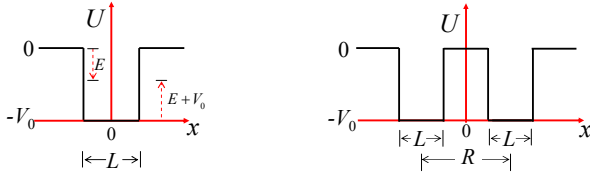


Appendix 1: 1D quantum wells

(1D atom, 1D molecule and 1D solid)



1D atom: single well

1D molecule: double well

(E = energy of particle in the potential well $U(x)$)

For these symmetric potentials, always set coordinates such that $U(-x) = U(x)$ (an even potential).

Then there are two types of solutions:

- (1) even wavefunction and
- (2) odd wavefunction.

Each type of solution must be

(a) for region $E > U(x)$,

$$\psi(x) \sim Ae^{ikx} + Be^{-ikx} \text{ or } A'\cos kx + B'\sin kx$$

(b) for region $E < U(x)$,

$$\psi(x) \sim Ce^{kx} + De^{-kx} \text{ or } C'\cosh kx + D'\sinh kx$$

Note: For different regions, k is defined by rearranging the time-independent Schrödinger equation (**TISE**).

The eigen-energy and wavefunctions can be obtained by matching ψ , $d\psi/dx$ at all boundaries (e.g. $x = \pm L/2$ for single well).

(A) 1D atom: Single well

Bound state energies E ($-V_0 \leq E < 0$) are solutions of the following equations:

(a) For **even wavefunctions**:

(corresponding to $n = 1, 3, 5, \dots$ of infinite well)

$$\tan\left(\frac{KL}{2}\right) = \frac{k}{K} \quad [1]$$

(b) For **odd wavefunctions**:

(corresponding to $n = 2, 4, 6, \dots$ of infinite well)

$$\tan\left(\frac{KL}{2}\right) = -\frac{K}{k} \quad [2]$$

$$\text{where } k = \sqrt{\frac{-2mE}{\hbar^2}} \quad \& \quad K = \sqrt{\frac{2m(E+V_0)}{\hbar^2}} \quad [3]$$

Solutions are obtained only by a graphic method.

If we choose the well bottom at $U = 0$, then the bound state energies E ($0 < E < V_0$) are solutions of the same equations shown above but with

$$k = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \quad \& \quad K = \sqrt{\frac{2mE}{\hbar^2}}$$

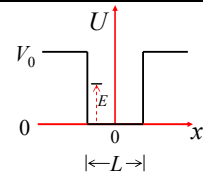
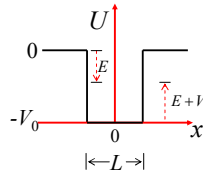
Solutions are obtained by a graphic method:

$$\text{Set } \xi \equiv \frac{KL}{2} = \frac{L}{2\hbar} \sqrt{2mE}$$

$$\text{Then for even } \psi \text{ (odd } n), \tan \xi = \frac{\sqrt{W - \xi^2}}{\xi} \quad \text{---} \quad W \equiv \frac{mV_0L^2}{2\hbar^2}$$

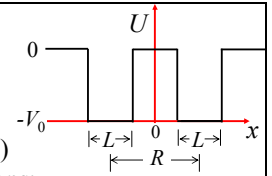
Plot $\tan \xi$ & $\sqrt{W - \xi^2} / \xi$ as a function of ξ .

The solutions are obtained by the value of ξ where the curves cross.



(B) 1D molecule: Double well

(Problem set 1)



Bound state energies E ($-V_0 \leq E < 0$)

are solutions of the following equations:

$$(a) \text{ For even wavefunctions: } \tan(KL) = \frac{kK(1+T)}{K^2 - k^2T} \quad [4]$$

$$(b) \text{ for odd wavefunctions: } \tan(KL) = \frac{kK(1+T)}{K^2T - k^2} \quad [5]$$

$$\text{where } k = \sqrt{\frac{-2mE}{\hbar^2}}, \quad K = \sqrt{\frac{2m(E+V_0)}{\hbar^2}} \quad [3]$$

$$\text{and } T \equiv \tanh\left[k\left(\frac{R-L}{2}\right)\right] \quad [6]$$

To find solutions of E , plot $\tan(KL)$ against KL

& plot $\frac{kK(1+T)}{K^2 - k^2T} \equiv \Theta_E$ against KL for even wavefunctions,

& plot $\frac{kK(1+T)}{K^2T - k^2} \equiv \Theta_O$ against KL for odd wavefunctions,

$$\text{Note: } k^2 + K^2 = \frac{2mV_0}{\hbar^2} \equiv k_0^2 \quad [7]$$

$$0 < K < k_0$$

The solutions of E can be obtained from the cross points of these curves.

Feature: each single-well level is split into 2 levels, one even & one odd. (See next graph)

Limiting case: $R \rightarrow \infty$

$$\Rightarrow T \rightarrow 1$$

The double well becomes two independent single well.

Then Eq. [3] & [4] becomes

$$\tan(KL) = \frac{2kK}{K^2 - k^2} \quad [7]$$

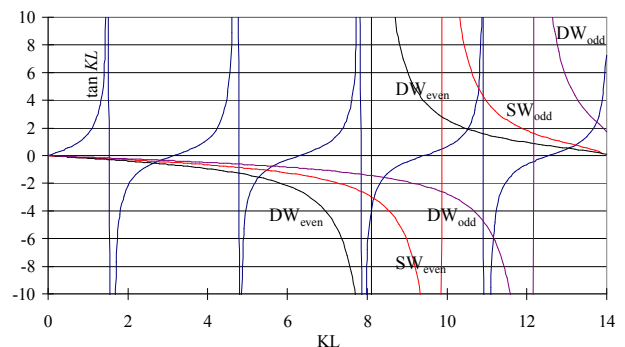
Eq. [7] is equivalent to Eq. [1] & [2] for single well:

$$\begin{aligned} \tan(KL) &= \frac{\sin(KL)}{\cos(KL)} = \frac{2\sin(\frac{1}{2}KL)\cos(\frac{1}{2}KL)}{\cos^2(\frac{1}{2}KL) - \sin^2(\frac{1}{2}KL)} \\ &= \frac{2\tan(\frac{1}{2}KL)}{1 - \tan^2(\frac{1}{2}KL)} = \frac{2(k/K)}{1 - (k/K)^2} \quad (\text{by [1]}) \\ &= \frac{2kK}{K^2 - k^2} \end{aligned}$$

Plots for solutions: electron in DW & SW

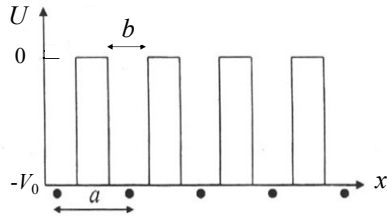
DW: double well, $R = 1.1L$, $L = 0.2 \text{ nm}$

V_0 is given by $k_0L = \sqrt{20\pi} \approx 14$



(C) 1D solid: Periodic well (Kronig-Penny model)

$$\psi_k(x) = e^{ikx} \cdot u_k(x)$$



Solutions for bound states ($E < 0$) and extended states ($E > 0$) can be found in many QM textbooks (e.g. Merzbacher, Quantum Mechanics, 2/e).

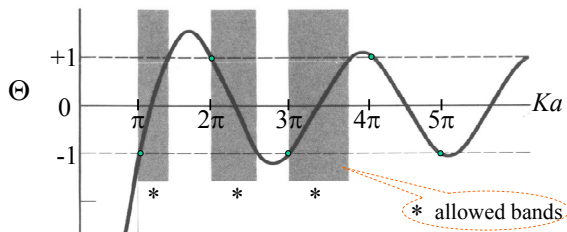
If $b \rightarrow 0$ & $V_0 \rightarrow \infty$, but with fixed and finite $G \equiv bV_0$, then the extended state solution ($E > 0$) is given by solving

$$\cos ka = \cos Ka - \frac{mGa \sin Ka}{\hbar^2 Ka}$$

where $K = \sqrt{\frac{2m}{\hbar^2} E}$ Note: $|\cos ka| \leq 1$

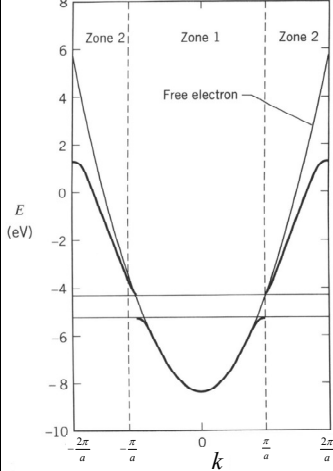
Plot $\Theta \equiv \cos Ka - \frac{mGa \sin Ka}{\hbar^2 Ka}$ against Ka

with a fixed G :



For an allowed K , we can calculate k using $\cos ka = \Theta$.
 E as a function of k is then obtained numerically:

Correct graph (by Slater)



wrong graph

(Bernstein-Fishbane-Gasiorowicz, Modern Physics)

