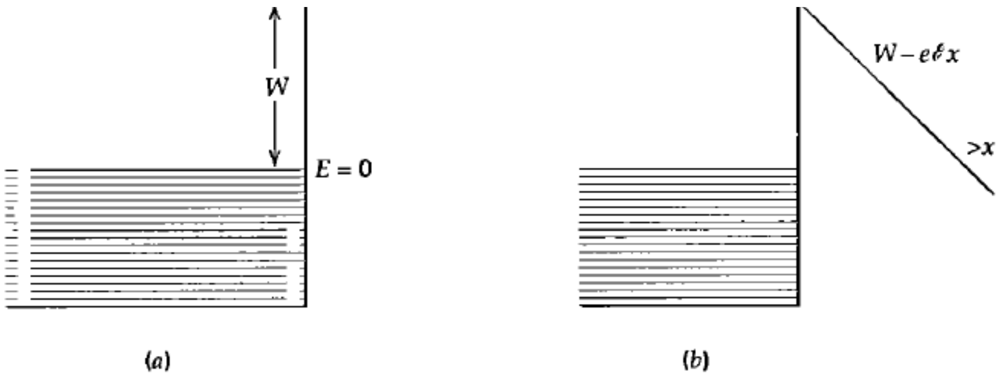


Figure 4-5 (a) Electronic levels in metal. We set the energy of the highest level $E = 0$. (b) Schematic sketch of how the potential is altered by an external electric field.

where a is the width of the barrier given by $V(a) \sim W - e\mathcal{E}a = 0$

$$a = \frac{W}{e\mathscr{E}} \tag{4-45}$$

The integral in (4-44) is easily evaluated. It leads to the result

$$P_T \sim C e^{-\frac{4\sqrt{2}}{3}\sqrt{mWa^2/\hbar^2}} = C e^{-\frac{4\sqrt{2}}{3}\sqrt{mW^3/\hbar^2}\frac{1}{e\mathcal{E}}} \tag{4-46}$$

The *Fowler-Nordheim formula*, as (4-46) is called, describes emission only qualitatively One effect, which is easily included, is the additional attraction of the electron to its image charge, which acts to pull it back to the plate. The other effect, much harder to handle, is that there are surface imperfections, which change the electric field locally, and since $\mathscr{E}$ appears in the exponent (in a) this can make a large difference.

triangular-shaped potential barrier. In this simple approximation, the probability of tunneling corresponding to Eqn. (11.49) is (P11.8)

$$P_T = \exp\left(-\frac{4}{3}\sqrt{\frac{2mW^3}{\hbar^2}}\frac{1}{e\mathcal{E}}\right) = \exp\left(-\frac{\mathcal{E}_0}{\mathcal{E}}\right) \tag{11.50}$$

This expression shows the strong dependence on the local value of the work function W at the surface. The resulting electron current due to quantum tunneling should be directly proportional to this probability, namely

$$I = I_0 e^{-\mathcal{E}_0/\mathcal{E}} \quad \text{or} \quad \log(I) = \log(I_0) - \frac{\mathcal{E}_0}{\mathcal{E}} \tag{11.51}$$

We compare this prediction with some of the data from one of the original experiments[1] in Fig. 11.11.

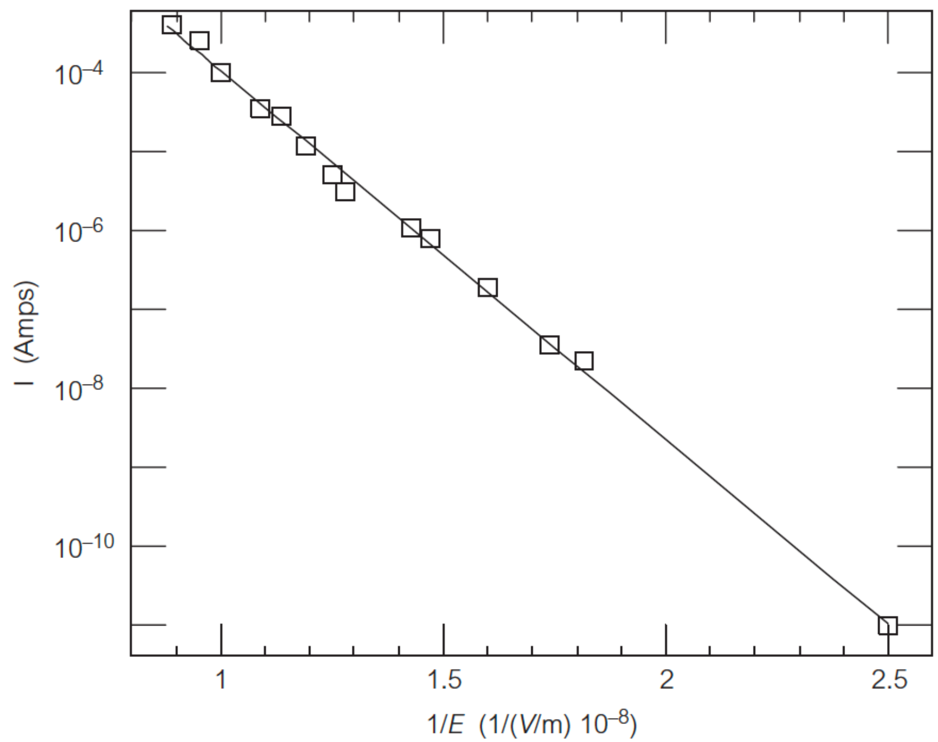


Figure 11.11. Semilog plot of tunneling current, I, versus $1/\mathcal{E}$ where $\mathcal{E}$ is the applied electric field, illustrating field emission. The data are taken from Millikan and Eyring (1926).

This effect is also used as the basis of an imaging device called the field ion microscope[2] (FIM), which was the first microscope to achieve atomic resolutions enabling one to "see" individual atoms. The device works roughly as follows:

- A sharp, metallic tip with radius of curvature in the range 100 to 200 Å is placed in a vacuum and charged to a large voltage, typically 1–20 kV; this process itself helps to smooth the surface by selective field ionization of the metal atoms to what can be called "atomic smoothness".
- A very dilute gas of noble gas atoms (often helium) is introduced; this is used as the imaging gas. These atoms are adsorbed onto the surface of the probe due to dipole–dipole attractions to the tip atoms (remember that both atomic species are initially neutral).
- The image gas atoms, once attached to a tip atom, can be ionized via field emission, losing an electron to the tip; the resulting positively charged *ions* are then accelerated by the electric field toward a phosphorescent screen some tens of centimeters, away forming the image. A schematic representation of the process is shown in Fig. 11.12 and an FIM image is shown in Fig. 11.13.
- In this device, the electron tunneling serves only to initiate ion formation and the electrons themselves do not participate in the image formation. In the original *field emission microscope*, the electrons emitted via field ionization were used to image the surface; this process relied on the local variations of

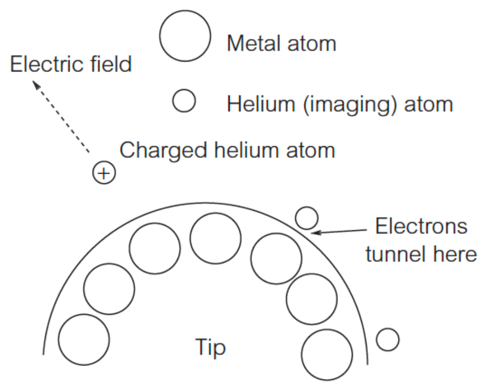


Figure 11.12. Schematic representation of field ion microscope. The metal atoms (large circles) forming the surface of the smooth probe tip attract (via dipole–dipole forces) the atoms of the imaging gas (small circles are helium). Once bound, electrons from the He can tunnel into the tip via field emission. The resulting charged ions travel along the electric field lines (the tip is held at a large electric potential) and form an image on the screen.

Figure 11.13. Field ion microscope image of a tungsten tip of radius $\sim$ 400 Å. The original image had a magnification of 3 million. (Photo courtesy of T. Tsong.

EXAMPLE 40.7 TUNNELING THROUGH A BARRIER

SOLUTION

A 2.0-eV electron encounters a barrier 5.0 eV high. What is the probability that it will tunnel through the barrier if the barrier width is (a) 1.00 nm and (b) 0.50 nm?

SOLUTION

IDENTIFY and SET UP: This problem uses the ideas of tunneling through a rectangular barrier, as in Figs. 40.19 and 40.20. Our target variable is the tunneling probability T in Eq. (40.42), which we evaluate for the given values $E = 2.0\ \text{eV}$ (electron energy), $U = 5.0\ \text{eV}$ (barrier height), $m = 9.11 \times 10^{-31}\ \text{kg}$ (mass of the electron), and $L = 1.00\ \text{nm}$ or $0.50\ \text{nm}$ (barrier width).

EXECUTE: First we evaluate G and κ in Eq. (40.42), using $E = 2.0\ \text{eV}$:

$$G = 16\left(\frac{2.0\ \text{eV}}{5.0\ \text{eV}}\right)\left(1 - \frac{2.0\ \text{eV}}{5.0\ \text{eV}}\right) = 3.8$$

$$U_0 - E = 5.0\ \text{eV} - 2.0\ \text{eV} = 3.0\ \text{eV} = 4.8 \times 10^{-19}\ \text{J}$$

$$\kappa = \frac{\sqrt{2(9.11 \times 10^{-31}\ \text{kg})(4.8 \times 10^{-19}\ \text{J})}}{1.055 \times 10^{-34}\ \text{J}\cdot\text{s}} = 8.9 \times 10^{9}\ \text{m}^{-1}$$

(a) When $L = 1.00\ \text{nm} = 1.00 \times 10^{-9}\ \text{m}$, we have $2\kappa L = 2(8.9 \times 10^{9}\ \text{m}^{-1})(1.00 \times 10^{-9}\ \text{m}) = 17.8$ and $T = Ge^{-2\kappa L} = 3.8e^{-17.8} = 7.1 \times 10^{-8}$.

(b) When $L = 0.50\ \text{nm}$, one-half of 1.00 nm, $2\kappa L$ is one-half of 17.8, or 8.9. Hence $T = 3.8e^{-8.9} = 5.2 \times 10^{-4}$.

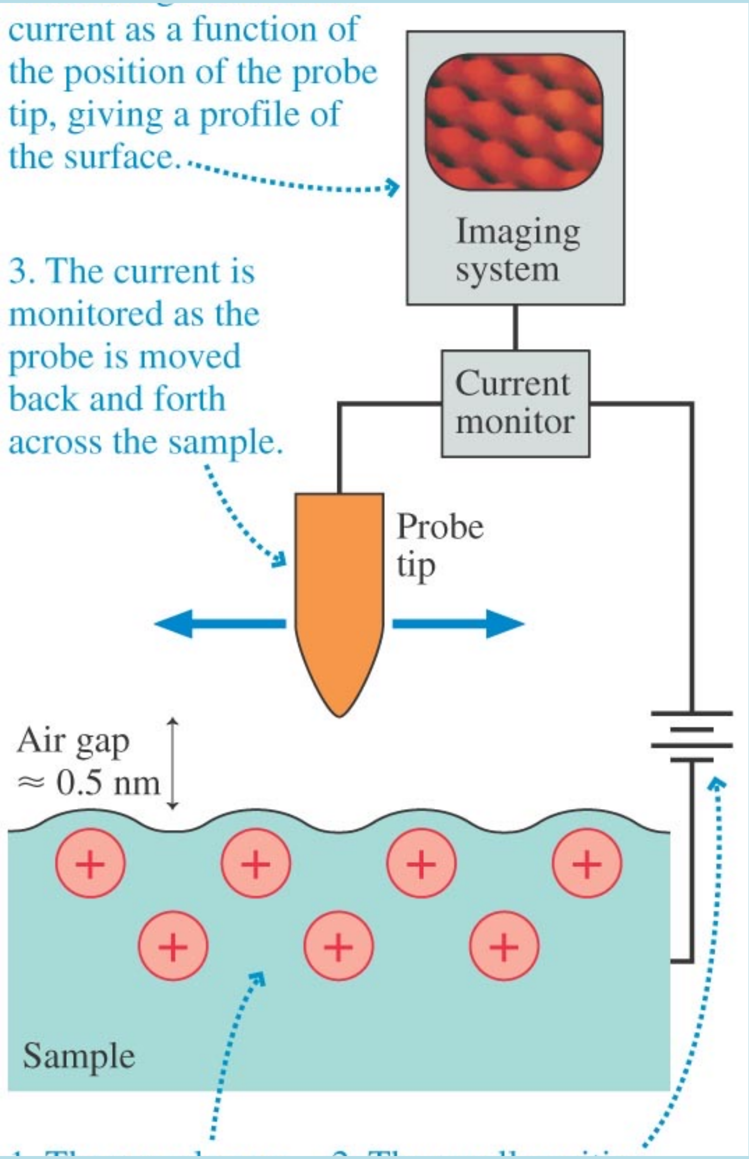
EVALUATE: Halving the width of this barrier increases the tunneling probability T by a factor of $(5.2 \times 10^{-4})/(7.1 \times 10^{-8}) = 7.3 \times 10^{3}$, or nearly ten thousand. The tunneling probability is an *extremely* sensitive function of the barrier width.

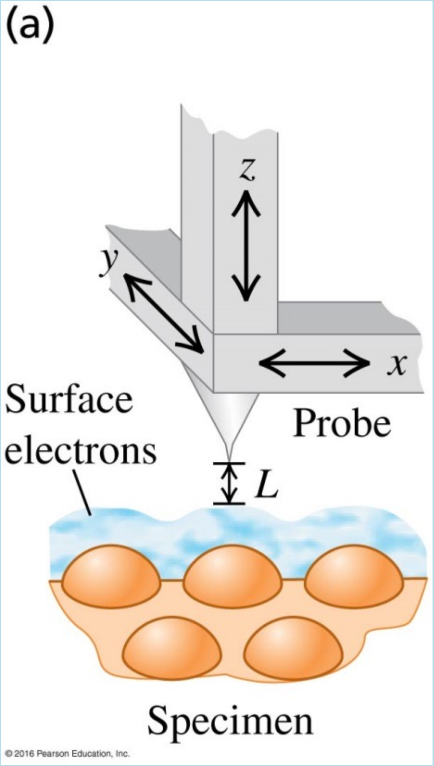
穿隧效應的應用

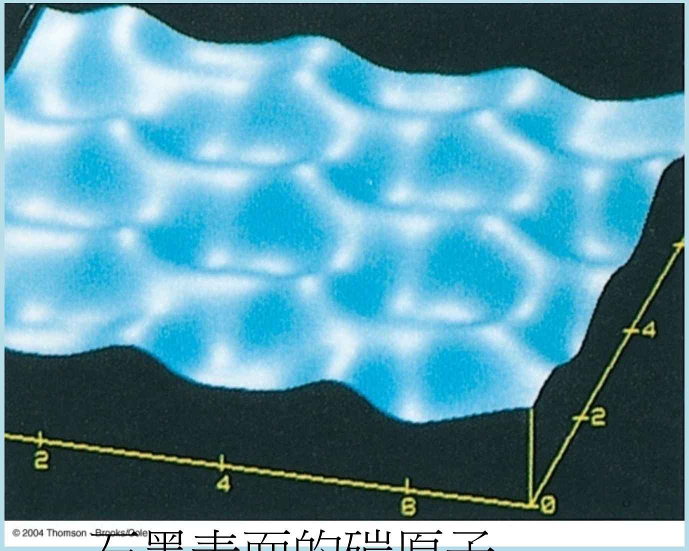
Scanning Tunneling Microscope 穿隧顯微鏡 STM

$$T \propto e^{-2\kappa a}$$

$$\kappa \equiv \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$







石墨表面的碳原子

11.4.2 Scanning Tunneling Microscopy

A newer technique which has had great success in obtaining images of atomic structures on (typically graphite or silicon) surfaces is *scanning tunneling microscopy*[3] (STM). A schematic representation of the physics involved is shown in Fig. 11.14:

1. Two metal electrodes are placed close together (often only Å's apart), one being the sample while the other is the tip.
2. Their Fermi surfaces differ and electrical equilibrium is reached only when enough electrons have tunneled through the junction (from left to right in this case). The resulting charge separation results in an electric field in the vacuum region between the electrodes.
3. An external voltage difference is applied to the tip shifting the Fermi energies again and allowing electron tunneling to occur.

As the tip is scanned over a plane surface, feedback circuits monitor the tunneling current, adjusting the tip height to maintain it at a constant value. The resulting height profile provides a map of the surface.

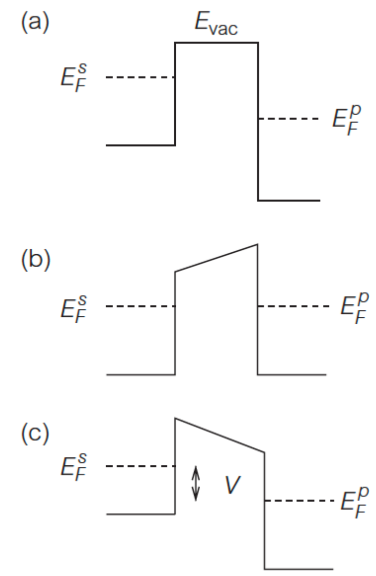


Figure 11.14. Schematic representation of the energy levels relevant for a scanning tunneling microscope (STM).

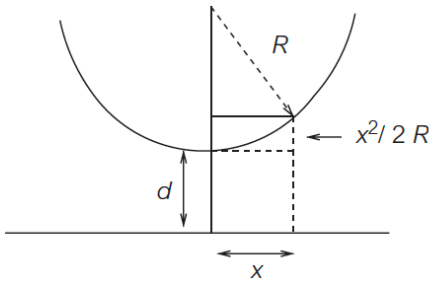
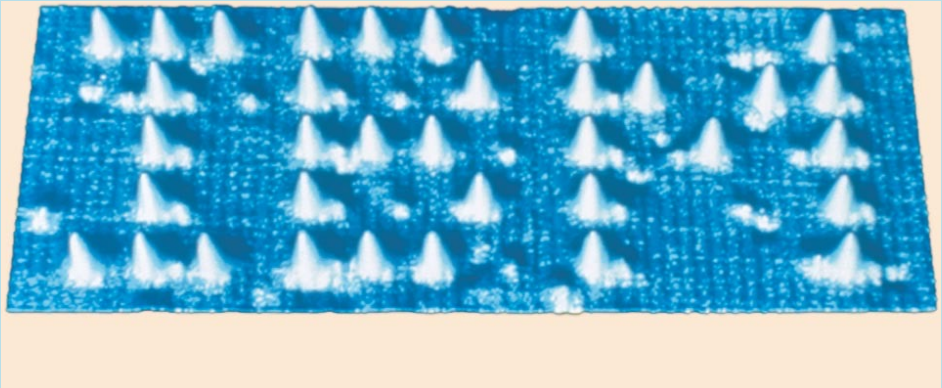


Figure 11.15. Typical geometry of the tip of an STM probe.

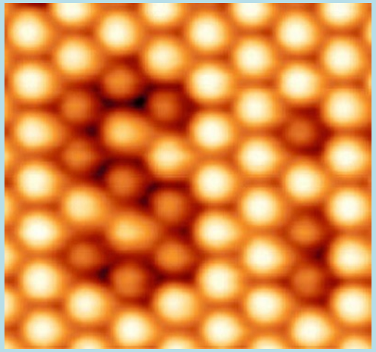
An estimate of the lateral resolution possible with this instrument can be made by assuming a simple shape for the STM tip probe as in Fig. 11.15. Assuming a parabolic probe with radius of curvature R of say 1000 Å, one finds a current profile as a function of distance away from the closest point d given by

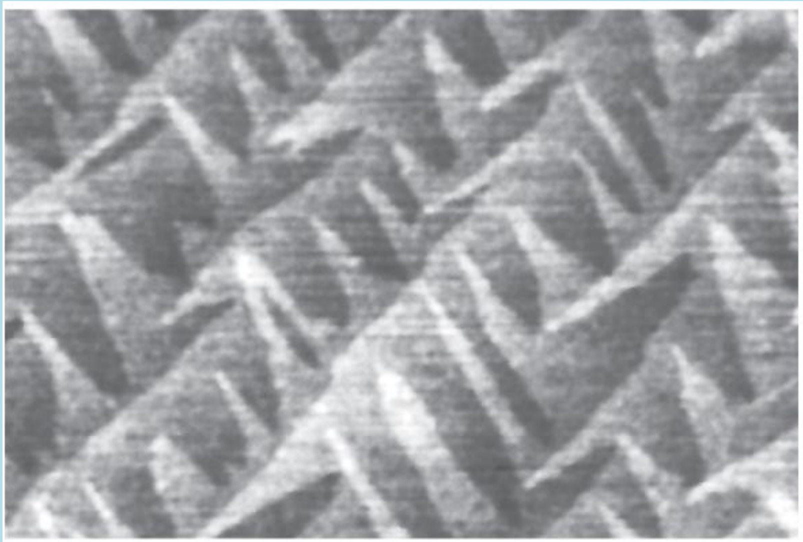
$$I(x) \propto e^{-2(d+x^2/2R)\kappa} \quad \propto \quad e^{-x^2\kappa/R} \quad \propto \quad e^{-x^2/\rho^2} \tag{11.52}$$

where $\rho \equiv \sqrt{R/\kappa}$; typically $\kappa \approx \sqrt{2mW/\hbar^2} \approx 1\,\text{Å}^{-1}$. This familiar Gaussian distribution has a spread in lateral position given by $\Delta x = \rho/\sqrt{2} \approx 20\,\text{Å}$. As mentioned above, even smaller tip sizes are possible, but because of the exponential sensitivity of the tunneling current to the tip-to-surface distance d, it can well be the case that the best images arise from the tunneling from a very few surface atoms forming an atomic-scale 'dimple' closest to the surface.

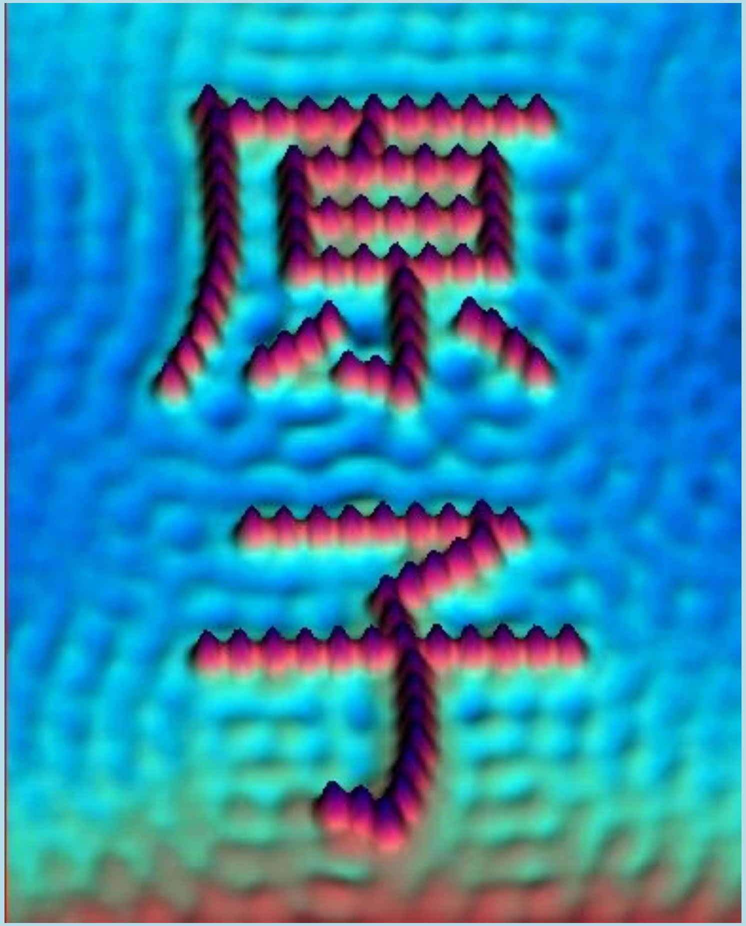


Xenon Atoms



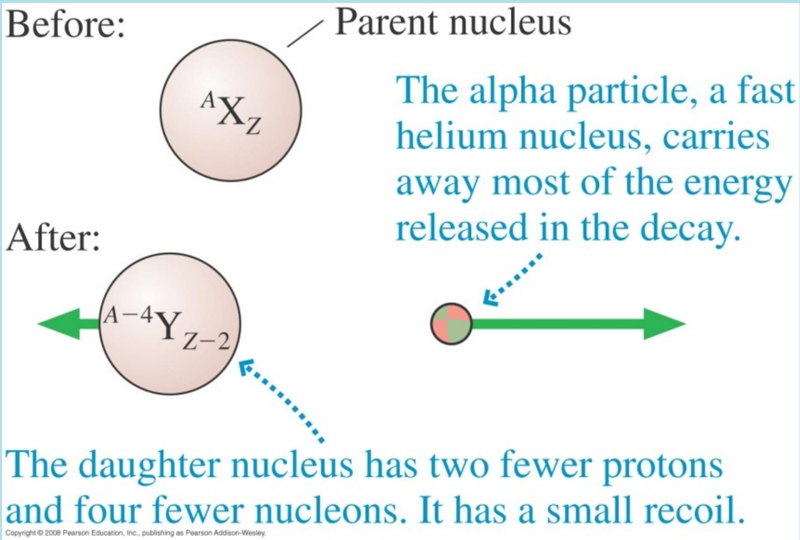


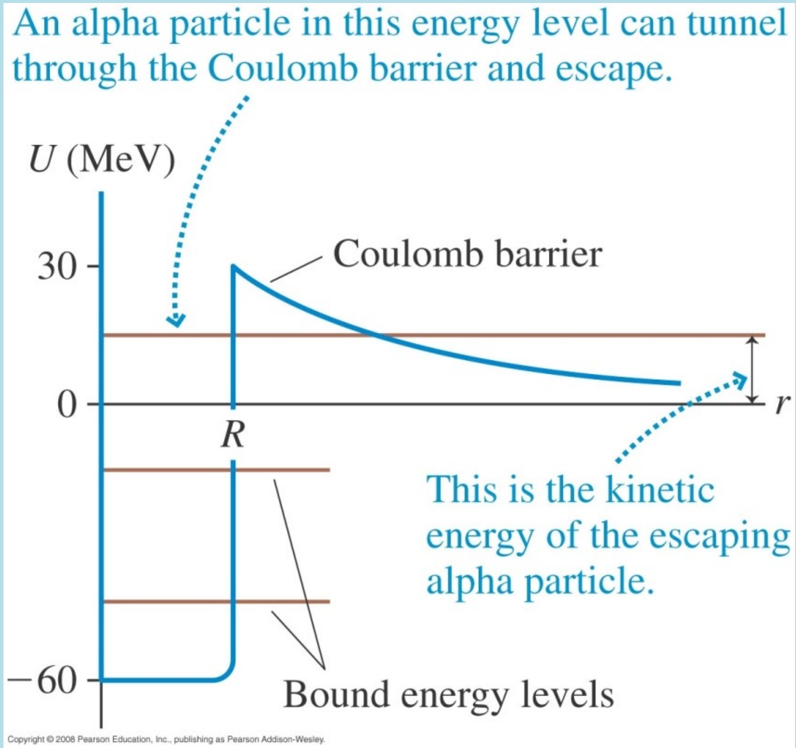
The surface of silicon



原子核的 α 衰變

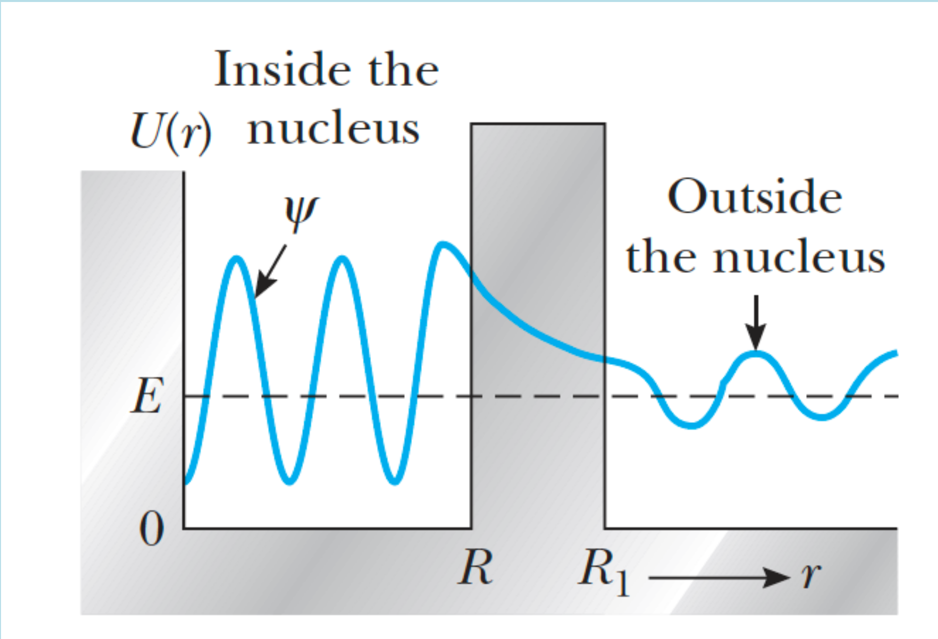
原子核的α衰變，可以將衰變原子核，看成α粒子與產物原子核的束縛態。
吸引的核力很強，對應很深的位能，但只有短距$r < R$。
長距$r > R$，位能則由排斥的庫倫位能取代。

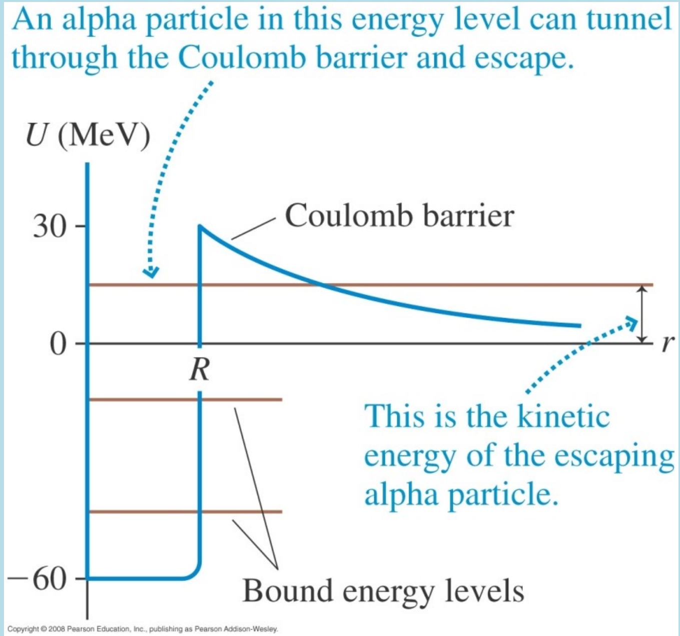




α粒子可以透過量子穿隧效應，自發地穿透放射離開。

因為是量子效應，因此發生的可能是由機率控制！





tunneling. In this process, a heavy nucleus decays to a lighter one by the emission of an α-particle, that is, the nucleus He^4. Using a compact notation, the process can be written as

$$ {}^{Z}_{N}X^{A} \longrightarrow {}^{(Z-2)}_{(N-2)}Y^{(A-4)} + {}^{2}_{2}\mathrm{He}^{4} \tag{11.53} $$

where Z, N, and A are, respectively, the numbers of protons, neutrons, and total nucleons in the nuclear species denoted by X (the "parent") or Y (historically the "daughter" nucleus).

Because this is a two-body decay, the energy of the emitted α is determined uniquely from conservation of energy and momentum, and can be calculated from a knowledge of the masses of the parent and daughter nuclear species. For the nuclei for which α-decay is an important decay mechanism, the range in numerical values for the appropriate dimensionful parameters in the problem is not very large,

$$ R \sim 2\text{–}4\, F, \quad E_\alpha \sim 2\text{–}8\, MeV, \quad \text{and} \quad Z \sim 50\text{–}100 \tag{11.54} $$

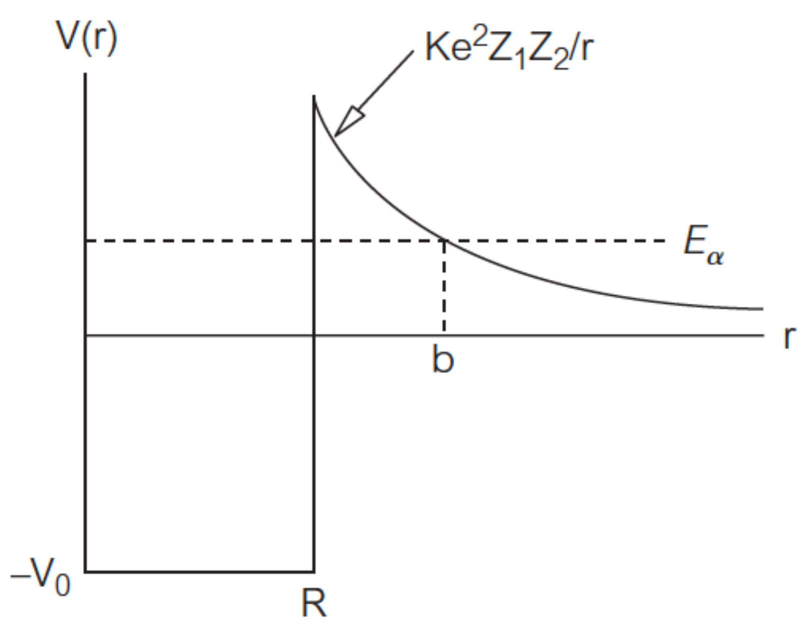
while the observed lifetimes have been measured over an incredibly large range

$$ \tau \sim 10^{17}\,\mathrm{s} - 10^{-12}\,\mathrm{s} \tag{11.55} $$

A simple model for this process assumes that the α-particle moves in the potential of the *daughter* nucleus, modeled by a combination of an attractive square well (as in Section 8.2), along with the mutual Coulomb repulsion. This can be written as

$$V(r) = \begin{cases} -V_0 & \text{for } r < R \\ Z_1 Z_2 K e^2/r & \text{for } R < r \end{cases} \tag{11.56}$$

We would then take $Z_1 = Z_\alpha = 2$ and $Z_2 = Z - 2$ where Z is the charge of the *parent* nucleus. This potential is illustrated in Fig. 11.16 and the α-particle is assumed to have positive energy E_α equal, to its observed final kinetic energy; the model pictures the α-particle as "rattling around" inside the nucleus with a small (exponentially so) quantum tunneling probability of escaping each time it "hits" the Coulomb barrier. The tunneling probability for this process is then



it "hits" the Coulomb barrier. The tunneling probability for this process is then given from Eqn. (11.49) by

$$P_T = \exp\left[-2\sqrt{\frac{2\mu}{\hbar^2}}\int_a^b dr\sqrt{\frac{Z_1 Z_2 K e^2}{r} - E}\right] = e^{-2G} \tag{11.57}$$

where the factor in the exponential (G) is known as the *Gamow factor*. The classical turning points are taken to be

$$a = R \quad \text{and} \quad b = \frac{Z_1 Z_2 K e^2}{E_\alpha} \tag{11.58}$$

and we have used the reduced mass μ as is appropriate for a two-body problem; since the daughter nucleus is much heavier than the α-particle, however, one has $\mu \approx m_\alpha$. The Gamow factor can be written in the form

$$G = Z_1 Z_2 \alpha \sqrt{\frac{2\mu c^2}{E_\alpha}} \int_{\omega^2}^1 d\eta \sqrt{\frac{1}{\eta} - 1} \tag{11.59}$$

where $\alpha = Ke^2/\hbar c$ as always and $\omega^2 \equiv R/b$. The integral can be done in closed form giving

$$\int_{\omega^2}^1 d\eta \sqrt{\frac{1}{\eta} - 1} = \frac{\pi}{2} - \sin^{-1}(\omega) - \sqrt{\omega^2(1-\omega^2)}$$

$$\downarrow$$

$$\frac{\pi}{2} \text{ for } \omega = \sqrt{b/R} << 1 \tag{11.60}$$

One then has very roughly that

$$2G \approx 4\frac{(Z-2)}{\sqrt{E_\alpha(\text{MeV})}} \tag{11.61}$$

The decay *lifetime* itself can be estimated by noting that there is roughly an e^{-2G} probability of a tunneling "escape" every time the α "hits" the electrostatic barrier. The time between such 'escape attempts' can be approximated as

$$T_0 \approx \frac{2R}{v_\alpha} \quad \text{where} \quad v_\alpha \approx \sqrt{\frac{2E_\alpha}{m_\alpha}} \approx \frac{1}{20}\,c \tag{11.62}$$

and $R \approx 5$–$8\,F$ is a typical (heavy) nuclear radius; this gives $T_0 \approx 10^{-21}$ s, which is indeed a typical nuclear reaction time. The lifetimes in this simple picture then scale as

$$\tau = T_0 e^{+2G} \quad \text{or} \quad \log(\tau) \approx \log(T_0) + 4\frac{(Z-2)}{\sqrt{E_\alpha(\text{MeV})}} \tag{11.63}$$

This behavior is most easily studied by examining the α-decay lifetimes of different isotopes of the same element (so that the value of Z is fixed and only E_α varies). We plot the lifetimes for several such series (on a log scale) versus $1/\sqrt{E_\alpha}$ in Fig. 11.17 (a so-called *Geiger–Nuttall* plot) and note the reasonable straight line fits. The simple approximations made here can be refined,[4] but they provide convincing evidence for the importance of quantum tunneling effects in nuclear decay processes.

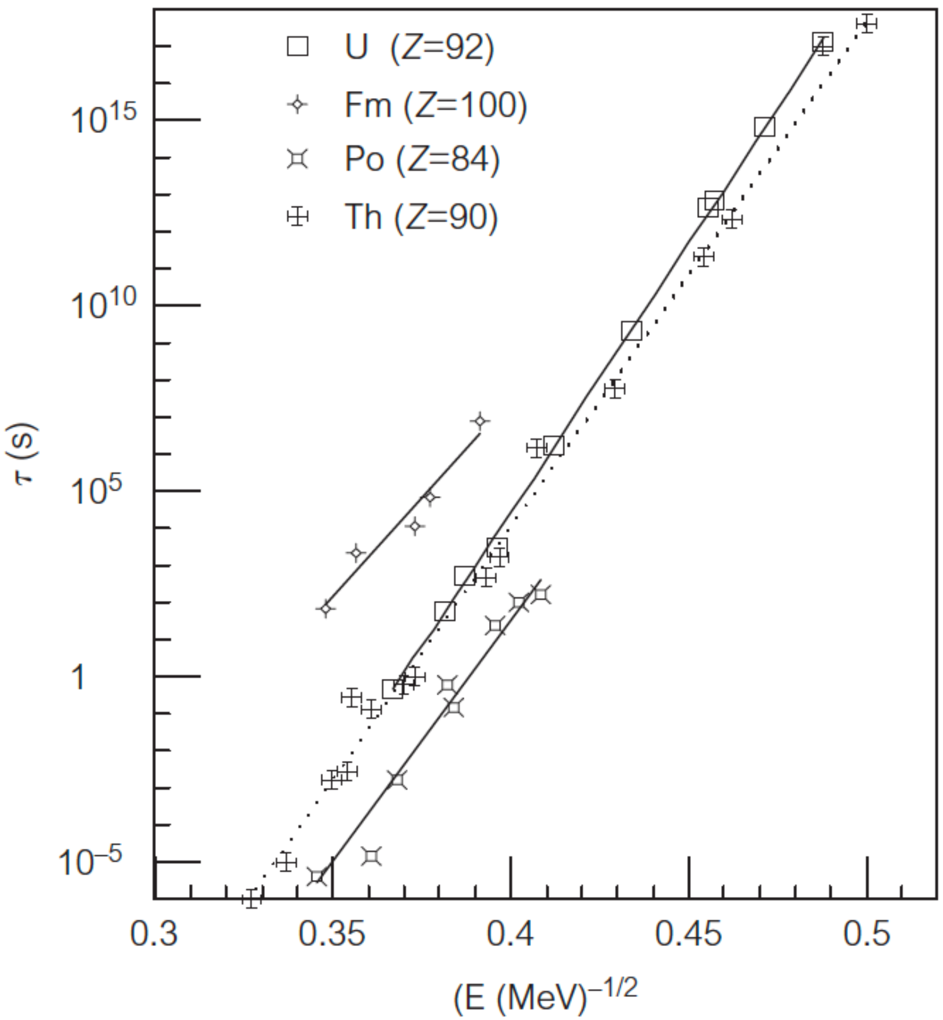


Figure 11.17. Semilog plot of α-decay lifetime (τ in seconds) versus $1/\sqrt{E_\alpha}$ (in MeV) for four different radioactive decay series, the so-called Geiger–Nutall plot. The data are taken from a recent edition of the Chart of the Nuclides (Walker (1983).)

$$\tau = T_0 e^{+2G} \quad \text{or} \quad \log(\tau) \approx \log(T_0) + 4\frac{(Z-2)}{\sqrt{E_\alpha(\text{MeV})}} \tag{11.63}$$

Tunneling is important in nuclear physics. Nuclei are very complicated objects, but under certain circumstances it is appropriate to view nucleons as independent particles occupying levels in a potential well. With this picture in mind, the decay of a nucleus into an α-particle (a He nucleus with $Z = 2$) and a daughter nucleus can be described as the tunneling of an α-particle through a barrier caused by the Coulomb potential between the daughter and the α-particle (Fig. 4B-1). The α-particle is not viewed as being in a bound state: if it were, the nucleus could not decay. Rather, the α-particle is taken to have positive energy, and its escape is only inhibited by the existence of the barrier.[1]

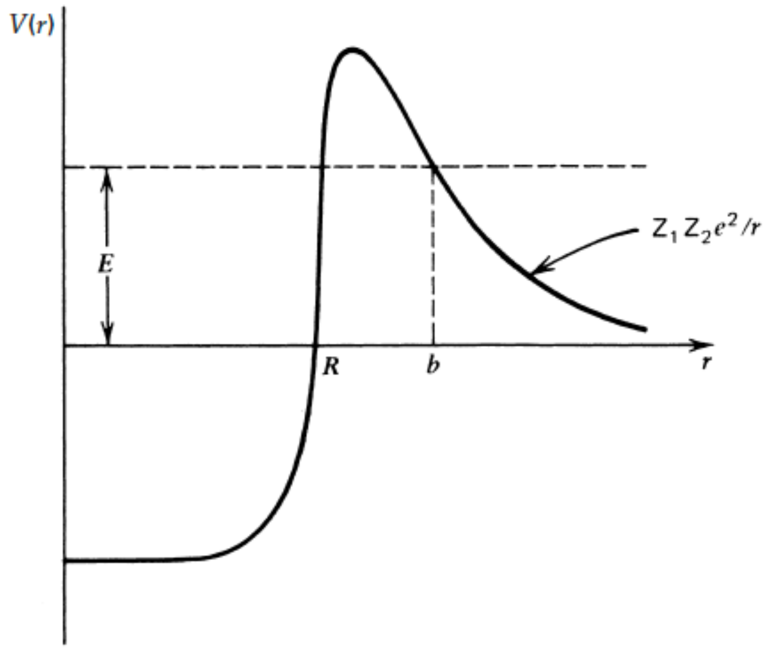


Figure 4B-1 Potential barrier for α decay.

If we write

$$|T|^2 = e^{-G} \tag{4B-1}$$

then

$$G = 2\left(\frac{2m}{\hbar^2}\right)^{1/2} \int_R^b dr \sqrt{\frac{Z_1 Z_2 e^2}{4\pi\varepsilon_0 r} - E} \tag{4B-2}$$

where R is the nuclear radius[2] and b is the turning point, determined by the vanishing of the integrand (4B-2); Z_1 is the charge of the daughter nucleus, and Z_2 (= 2 here) is the charge of the particle being emitted. The integral can be done exactly

$$\int_R^b dr\left(\frac{1}{r} - \frac{1}{b}\right)^{1/2} = \sqrt{b}\left[\cos^{-1}\left(\frac{R}{b}\right)^{1/2} - \left(\frac{R}{b} - \frac{R^2}{b^2}\right)^{1/2}\right] \tag{4B-3}$$

At low energies (relative to the height of the Coulomb barrier at $r = R$), we have $b \gg R$, and then

$$G = \frac{2}{\hbar}\left(\frac{2mZ_1Z_2e^2b}{4\pi\varepsilon_0}\right)^{1/2}\left[\frac{\pi}{2} - \sqrt{\frac{R}{b}}\right] \tag{4B-4}$$

with $b = Z_1Z_2e^2/4\pi\varepsilon_0 E$. If we write for the α-particle energy $E = mv^2/2$, where v is its final velocity, then

$$G = \frac{2\pi Z_1 Z_2 e^2}{4\pi\varepsilon_0 \hbar v} = 2\pi\alpha Z_1 Z_2\left(\frac{c}{v}\right) \tag{4B-5}$$

The time taken for an α-particle to get out of the nucleus may be estimated as follows: the probability of getting through the barrier on a single encounter is e^{-G}. Thus the number of encounters needed to get through is $n \simeq e^G$. The time between encounters is of the order of $2R/v$, where R is again the nuclear radius, and v is the α velocity inside the nucleus. Thus the lifetime is

$$\tau \simeq \frac{2R}{v} e^G \tag{4B-6}$$

The velocity of the α inside the nucleus is a rather fuzzy concept, and the whole picture is very classical, so that the factor in front of the e^G cannot really be predicted without a much more adequate theory. Our considerations do give us an order of magnitude for it. For a 1-MeV α-particle,

$$v = \sqrt{\frac{2E}{m}} = c\sqrt{\frac{2E}{mc^2}} = 3 \times 10^8 \sqrt{\frac{2}{4 \times 940}} \simeq 7.0 \times 10^6 \text{ m/s}$$

so that one predicts, for low energy α's, the straight-line plot

$$\log_{10}\frac{1}{\tau} \simeq \text{const} - 1.73\,\frac{Z_1}{\sqrt{E(\text{MeV})}} \tag{4B-7}$$

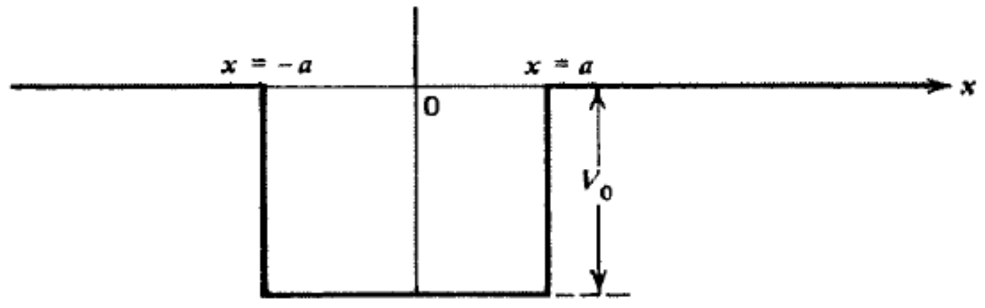
with the constant in front of the order of magnitude 27–28 when τ is measured in years instead of seconds. A large collection of data shows that a good fit to the lifetime data is obtained with the formula

$$\log_{10}\frac{1}{\tau} = C_2 - C_1\frac{Z_1}{\sqrt{E}} \tag{4B-8}$$

Here $C_1 = 1.61$ and C_2 lying between 55 and 62. The exponential part of the fit differs slightly from our derivation, but given the simplicity of our model, the agreement has to be rated as good.

For larger α energies, the G factor depends on R, and with $R = r_0A^{1/3}$, one finds that r_0 is a constant—that is, that the notion of a Coulomb barrier taking over the role of the potential beyond the nuclear radius has some validity. Again, simple qualitative considerations explain the data.

有限位能井 Finite Potential Well

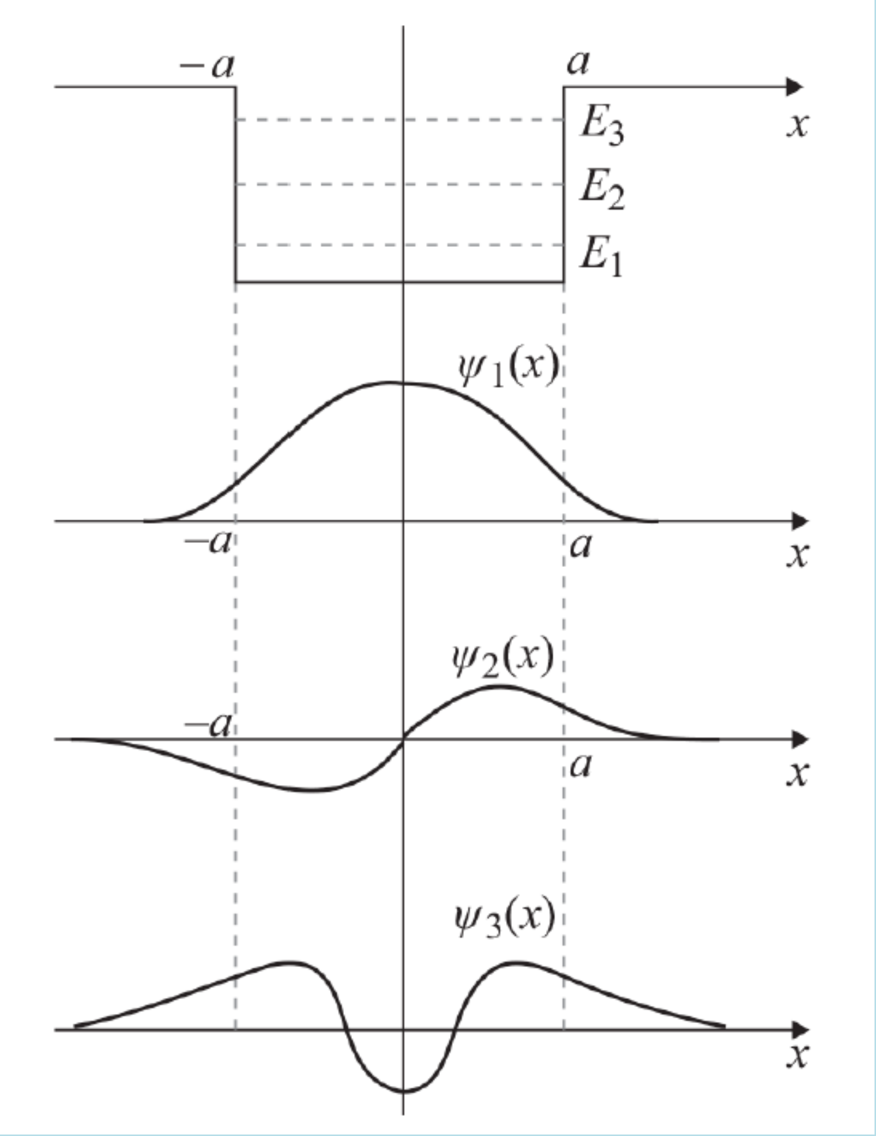


$$V(x) = 0 \qquad x < -a$$
$$= -V_0 \qquad -a < x < a$$
$$= 0 \qquad a < x$$

functions. To solve the Schrödinger equation, we have to examine how the equation looks in the various regions where the potential is constant and then use boundary conditions to match the solutions across the points where the potential is discontinuous. We have the equation

一維位能的問題有時可以分解為一段段常數位能的區域，可以分開求解。
然後在邊界處，以連續條件將得到的各個解聯(match)起來。

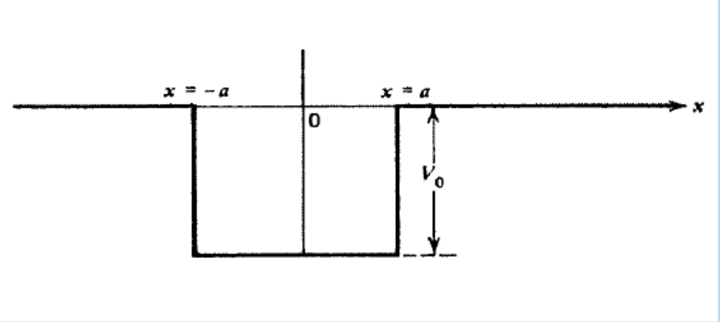
首先考慮$E < 0$，能量可能為離散的定態



在位能井內，電子如同自由粒子！

$-a < x < a$ 　　 $0 > E > V = -V_0$

在此區域古典的粒子可以存在。



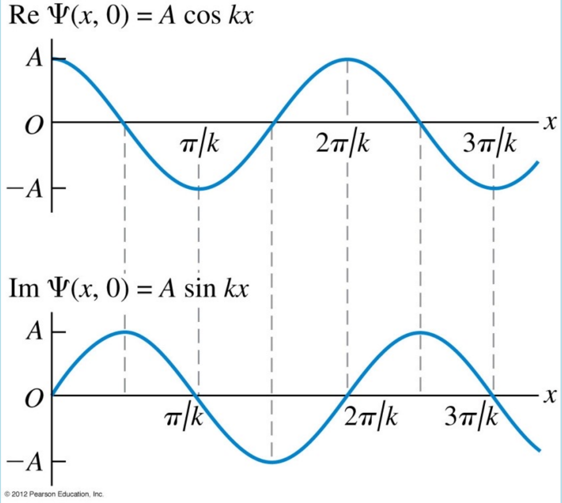
$$\frac{d^2\psi_E}{dx^2} = \frac{2m}{\hbar^2}[V - E]\psi_E = -\frac{2m}{\hbar^2}[V_0 - |E|]\psi_E$$

$$\frac{d^2\psi_E}{dx^2} = -q^2\psi_E \qquad q \equiv \sqrt{\frac{2m}{\hbar^2}(V_0 - |E|)}$$

解也如同自由粒子波！

$$\psi_E = C_1 e^{iqx} + C_2 e^{-iqx}$$

$$= A\cos qx + B\sin qx$$



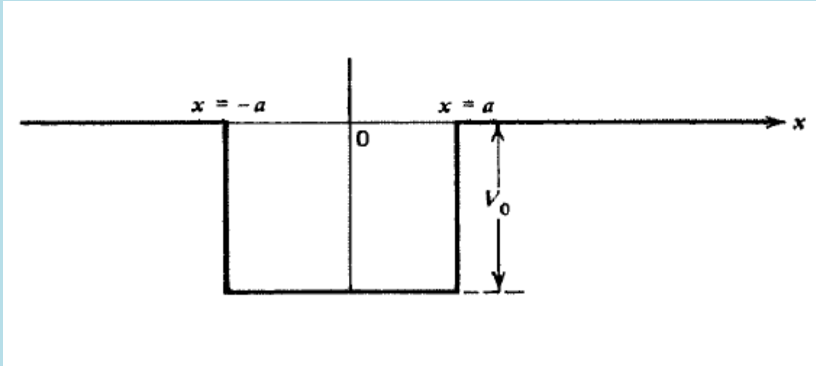
這兩個解分別是偶函數與奇函數。

可以分開考慮！

從偶函數開始： $\psi_E = A\cos qx$

在位能井外：

$x < -a,$ 及 $x > a$ $E < V = 0$



古典的粒子不能存在這樣的區域，

方程式差一個負號！

$$\frac{d^2\psi_E}{dx^2} = \alpha^2\psi_E \quad E)\psi_E \equiv \alpha^2\psi_E$$

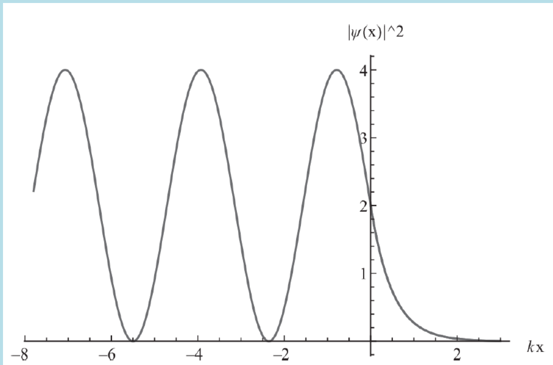
$$\alpha \equiv \sqrt{\frac{2m}{\hbar^2}|E|}$$

$$\psi_E(x) = C_1e^{\alpha x} + C_2e^{-\alpha x}$$

為使無限遠處，波函數不發散：

$x > a$ $\psi_E(x) = C_2e^{-\alpha x}$

$x < -a$ $\psi_E(x) = C_1e^{\alpha x}$



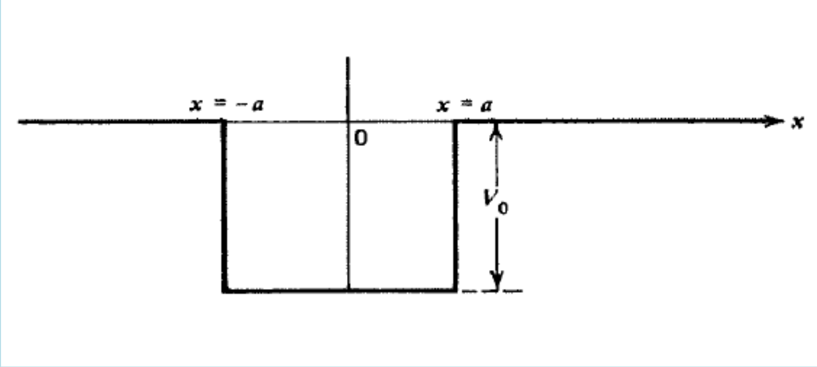
古典粒子不能存在，就表現在波函數指數遞減之上！

在量子力學中，此區域波函數還是有解，只是不再是正弦波，而是指數函數。

在位能井邊界上：

$x = -a$, 及 $x = a$

$\psi(x)$必須連續！



否則微分會是無限大，微分決定流量，不能是無限大。

先從偶函數開始討論：Even Function。

$x = a$

$\psi_E(x) = A\cos qx$

$\psi_E(x) = C_2 e^{-\alpha x}$

$A\cos qa = C_2 e^{-\alpha a}$

$x = -a$

$\psi_E(x) = A\cos qx$

$\psi_E(x) = C_1 e^{\alpha x}$

$A\cos qa = C_1 e^{-\alpha a}$

兩邊對稱，解是一樣的！只要考慮一邊即可。

$x = a$ $\psi(x)$與其微分都必須連續！

$\psi'_E(x) = -Aq\sin qx$

$\psi'_E(x) = -\alpha C_2 e^{-\alpha x}$

$Aq\sin qa = \alpha C_2 e^{-\alpha a}$

$$\alpha \equiv \sqrt{\frac{2m}{\hbar^2}|E|}$$

$\psi(x)$連續的條件：

$A\cos qa = C_2 e^{-\alpha a}$

$$q \equiv \sqrt{\frac{2m}{\hbar^2}(V_0 - |E|)}$$

兩式相除，即消去常數：

$q\tan qa = \alpha$

注意角波數q與α都是隨能量E變化的變數，而E是我們要由上式求解的對象。

角波數q，可轉為無單位的數值變數 y ：定義 $qa \equiv y$

$y\tan y = \alpha a$

另一個變數α可以用y表示出來，因為：

$$\alpha^2 + q^2 = \frac{2mV_0}{\hbar^2}$$

λ是常數！

$$\alpha a = \sqrt{\frac{2mV_0 a^2}{\hbar^2} - y^2} \equiv \sqrt{\lambda - y^2}$$

⬇

$y\tan y = \sqrt{\lambda - y^2}$

$$y\tan y = \sqrt{\lambda - y^2} \quad \Rightarrow \quad \tan y = \frac{\sqrt{\lambda - y^2}}{y}$$

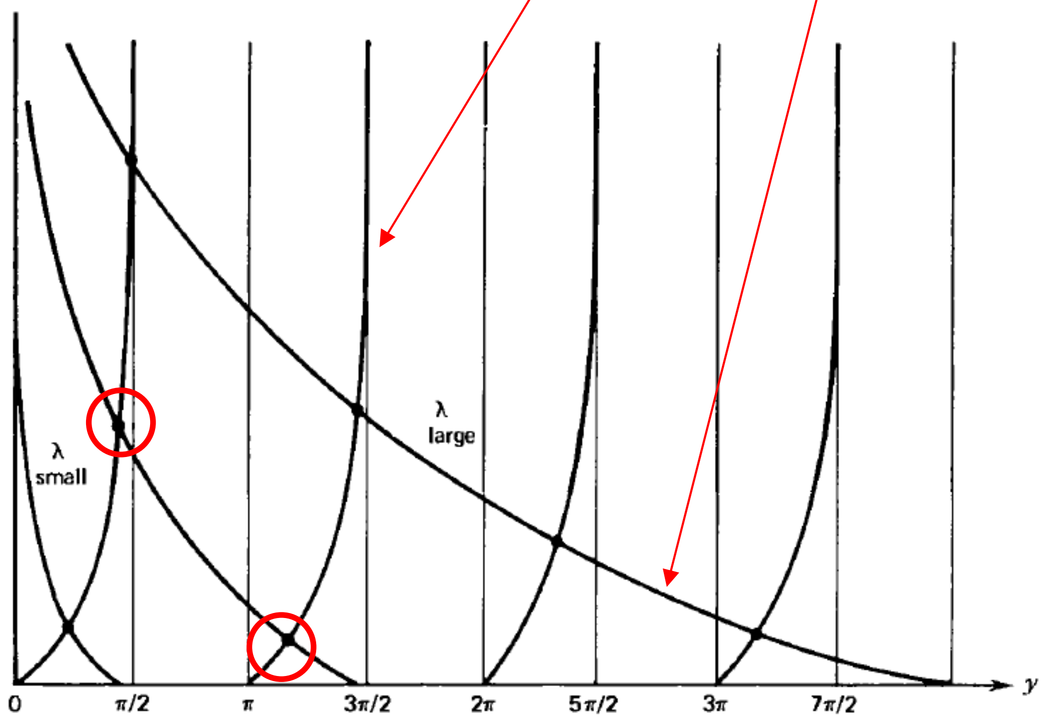


Figure 4-7 Location of discrete eigenvalues for even solutions in a square well. The rising curves represent tan y; the falling curves are $\sqrt{\lambda - y^2}/y$ for different values of λ.

$qa \equiv y$ 由y的解即得到q，也就得到E。

$x = a$ Odd Function

$$\psi_E(x) = A \sin qx$$

$$\psi_E'(x) = Aq \cos qx$$

$$\psi_E(x) = C_2 e^{-\alpha x}$$

$$\psi_E'(x) = -\alpha C_2 e^{-\alpha x}$$

$$\alpha \equiv \sqrt{\frac{2m}{\hbar^2}|E|}$$

$$q \equiv \sqrt{\frac{2m}{\hbar^2}(V_0 - |E|)}$$

$$A \sin qa = C_2 e^{-\alpha a}$$

$$Aq \cos qa = -\alpha C_2 e^{-\alpha a}$$

兩式相除，即消去常數：

$$q \cot qa = -\alpha$$

角波數q，可轉為無單位的數值變數 y ：定義 $qa \equiv y$

$$y \cot y = -\alpha a$$

另一個參數α可以用 y 表示出來，因為：

$$\alpha^2 + q^2 = \frac{2mV_0}{\hbar^2}$$

λ是常數！

$$\alpha a = \sqrt{\frac{2mV_0 a^2}{\hbar^2} - y^2} \equiv \sqrt{\lambda - y^2}$$

$$y \cot y = \sqrt{\lambda - y^2}$$

$$y\cot y = -\sqrt{\lambda - y^2} \quad \Rightarrow \quad -\cot y = \frac{\sqrt{\lambda - y^2}}{y}$$

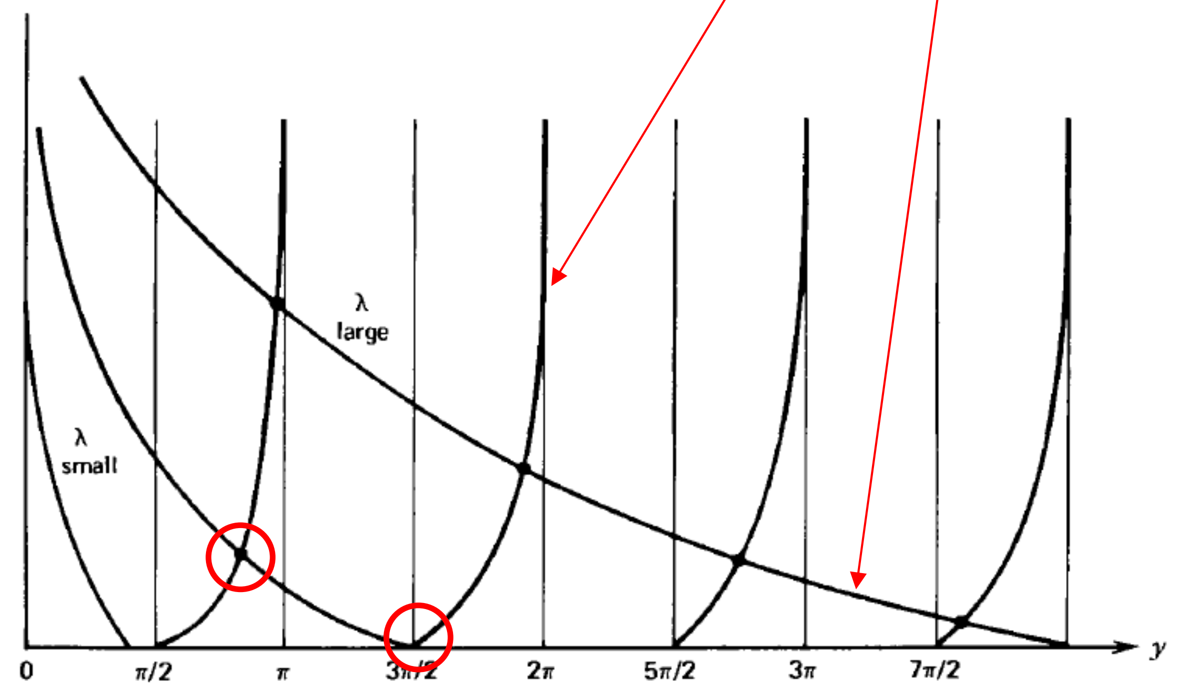
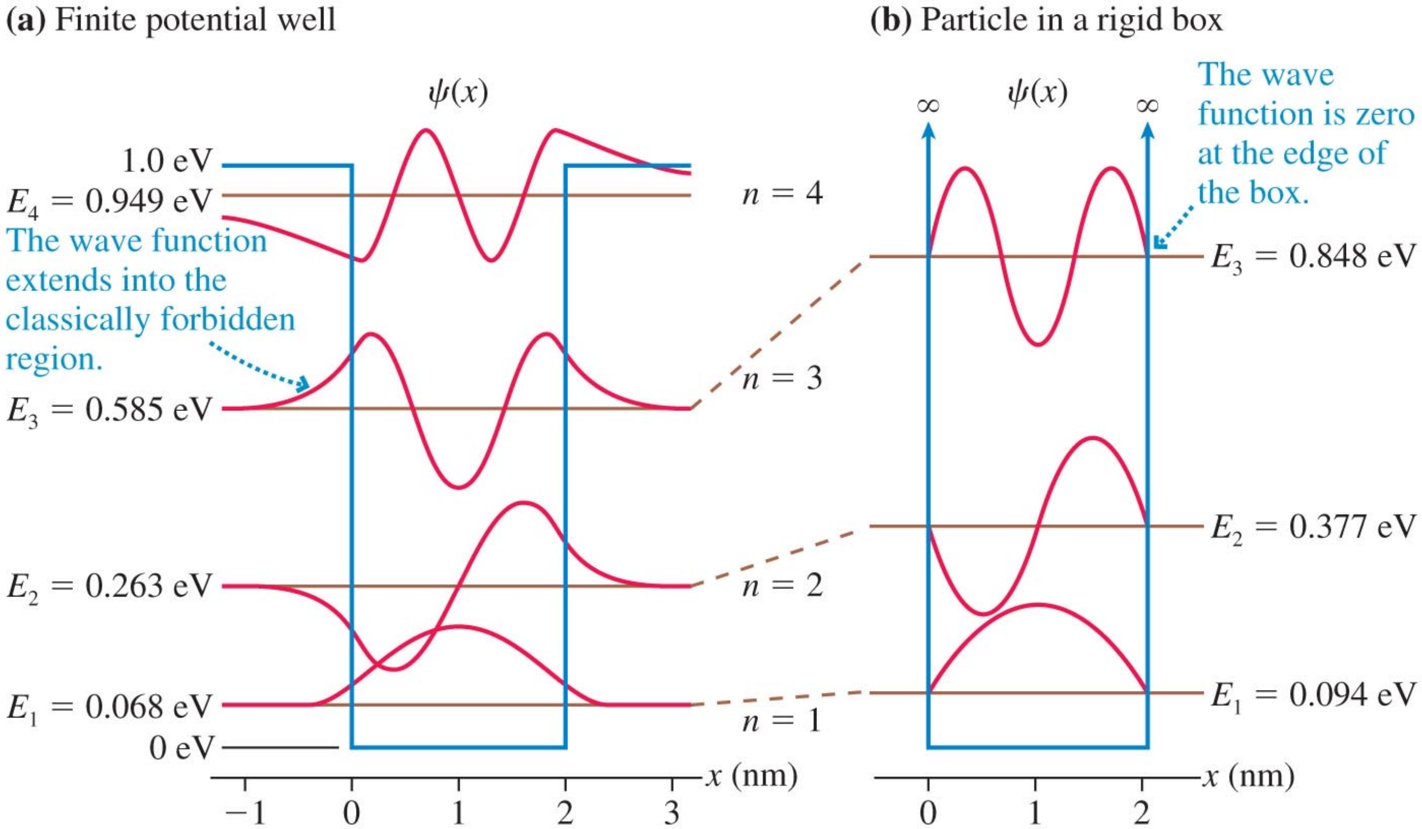
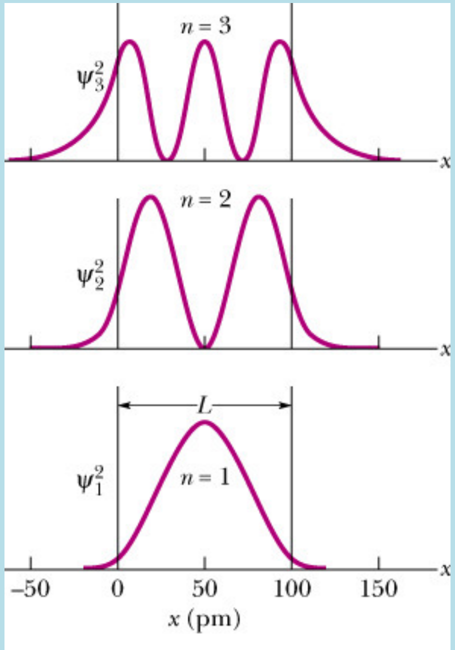


Figure 4-8 Location of discrete eigenvalues for odd solutions in a square well. The rising curves represent $-\cot y$; the falling curves are $\sqrt{\lambda - y^2}/y$ for different values of λ. Note that there is no eigenvalue for $\lambda < (\pi/2)^2$.

$qa \equiv y$　　由y的解即得到q，也就得到E。



(a) Finite potential well
(b) Particle in a rigid box
ψ(x)
1.0 eV
E4 = 0.949 eV
The wave function extends into the classically forbidden region.
E3 = 0.585 eV
E2 = 0.263 eV
E1 = 0.068 eV
0 eV
n = 4
n = 3
n = 2
n = 1
x (nm)
−1 0 1 2 3
∞
The wave function is zero at the edge of the box.
E3 = 0.848 eV
E2 = 0.377 eV
E1 = 0.094 eV
0 1 2



n = 3
ψ3²
n = 2
ψ2²
L
n = 1
ψ1²
x
–50 0 50 100 150
x (pm)

現在考慮$E > 0$，能量可能為連續的定態

在位能井內外，電子都如同自由粒子！

$E > V$

$x < -a$

$$\frac{d^2\psi_E}{dx^2} = -k_1^2\psi_E \qquad k_1 \equiv \sqrt{\frac{2m}{\hbar^2}E}$$

解如同自由粒子波！

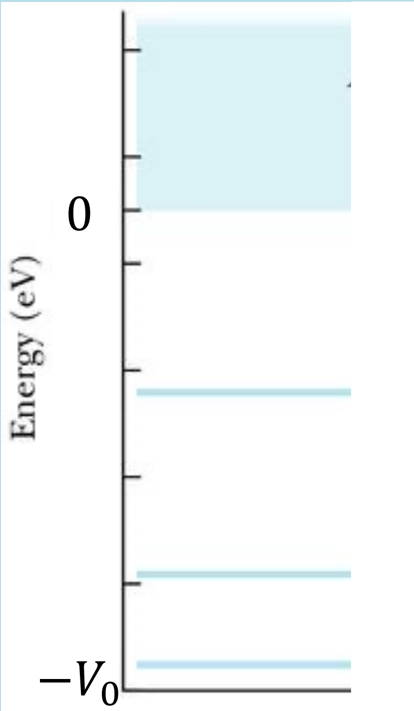
$$\psi_E = A_1 e^{ik_1x} + A_2 e^{-ik_1x}$$

$-a < x < a$

$$\frac{d^2\psi_E}{dx^2} = -k_2^2\psi_E \qquad k_2 \equiv \sqrt{\frac{2m}{\hbar^2}(V_0 + E)}$$

解也如同自由粒子波！

$$\psi_E = C_1 e^{ik_2x} + C_2 e^{-ik_2x}$$



任何的E都會有解，能階是連續的。這樣的定態，主要用於描述散射！

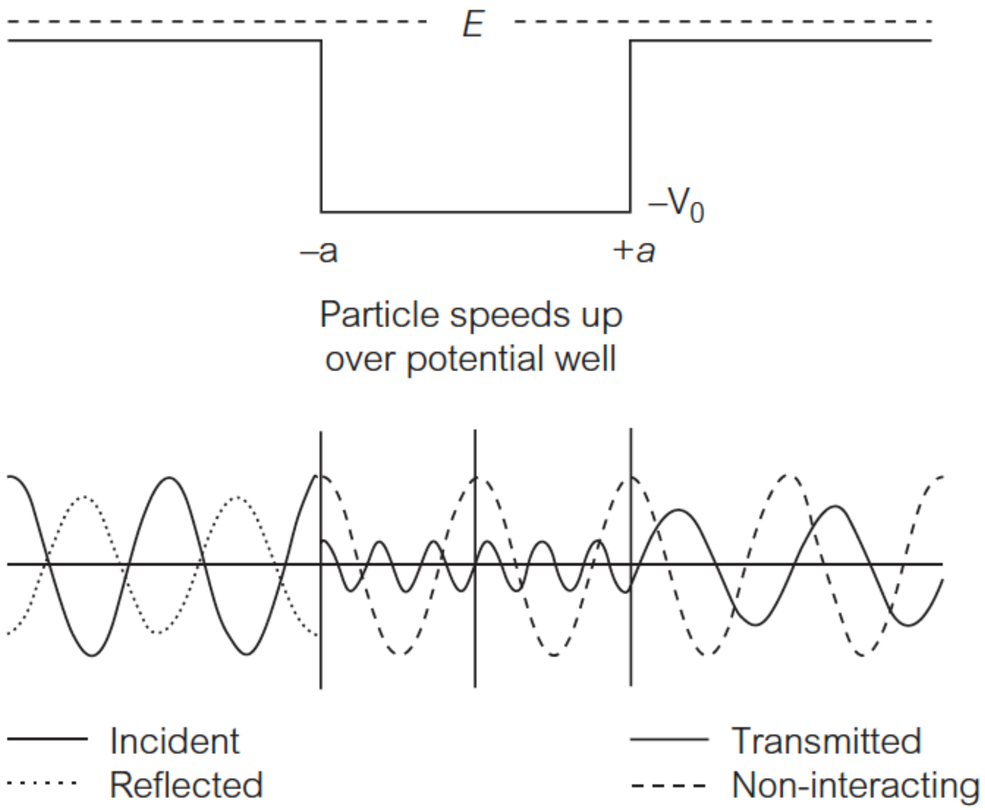
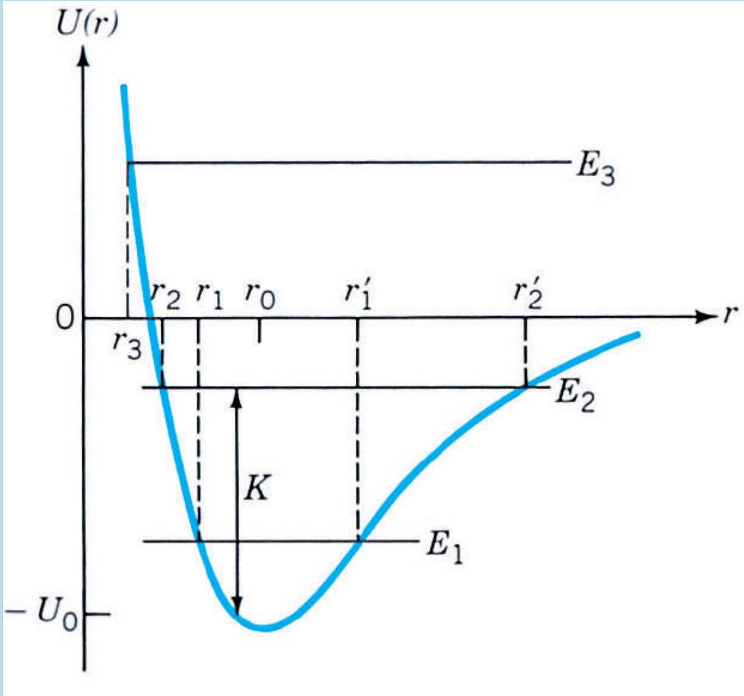


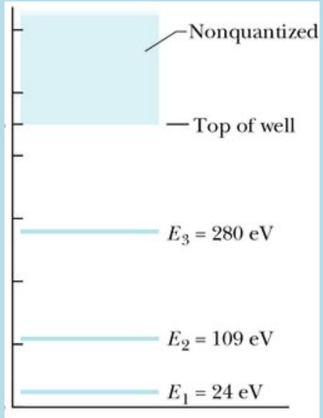
Figure 11.6. The real part of the incident, reflected, and transmitted plane wave solutions for a finite well. For $x < -a$ the dotted curve represents the reflected wave; for $x > -a$ the dashed curve simply continues the incident wave showing an unscattered wave for comparison.

Attractive Well

當位能在古典狀況下，使電子形成束縛態，本徵值E就不是連續，而是量子化的。

束縛態：運動範圍被限制於一個區域內，機械能小於無限遠處的位能



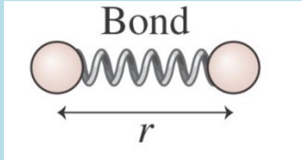


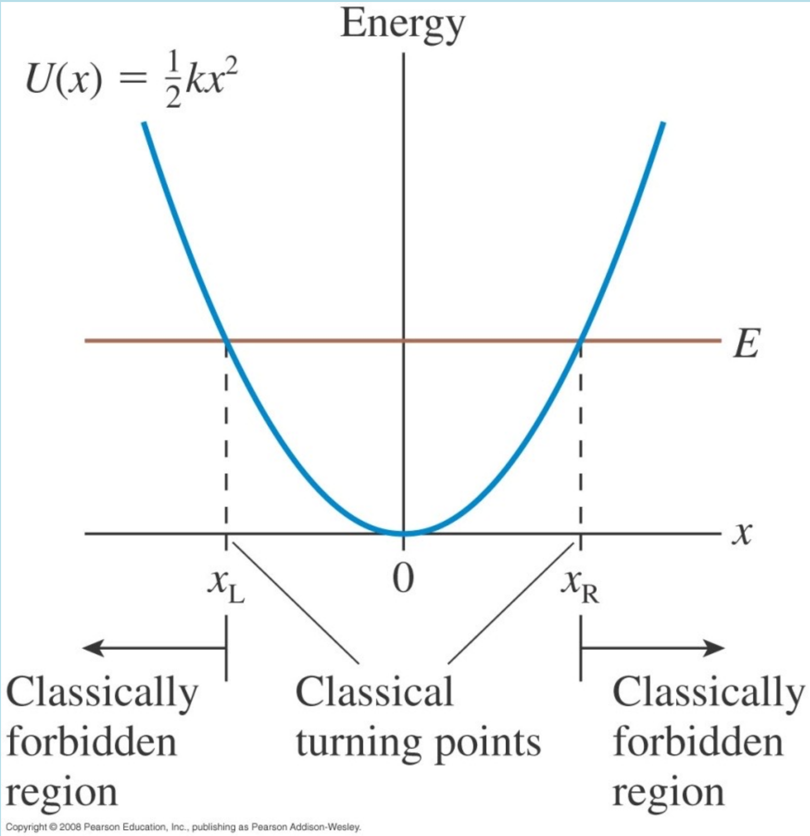
以此位能為例：$E < 0$ 束縛態，能量本徵值是量子化的

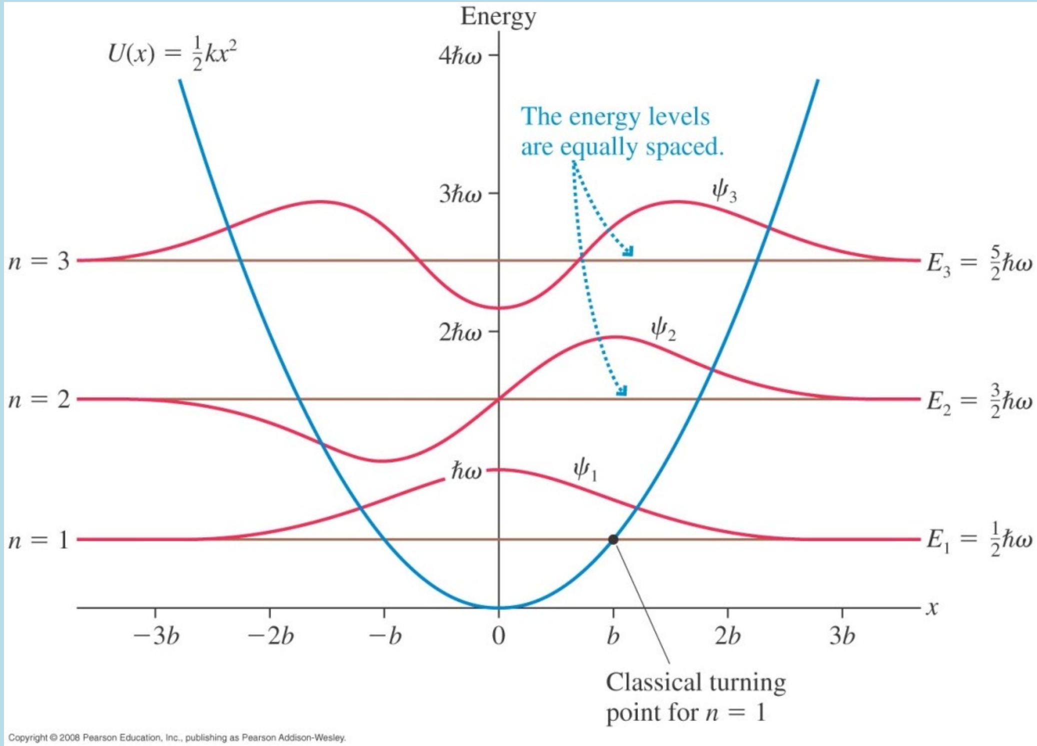
$E > 0$ 自由態，能量本徵值是連續的

簡諧振盪器、量子彈簧、古典完全是束縛態，預期定態能量完全量子化。

$$\frac{d^2\psi_E}{dx^2} = \frac{2m}{\hbar^2}\left(\frac{1}{2}kx^2 - E\right)\psi_E$$

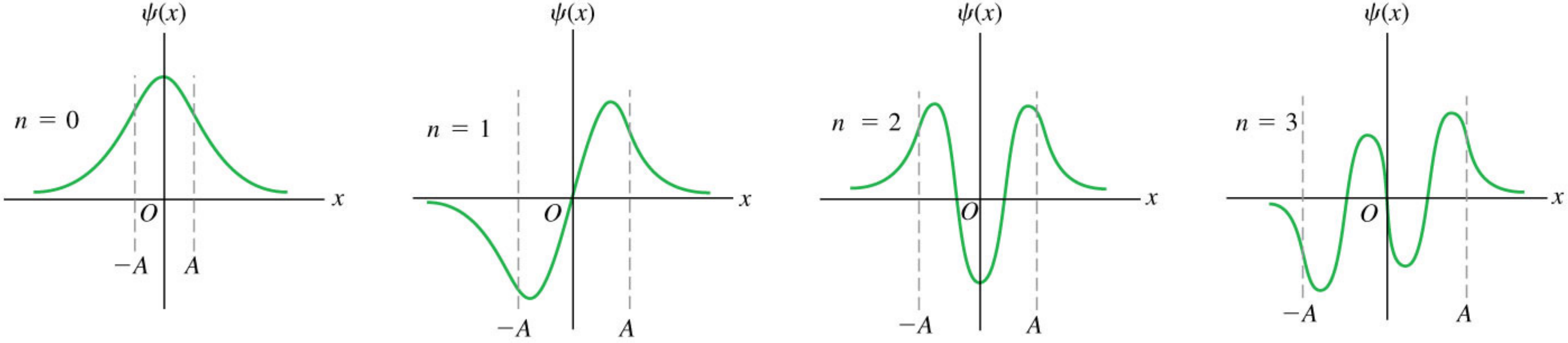


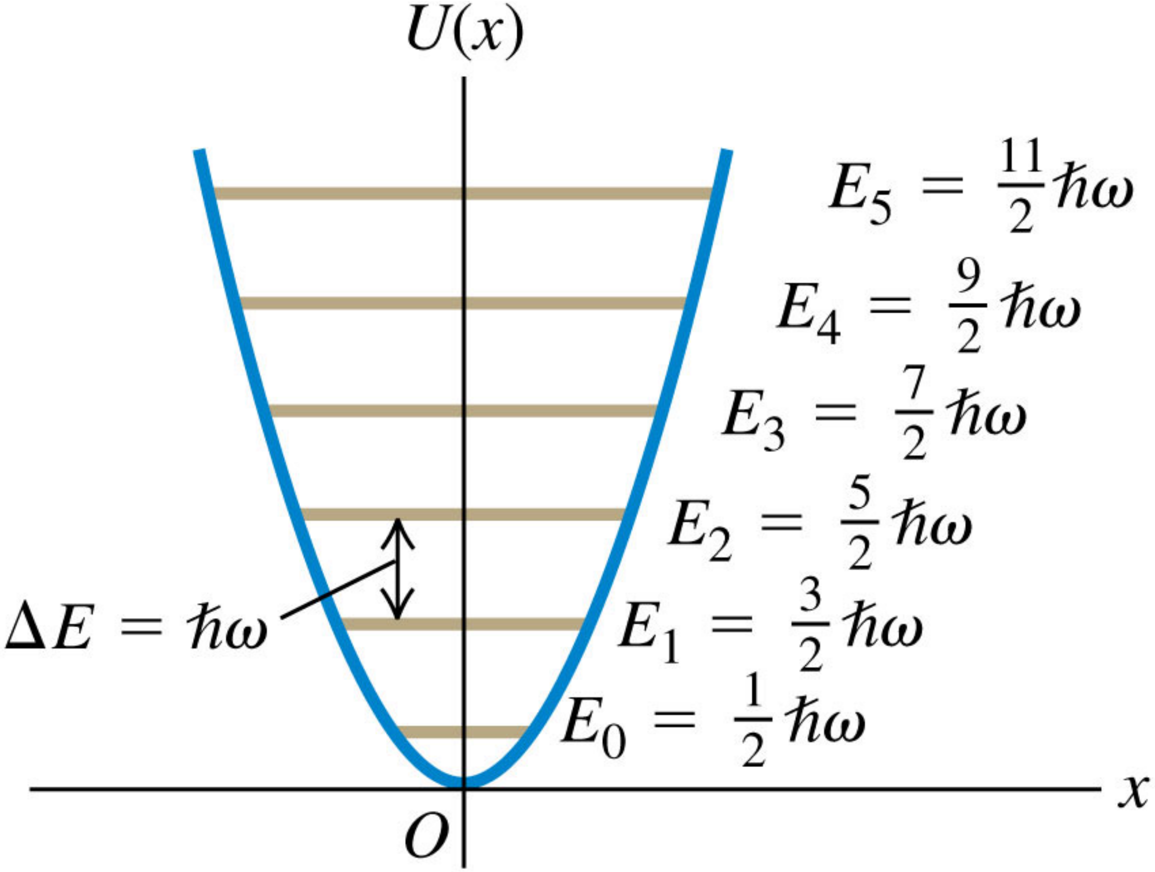


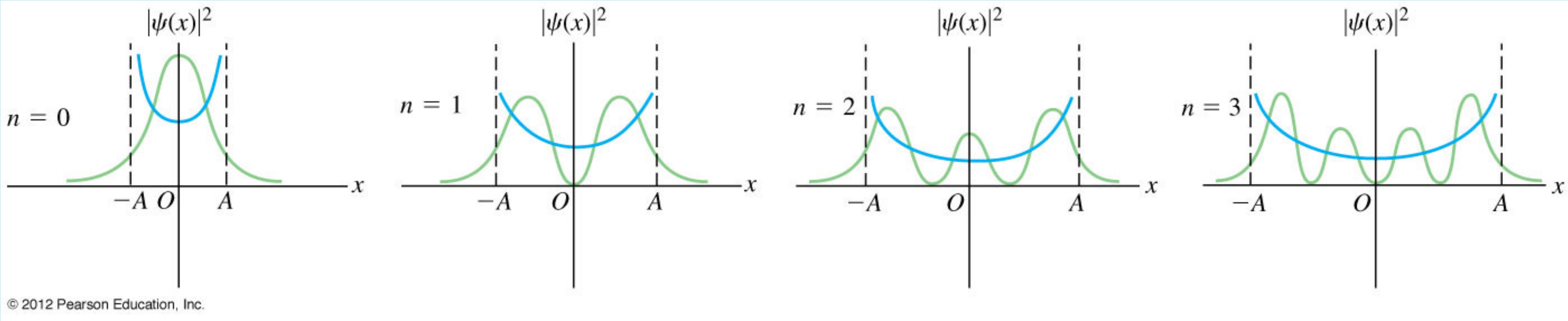


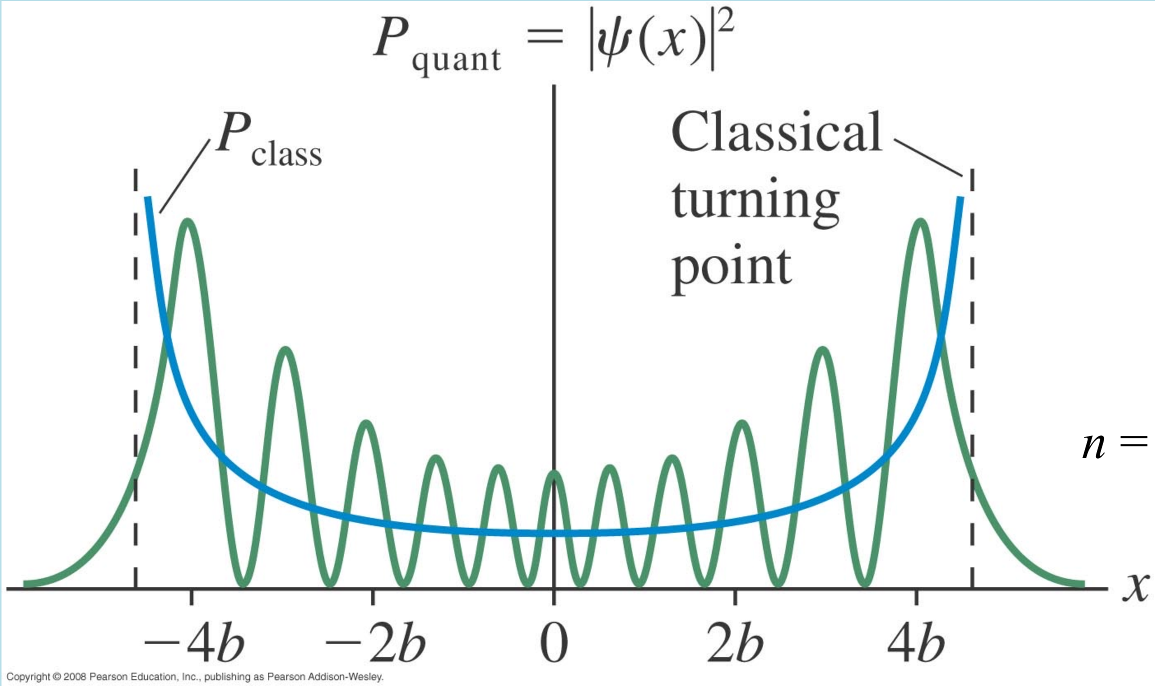
Energy is quantized

$$E_n = \left(n - \frac{1}{1}\right)\hbar\omega$$


ψ(x)
n = 0
n = 1
n = 2
n = 3
x
O
−A
A


U(x)
$E_5 = \frac{11}{2}\hbar\omega$
$E_4 = \frac{9}{2}\hbar\omega$
$E_3 = \frac{7}{2}\hbar\omega$
$E_2 = \frac{5}{2}\hbar\omega$
$E_1 = \frac{3}{2}\hbar\omega$
$E_0 = \frac{1}{2}\hbar\omega$
$\Delta E = \hbar\omega$
O
x

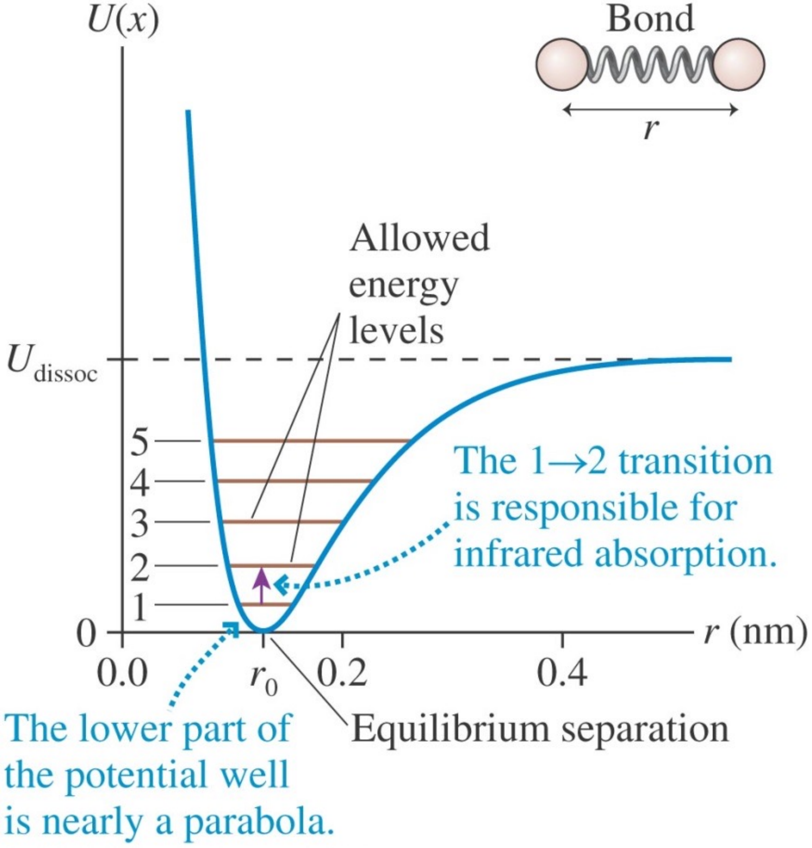


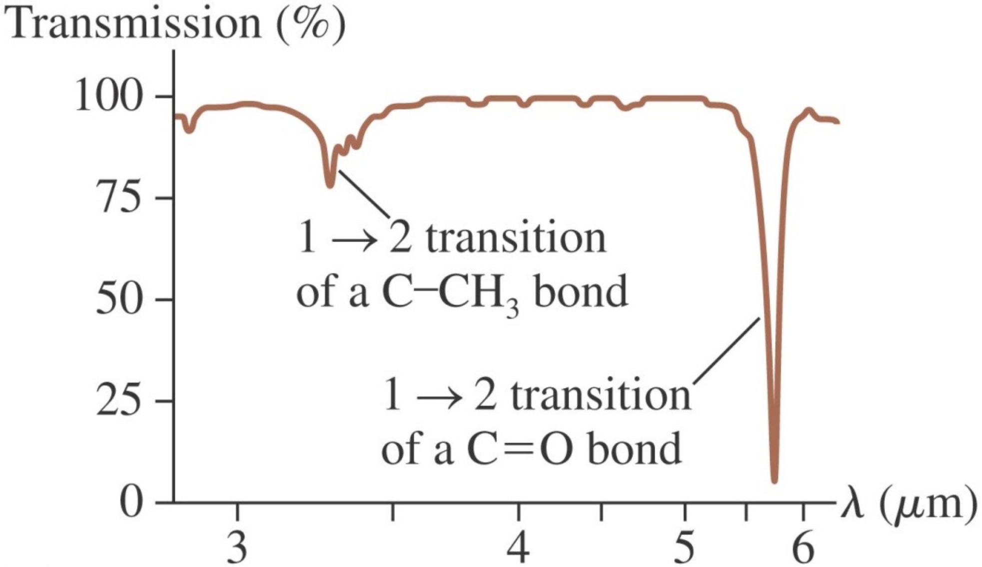


$n = 11$ State

For large n, the quantum probability is similar to the classical one.

Molecular Vibration





Delta Potential

是否有$E < 0$的解？

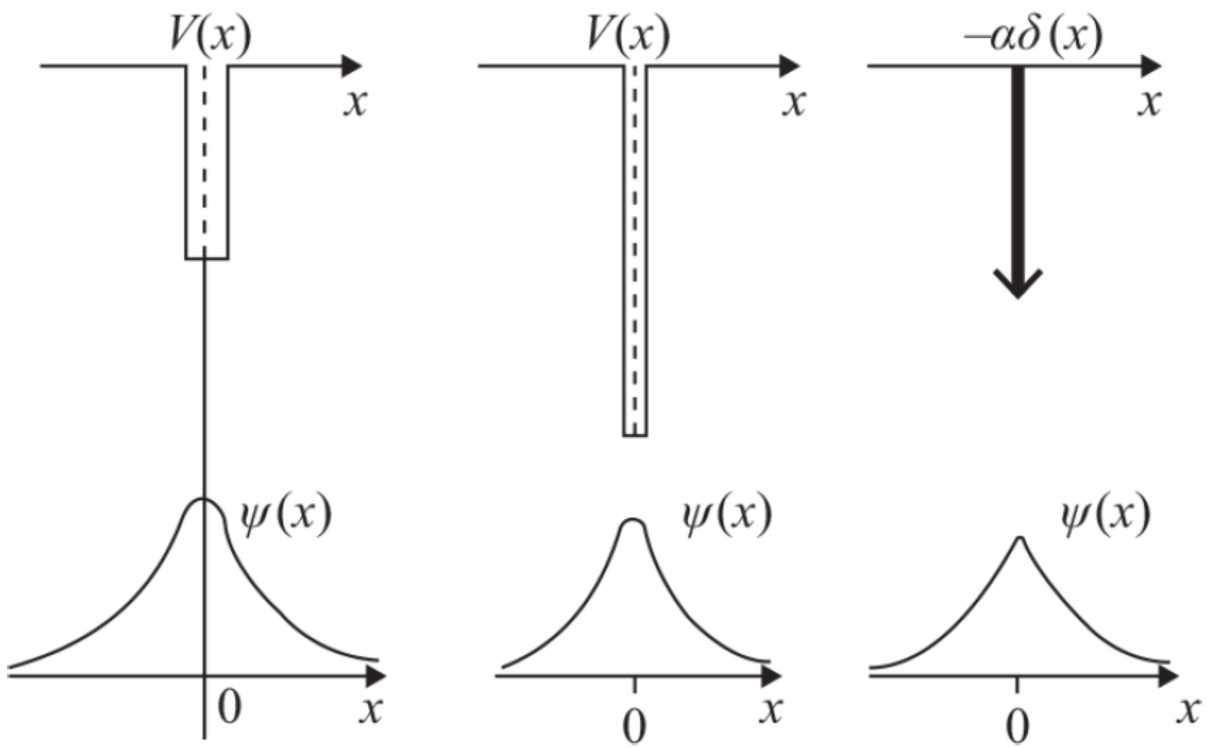
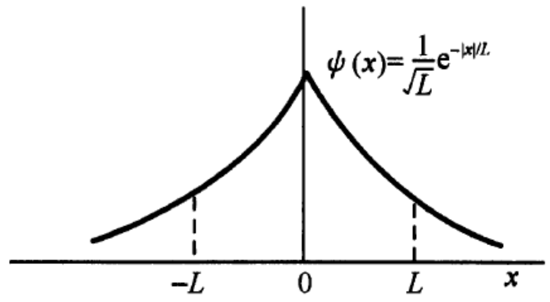


Figure 6.9
The delta function potential as the limit where the finite square well becomes narrower and deeper simultaneously. We expect to get a wave function with a discontinuous derivative.

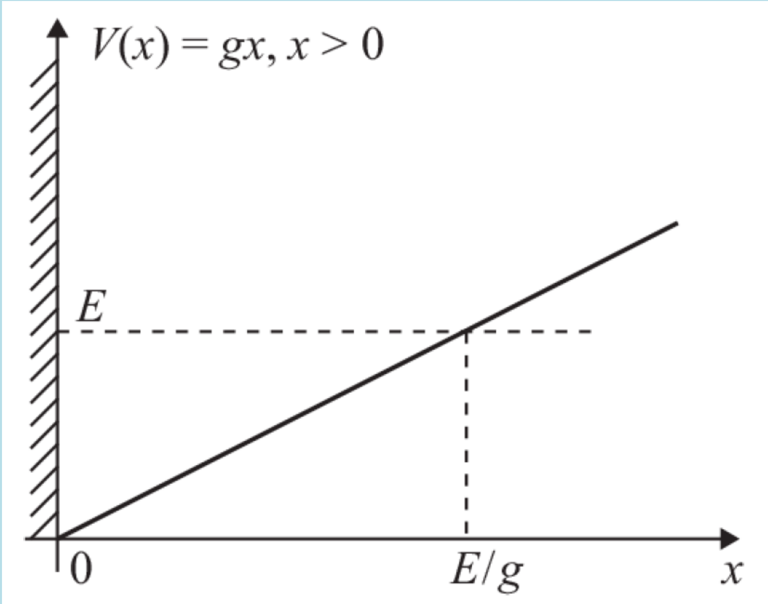


ψ'不連續。有一束縛態解。

$$\psi(x) = A e^{-\kappa|x|}.$$

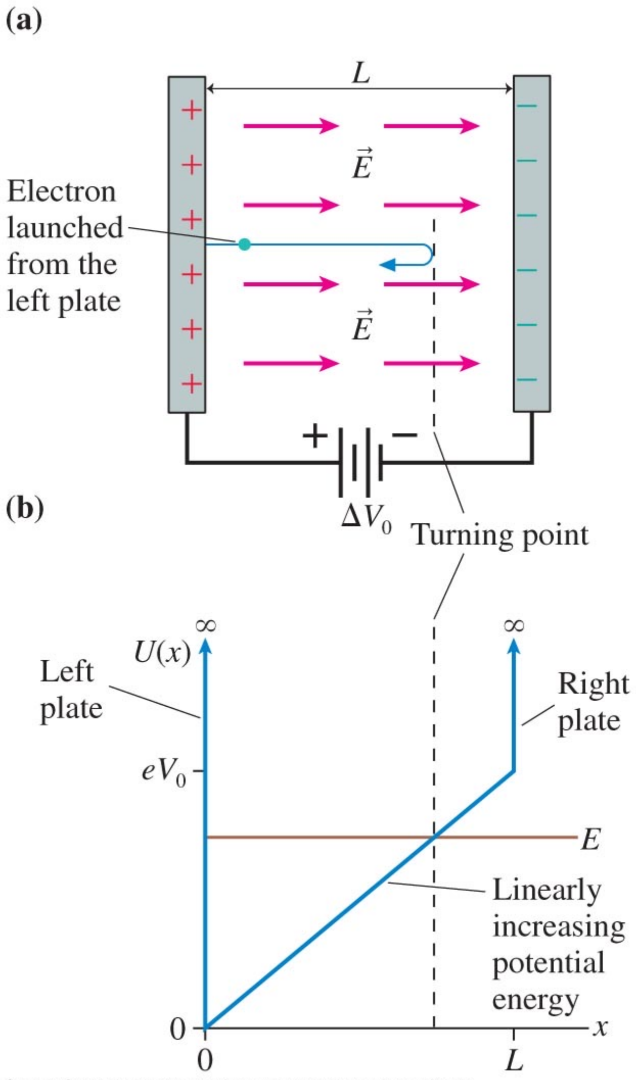
Linear Potential

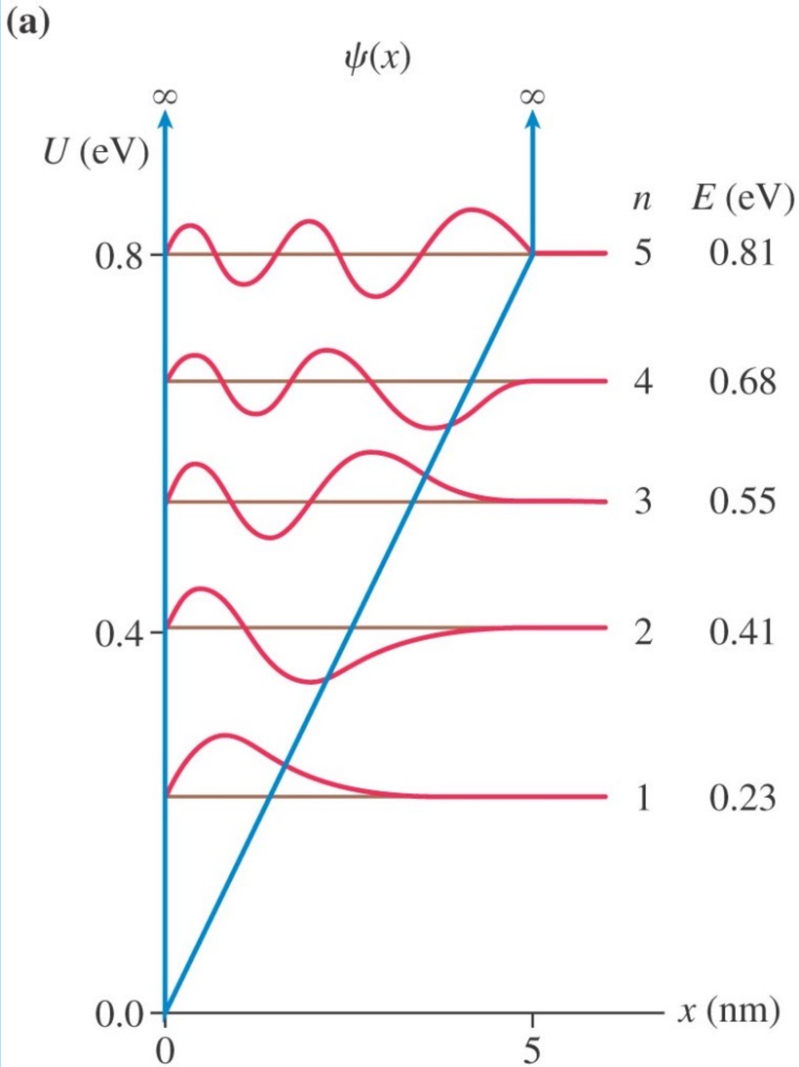
束縛態，能量量子化！



向右波長會變長。

電容器中的電子

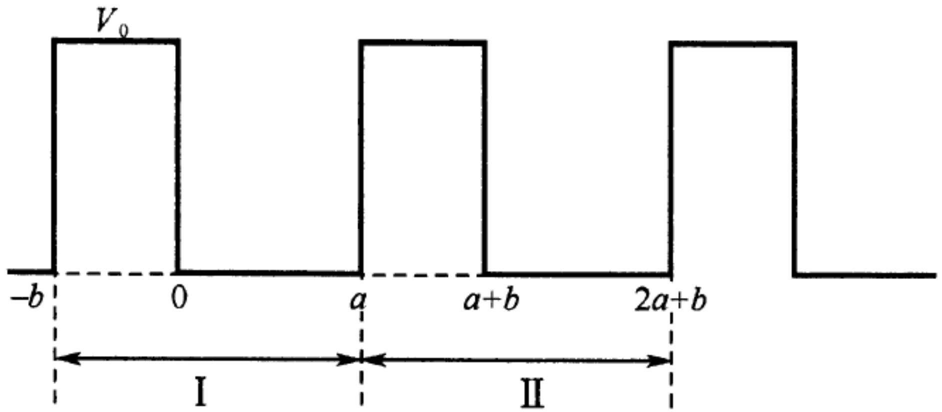

(a)
L
$\vec{E}$
Electron launched from the left plate
ΔV_0
Turning point
(b)
$U(x)$
∞
Left plate
Right plate
eV_0
E
Linearly increasing potential energy
0
L
x


(a)
$\psi(x)$
∞
U (eV)
n
E (eV)
0.8
0.4
0.0
5 0.81
4 0.68
3 0.55
2 0.41
1 0.23
0
5
x (nm)

Periodic Potential

例 考虑下列周期方势场(周期 $a+b$)中粒子(图 3.32),

$$V[x+n(a+b)] = V(x)$$



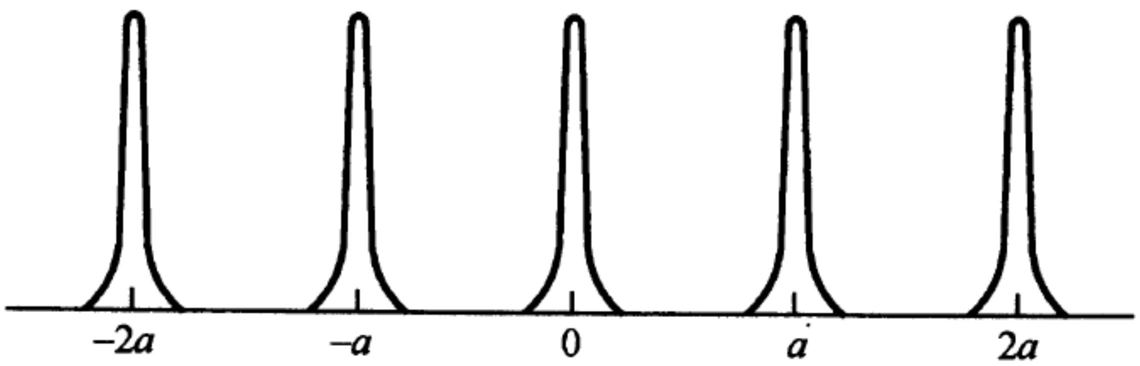
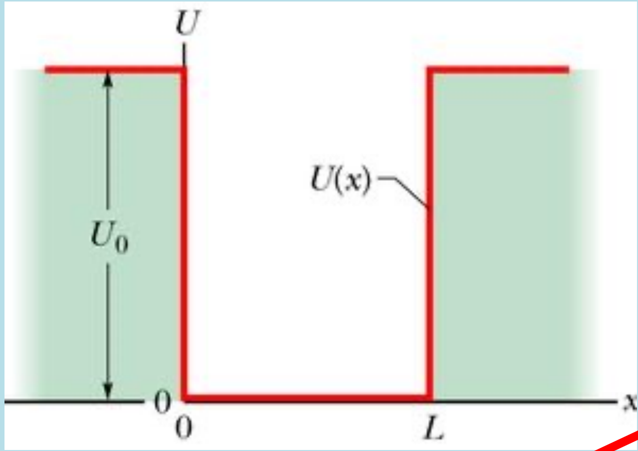
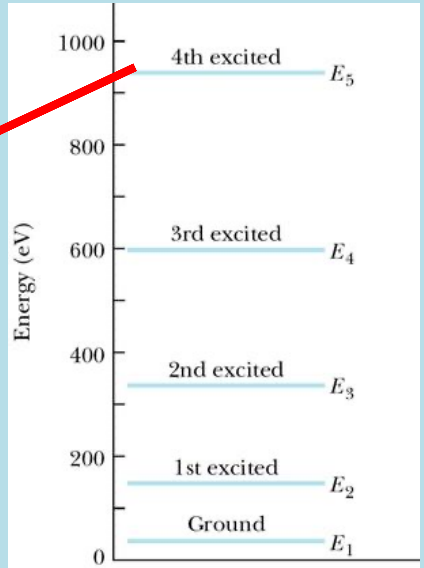
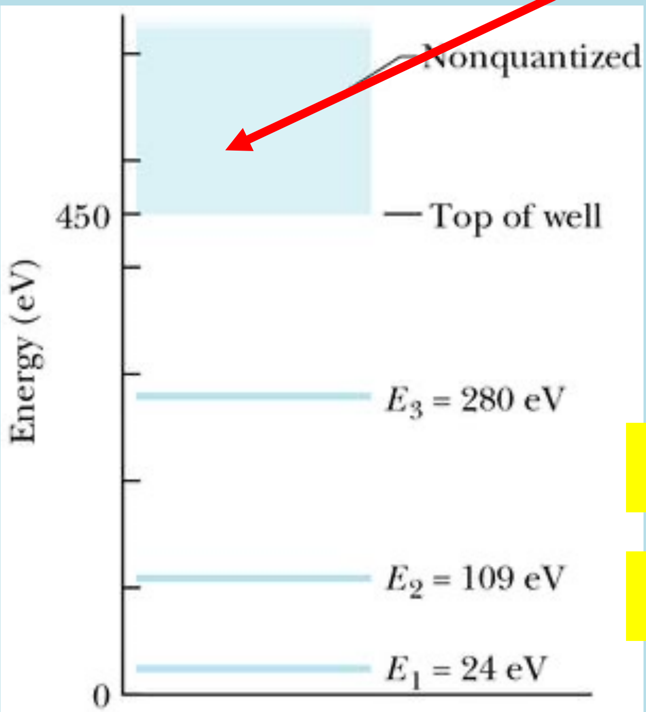


图 3.33 Dirac 梳

摘要







電子被拘限於一定區域時，能量為離散的能階

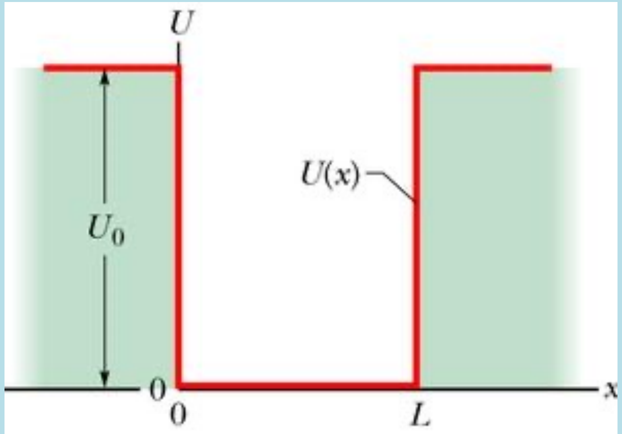
電子不被拘限於一定區域時，能量為連續

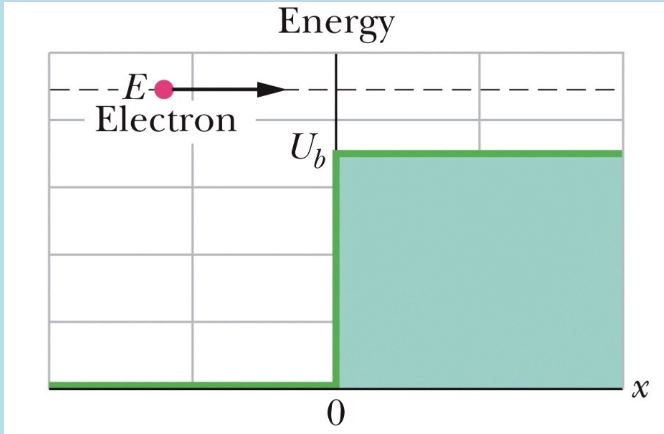
如果是有限大位能井，能量就會同時有連續與離散的部分！

因為能階高到一定值後，就不再被束縛了

摘要

一維階梯狀位能下的定態





束縛的定態將展現能量量子化！

在非束縛的情況中，定態能組成入射波包，可以描述散射問題！

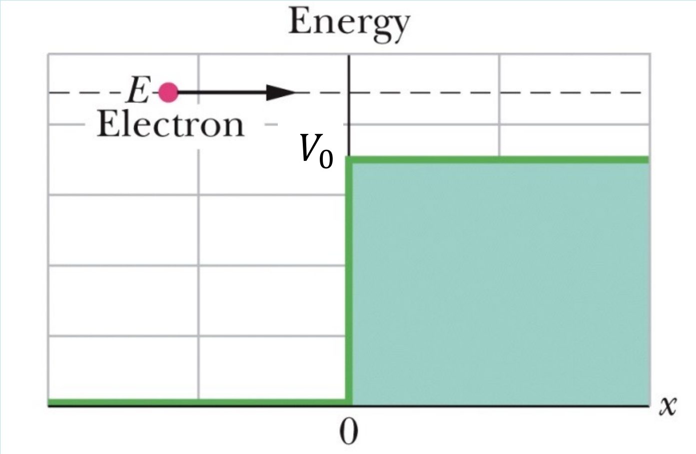
這些問題的物理意義差別很大：但在數學解法上卻非常類似！

這些問題都可以分解為一段段常數位能的區域，分開求解。

然後在邊界處，以連續條件將得到的各個解聯(match)起來。

反射與透射　摘要

在兩個區域內分別都是自由粒子，自由電子波定態解可以適用：



$x < 0$　$\psi_E = Ae^{ikx} + Re^{-ikx}$

$$k \equiv \sqrt{\frac{2mE}{\hbar^2}}$$

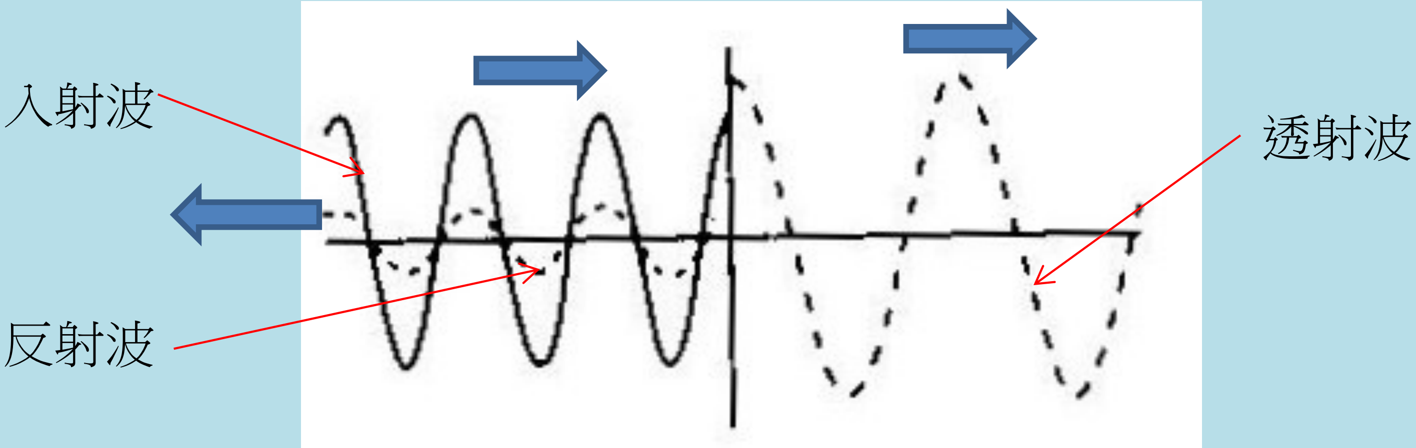
$x > 0$　$\psi_E = Te^{iqx}$

$$q \equiv \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$$

若只考慮由左入射的波，e^{-iqx}的部分可忽略。

$k > q$　　$\lambda_1 < \lambda_2$

由左向右入射的正弦波，在邊境產生向右的透射波，及向左的反射波。



摘要

但我們先以自由電子波e^{ikx}近似，所以就取$A = 1$。

$x < 0$ $\psi_E = e^{ikx} + Re^{-ikx}$ $\psi' = ike^{ikx} - ikRe^{-ikx}$

$x > 0$ $\psi_E = Te^{iqx}$ $\psi' = iqTe^{iqx}$

ψ及ψ'在邊界原點連續，可以得到兩個連續條件，正好求解得R, T。

$1 + R = T$

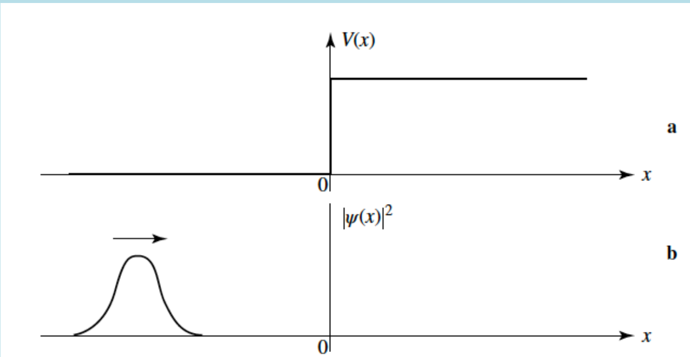
$k - kR = qT$

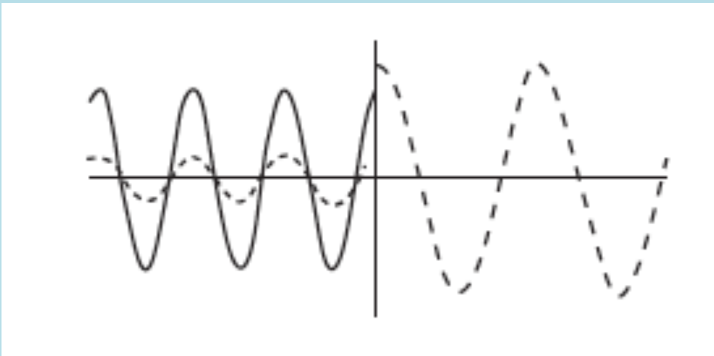
$$R = \frac{k-q}{k+q}$$

$$T = \frac{2k}{k+q}$$

$k > q, T > 1$

R決定了反射波強度，T決定了透射波強度。





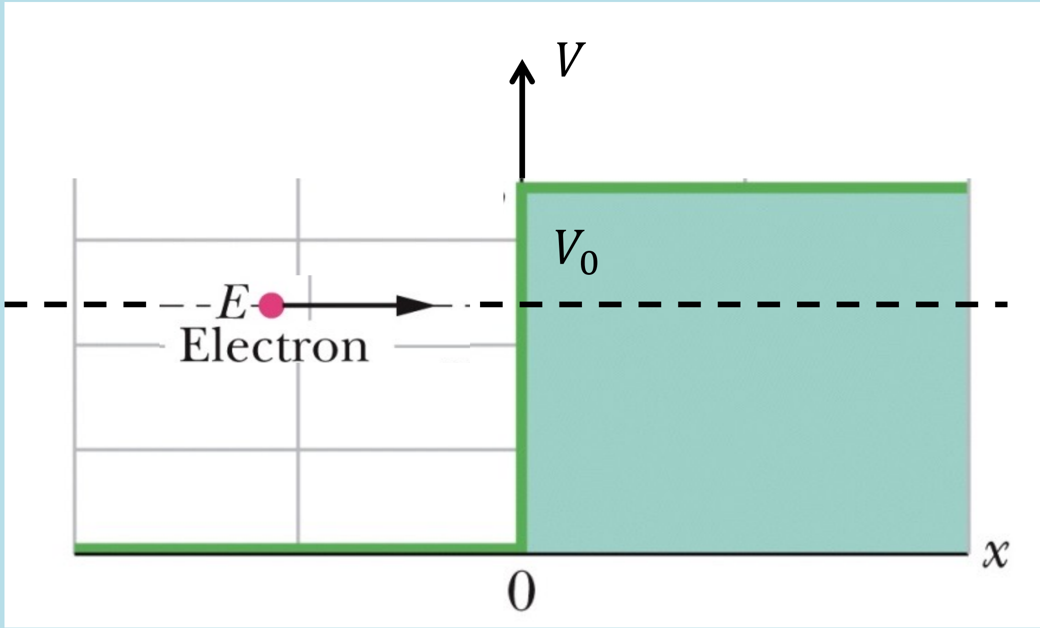
摘要

階梯狀位能全反射

$V = 0, \quad x < 0$

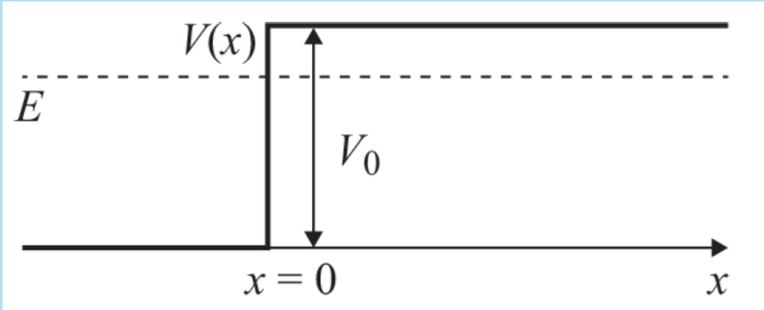
$V = V_0, \quad x > 0$

如果 $E < V_0$



$x < 0$ $\psi_E = e^{ikx} + Re^{-ikx}$ $k \equiv \sqrt{\frac{2mE}{\hbar^2}}$

摘要



$x > 0$ $E < V_0$ 古典粒子不能存在這樣的區域

但與時間無關的薛丁格方程式依舊有解：

$$\frac{d^2\psi_E}{dx^2} = \kappa^2\psi_E \;) - E]\psi_E \equiv \kappa^2\psi_E$$

$$\kappa \equiv \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

$$\psi_E = Ce^{-\kappa x} + De^{\kappa x}$$

在量子力學中，波函數還是有解，只是不再是正弦波，而是指數函數。

波函數若向右隨x增加，則在無限遠處波函數發散，不可能，因此$D = 0$。

$$\psi_E = Te^{-\kappa x}$$

進入折返點內禁止區後，振幅會指數遞減！

$\psi_E = e^{ikx} + Re^{-ikx}$　　$x < 0$

摘要

$\psi_E = Te^{-\kappa x}$　　$x > 0$

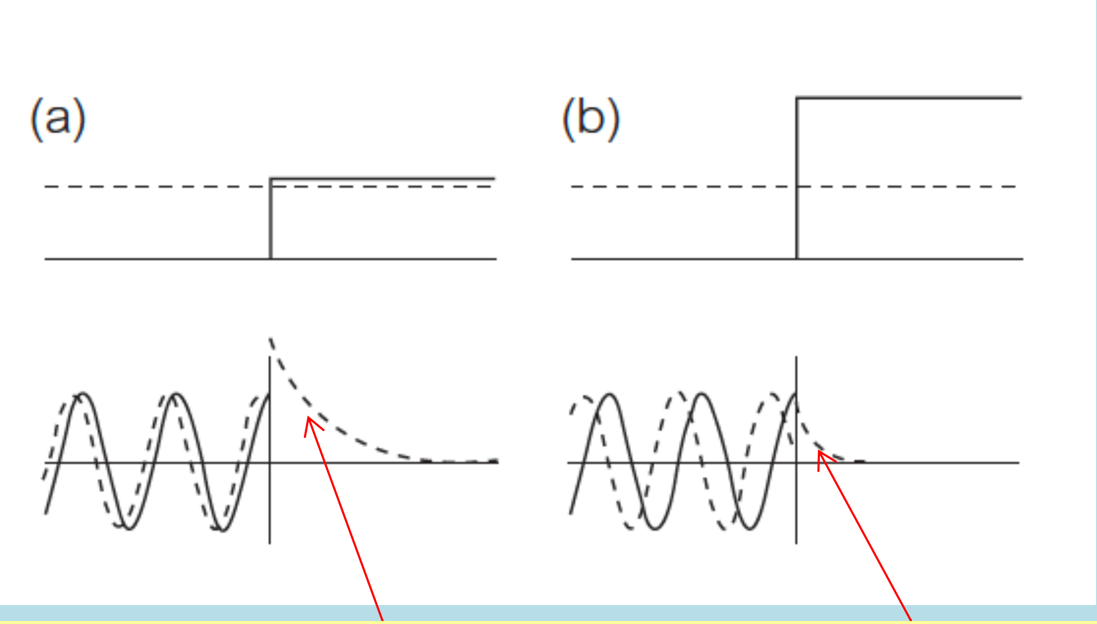
$$R = \frac{k - i\kappa}{k + i\kappa}$$

$$T = \frac{2k}{k + i\kappa}$$

同樣要求ψ及ψ'在邊界原點連續，

$1 + R = T$　　$k - kR = -i\kappa T$

與之前式子相同，只要以$i\kappa$替代q即可！



$$P = |\Psi|^2 = \left|\psi_E(x) \cdot e^{-i\frac{E}{\hbar}t}\right|^2 = |\psi_E(x)|^2 \left|e^{-i\frac{E}{\hbar}t}\right|^2 = |\psi_E(x)|^2 = |T|^2 e^{-2\kappa x}$$

在禁止區，機率密度不再是常數，而是隨滲透距離x指數遞減了！

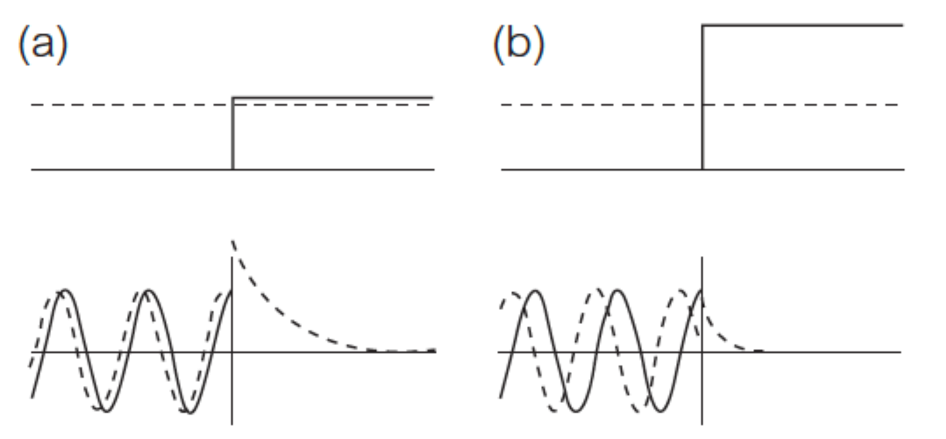


Figure 11.4. Same as for Fig. 11.3, but for two cases where $V_0 > E > 0$.

摘要

$$k - i\kappa \equiv |k - i\kappa| e^{i\delta}$$

$$R = \left|\frac{k - i\kappa}{k + i\kappa}\right| e^{2i\delta} = e^{2i\delta}$$

反射波與入射波振幅相同，但相差一個相角2δ！δ由E決定。

$$\psi_E = e^{ikx} + Re^{-ikx} = e^{ikx} + e^{-i(kx-2\delta)}$$

$$|R|^2 = \left|e^{2i\delta}\right|^2 = 1$$

反射率為1，完全反射。透射率是零。

在禁止區，雖然有滲透機率，可算出機率流為零，並沒有機率流進去！

$$j = -i\frac{\hbar}{2m}\left(\frac{\partial\psi^*}{\partial x}\cdot\psi - \psi^*\cdot\frac{\partial\psi}{\partial x}\right)$$

對實數的ψ，兩項抵消， $j = 0$。

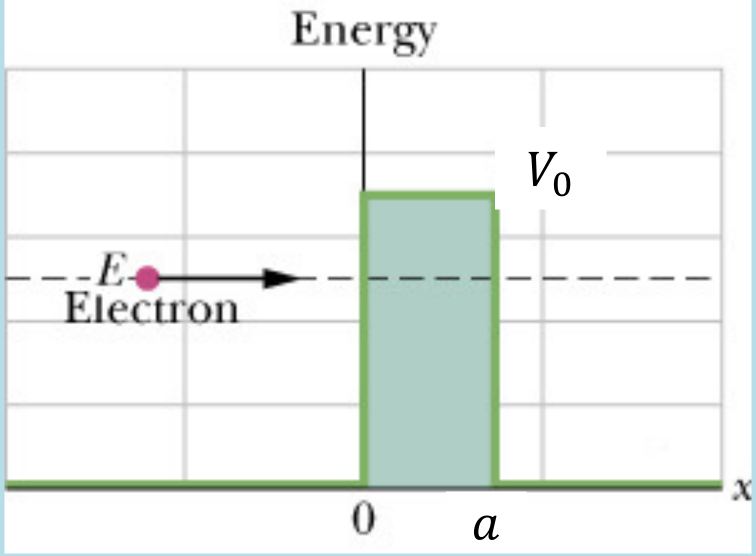
摘要

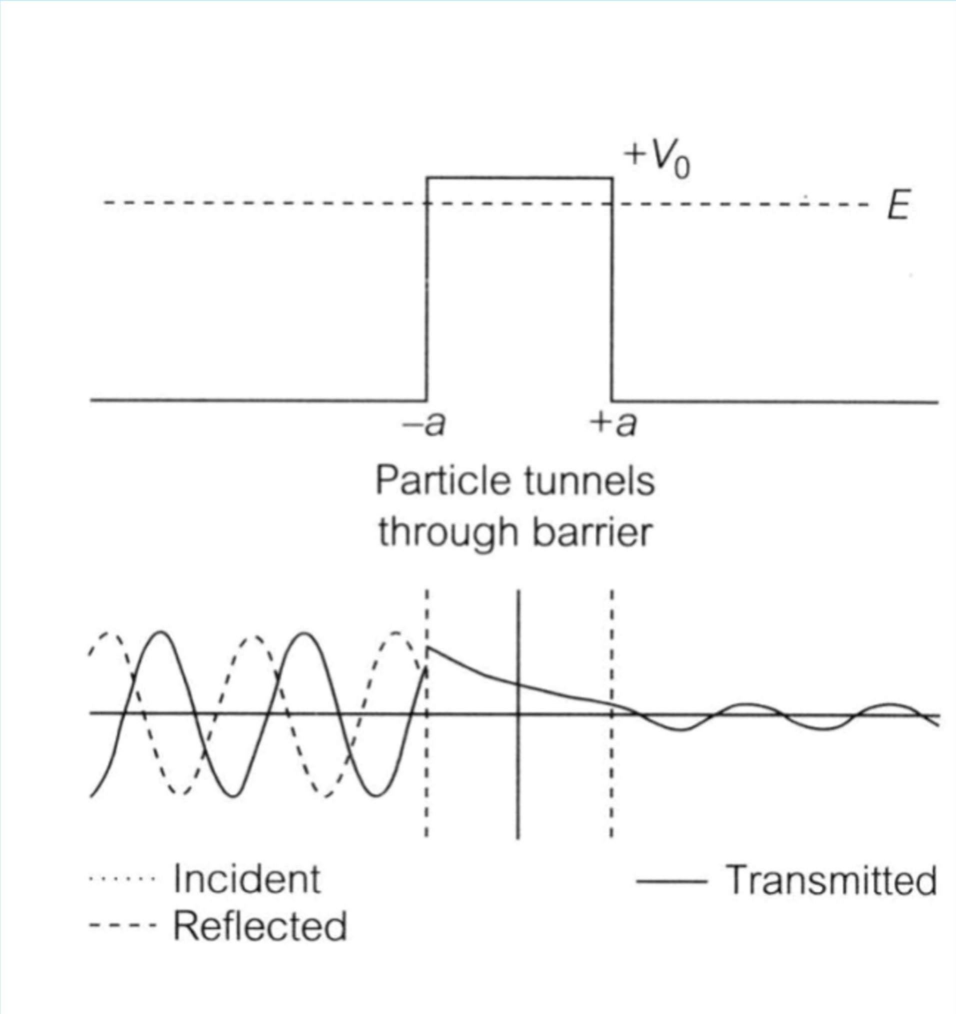
穿隧效應 Tunneling Effect

在禁止區，雖然有滲透機率，可算出機率流為零，並沒有機率流進去！

但如果這位能只持續很小一個範圍，位能很薄，粒子便能滲透過去，

在位能壘後方形成一個自由粒子波！

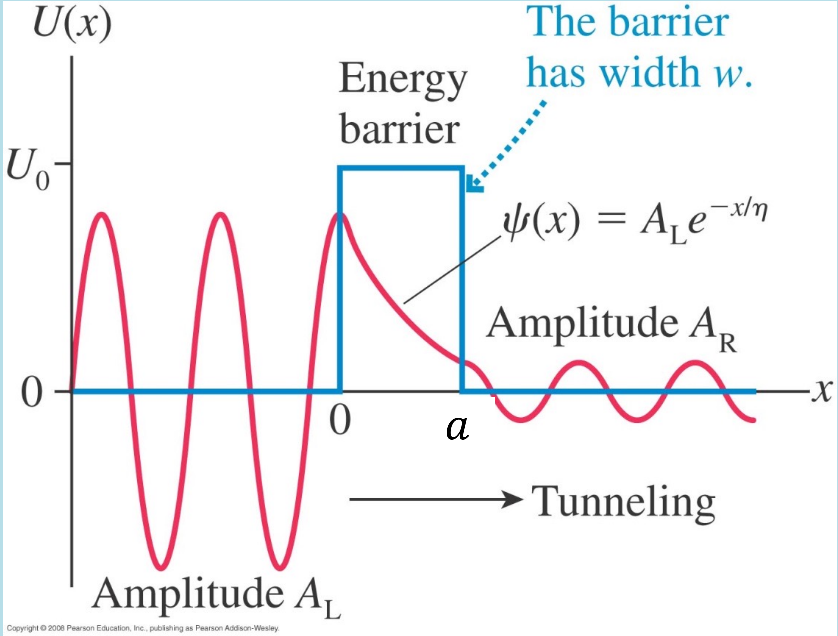




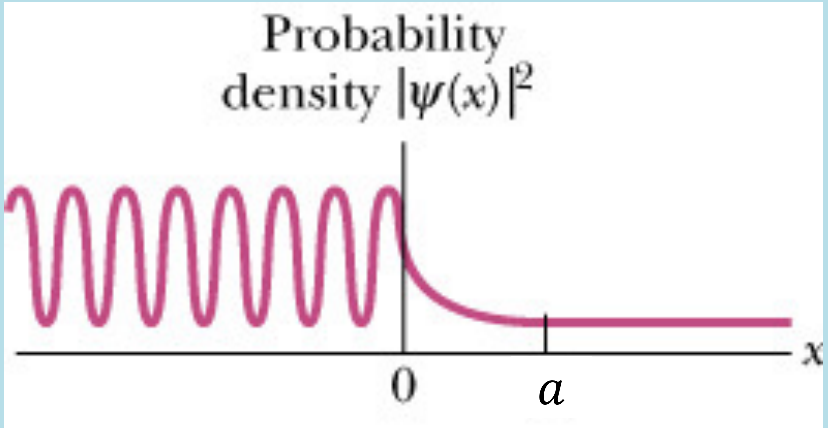
$+V_0$
E
$-a$
$+a$
Particle tunnels through barrier
Incident
Reflected
Transmitted

摘要

Tunneling effect 穿隧效應



摘要



在位壘中 $\psi_E(x) \sim A e^{-\kappa x}$

機率密度 $P = |\psi_E|^2 = |A|^2 e^{-2\kappa x}$

隨距離而指數遞減。在$x = a$，ψ_E要連續。

穿透後$x > a$機率 $\sim |\psi_E(a)|^2 \propto e^{-2\kappa a}$

一個電子有這麼多的機率會穿透，其餘的機率則反彈回來！

$$\kappa \equiv \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

能量差距越小，κ越小，穿透率越大！

$$|S|^2 \sim \left(\frac{4\kappa k}{k^2+\kappa^2}\right)^2 e^{-2\kappa a}$$

摘要

估算. 设 $\kappa a \gg 1$，此时 $\mathrm{sh}\kappa a \approx \frac{1}{2}e^{\kappa a} \gg 1$，式(3.3.16)可近似表示成

$$|S|^2 \approx \frac{16k^2\kappa^2}{(k^2+\kappa^2)^2}e^{-2\kappa a} = \frac{16E(V_0-E)}{V_0}\exp\left[-\frac{2a}{\hbar}\sqrt{2m(V_0-E)}\right] \qquad (3.3.19)$$

可以看出 T 与势垒宽度 a，(V_0-E)，以及粒子质量 m 的依赖关系都很敏感. 随势垒宽度 a 和粒子质量 m 增大，T 将指数衰减，$T \propto e^{-a\sqrt{m}}$. 所以，在宏观实验中，不容易观测到粒子穿透势垒的现象.

例如，对于电子，设 $E=1\mathrm{eV}$，$V_0=2\mathrm{eV}$，$a=2\times10^{-8}\mathrm{cm}$，可以估算出 $T\approx0.51$. 若 $a=5\times10^{-8}\mathrm{cm}$，则 $T\sim0.024$，迅速变小. 若电子换成质子，因为 $m_p/m_e\approx1840$，$a=2\times10^{-8}\mathrm{cm}$，可估算出 $T\approx2.6\times10^{-38}$.

对于 $E>V_0$ 情况（图 3.13），只需在式(3.3.16)中，把 $\kappa\to ik'$，k'为实数

$$k' = \sqrt{2m(E-V_0)/\hbar^2} \qquad (3.3.20)$$

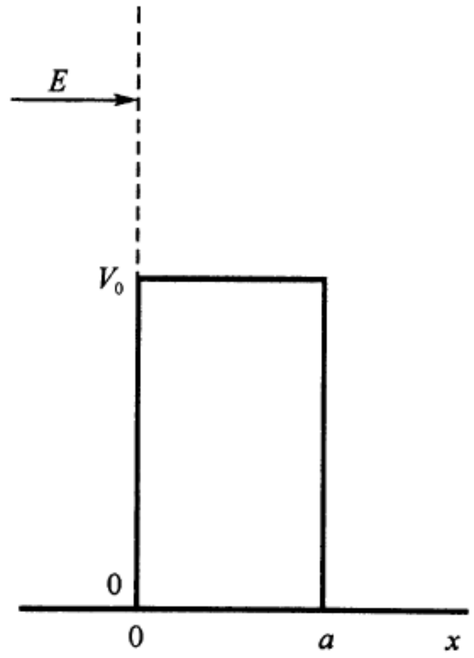


图 3.13

再利用 $\mathrm{sh}(ik'a)=i\sin k'a$，可得

$$|S|^2 = \frac{4k^2k'^2}{(k^2-k'^2)^2\sin^2k'a+4k^2k'^2} = \frac{1}{1+\frac{1}{4}\left(\frac{k}{k'}-\frac{k'}{k}\right)^2\sin^2k'a} \quad (k'\leqslant k) \qquad (3.3.21)$$