ECE/MAT 211A winter 07

HWK#1 solutions

#1·1-3: Photodissociation

The minimum photon energy must correspond to zero transverse momentum for each of the two fragments: any non-zero transverse momentum would not change the requirements imposed by longitudinal momentum conservation, but would make a positive contribution to the total kinetic energy of the two fragments, and hence to the photon energy required.

(a)

Energy conservation requires:

$$\hbar w = \varepsilon_0 + \frac{p_1^2}{2M_1} + \frac{p_2^2}{2M_2} \tag{1}$$

Momentum conservation requires

$$p_{photon} = p_1 + p_2 \tag{2}$$

thus the photon energy can be written as

$$\varepsilon_{photon} = \hbar w = c p_{photon} = c \cdot (p_1 + p_2) \tag{3}$$

From (1) and (3) we get:

$$\hbar w = \varepsilon_0 + \frac{p_1^2}{2M_1} + \frac{p_2^2}{2M_2} = c \cdot (p_1 + p_2) \tag{4}$$

Taking differentials:

$$\hbar \cdot dw = \frac{p_1 \cdot dp_1}{M_1} + \frac{p_2 \cdot dp_2}{M_2} = c \cdot (dp_1 + dp_2) \tag{5}$$

At the photon energy minimum, dw = 0, which implies $dp_2 = -dp_1$, and hence

$$\frac{p_1}{M_1} = \frac{p_2}{M_2} = v \tag{6}$$

that is, the two fragments have the same velocity. Insert (6) into (4),

$$\hbar w = \varepsilon_0 + \frac{1}{2} M v^2 = Mcv \tag{7}$$

where $M=M_1+M_2$

Because we had specified $\varepsilon_0 << Mc^2$, which implies v << c, the Mv^2-term will be small compared to the Mcv-term and compared to ε_0. The velocity would simply be:

$$v = \frac{1}{Mc}(\varepsilon_0 + \frac{1}{2}Mv^2) \approx \frac{\varepsilon_0}{Mc} \tag{8}$$

and if this is inserted into (7), we obtain the minimum excess photon energy

$$\boxed{(\Delta\varepsilon)_{\min} = \frac{1}{2}Mv^2 = \frac{\varepsilon_0^2}{2Mc^2}}$$

(b)

Transverse recoil velocities and momenta will be $\boxed{0}$.

Longitudinal recoil velocity will be $\boxed{v = \frac{\varepsilon_0}{Mc} = \frac{\varepsilon_0}{(M_1 + M_2)c}}$ for both fragments, and longitudinal recoil momenta will be $\boxed{\frac{M_1\varepsilon_0}{(M_1 + M_2)c}}$ and $\boxed{\frac{M_2\varepsilon_0}{(M_1 + M_2)c}}$.

(c)

For deuteron,

$v_D = 3.54\times10^5$ m/sec

$(\Delta\varepsilon)_D \sim 1.30$ keV

For hydrogen atom,

$v_H = 4.34$ m/sec

$(\Delta\varepsilon)_H \sim 9.93\times10^{-8}$ eV

For comparison, $k_BT \sim 0.0258$ eV around room temperature.

#1·5-2: Reflections at Semiconductor Hetero-Interfaces

Instead of (1·4-19a,b):

$$i\frac{k}{m_-^*}(A - B) = i\frac{k'}{m_+^*}C$$

which differs from (1·4-19a,b) by the substitutions

$$k \to \frac{k}{m_-^*} = \frac{v}{\hbar}$$

$$k' \to \frac{k'}{m_+^*} = \frac{v'}{\hbar}$$

where the v-s are the velocities on the two sides.

The remainder of the math in Sec. 1.4 remains valid, if these substitutions are made everywhere. Hence from (1·5-15),

$$\boxed{\begin{aligned} R &= \left|\frac{v-v'}{v+v'}\right|^2 \\ T &= \frac{4vv'}{(v+v')^2} = 1-R \end{aligned}}$$

Note that there are no reflections when v'=v.

#2·2-2: Energy Eigenvalues in a Symmetric Well with Finite Barrier Height

(a)

From Fig. 2·2-6 we see that the ka-value for the n-th state falls into the interval

$$(n-1)\cdot\frac{\pi}{2} < ka < n\cdot\frac{\pi}{2}$$

With $ka<k_0a$, this implies that $N = n_{max}$ is the largest integer that satisfies

$$N-1 < \frac{2k_0a}{\pi}$$

which is equivalent to

$$N = 1 + Int\left(\frac{2k_0a}{\pi}\right) = 1 + Int\left(\frac{2a}{\pi}\sqrt{\frac{2MV_0}{\hbar^2}}\right) = 1 + Int\left(1.63\cdot\frac{2a}{1nm}\sqrt{\frac{M}{m_e}\cdot\frac{V_0}{1eV}}\right)$$

The numerical value 1.63 is obtained by inserting 2a = 1nm and V_0 = 1eV.

(b)

The eigenstates can be solved easily by computer programming.

Here is the reference code in MATLAB, in which we use 'fzero' function to solve equations numerically.

<q2point2_2.m>

```
function q2point2_2(M, a, V0)
%  this function calculates the bound states according to (2.2-28a,b)
%  for a finite potential well which is V0 deep and 2a wide
%  and draws a Figure like Fig 2.2-6
%  M in the unit of electron mass
%  a in the unit of nm
%  V0 in the unit of eV
```

```
options.Display = 'off';

h_bar = 6.626e-34/(2*pi);
me = 9.1e-31;
e = 1.6e-19;

k0 = sqrt(2*(M*me)*(V0*e)/(h_bar^2));

N = 1 + floor(2*k0*a*(1e-9)/pi);        % number of bound states

data = zeros(N,4);
% create a N*3 matrix to store the results
% data(:,1) = state index  (1, 2, ... N)
% data(:,2) = k value
% data(:,3) = energy
% data(:,4) = y coordinate of the crosssections

for i = 1:N
    left_bound = (i-1)*(pi/2);
    right_bound = i*(pi/2);

    switch mod(i,4)
        case 1
            data(i,2) = fzero('even_parity', [left_bound right_bound], options, k0, a*1e-9, 0);
            data(i,4) = data(i,2)/(k0*1e-9);
        case 2
            data(i,2) = fzero('odd_parity', [left_bound right_bound], options, k0, a*1e-9, 0);
            data(i,4) = data(i,2)/(k0*1e-9);
        case 3
            data(i,2) = fzero('even_parity', [left_bound right_bound], options, k0, a*1e-9, 1);
            data(i,4) = -data(i,2)/(k0*1e-9);
        case 0
            data(i,2) = fzero('odd_parity', [left_bound right_bound], options, k0, a*1e-9, 1);
            data(i,4) = -data(i,2)/(k0*1e-9);

    end
    data(i,1) = i;
end

data(:,3) = ((h_bar^2)*(data(:,2)/(a*1e-9)).^2)/(2*M*me*e);

% display the result
data(:,1:3)

x = linspace(0, k0*a*1e-9, 1000)/pi;
even = cos(x*pi);
odd = sin(x*pi);

% plot a figure like Fig 2.2-6
plot(x,even, 'b-', x, odd, 'b-', data(:,2)/pi, data(:,4),'ro', x, x*pi/(k0*1e-9), 'c-', x, -x*pi/(k0*1e-9), 'c-');
xlabel('ka(π)');
grid on;

end
```

<odd_parity.m>

```
function result = odd_parity(ka, k0, a, sign)
% sign = 0 means line with + slope on Fig 2.2-6
% sign = 1 means line with - slope on Fig 2.2-6

  result = sin(ka)-((-1)^sign)*(ka/k0/a);

end
```

<even_parity.m>

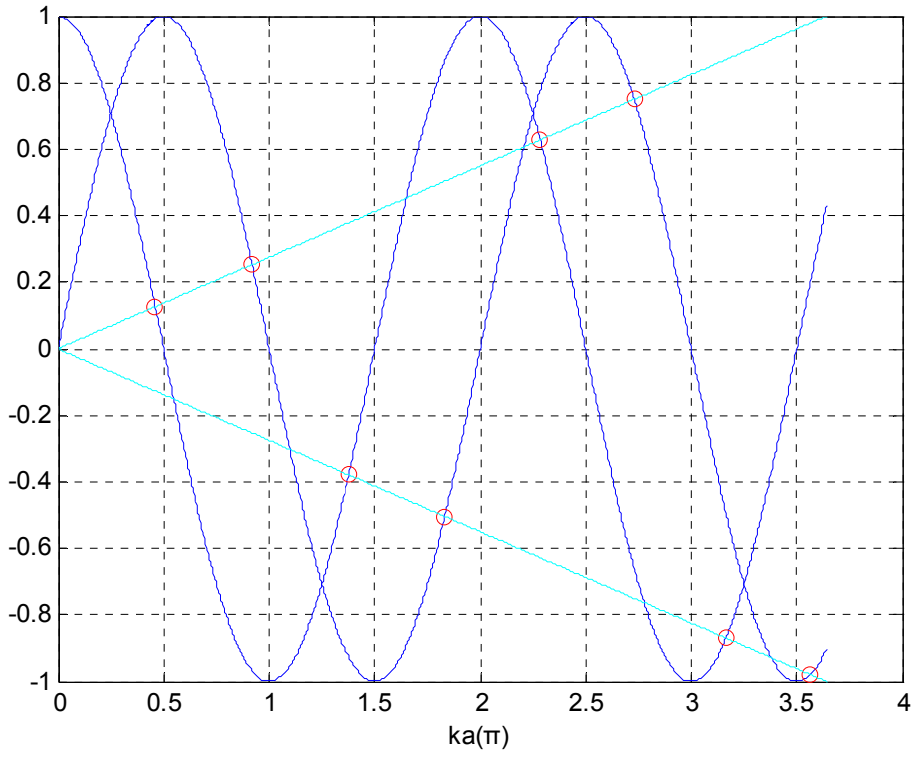
```
function result = even_parity(ka, k0, a, sign)
% sign = 0 means line with + slope on Fig 2.2-6
% sign = 1 means line with - slope on Fig 2.2-6

  result = cos(ka)-((-1)^sign)*(ka/k0/a);

end
```

The results for an electron well with 2a = 2nm and a depth V_0 = 5eV are.

state #	ka	Energy(eV)
1	1.4442	0.0797
2	2.8866	0.3182
3	4.3248	0.7143
4	5.7561	1.2653
5	7.1761	1.9666
6	8.5773	2.8096
7	9.9425	3.7752
8	11.2012	4.7916



#2·3-2: Pulsating Harmonic Oscillator Wave Packet

The specifications call for the superposition of two even-parity states with relative amplitudes such as to cause a periodic cancellation of the two contributions at x = 0. The simplest solution is

$$\boxed{\Psi(x,t) = a_0\psi_0(x)\cdot\exp\left(-\frac{i}{2}wt\right) + a_2\psi_2(x)\cdot\exp\left(-\frac{5i}{2}wt\right)}$$

where

$$\frac{a_0}{a_2} = \frac{\psi_2(0)}{\psi_0(0)} = -\sqrt{\frac{1}{2}},$$

with the help of (2·3-30a). With normalization,

$$a_0 = \sqrt{\frac{1}{3}} \quad \text{and} \quad a_2 = -\sqrt{\frac{2}{3}} \ .$$

The oscillation period is T = π/w. At t = 0 and t = T

$$|\Psi(x,0)|^2 = |\Psi(x,T)|^2 = |a_0\psi_0(x) + a_2\psi_2(x)|^2 .$$

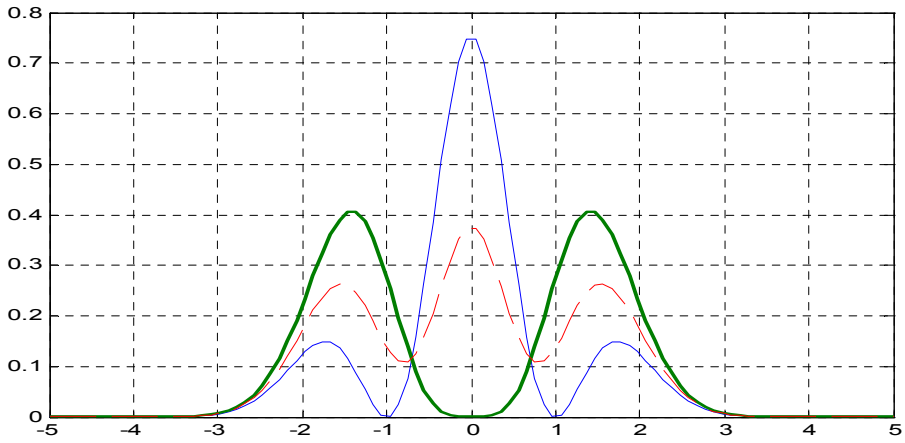
At t = T/2

$$|\Psi(x,T/2)|^2 = |a_0\psi_0(x) - a_2\psi_2(x)|^2 .$$

At t = T/4 and 3T/4

$$|\Psi(x,T/4)|^2 = |\Psi(x,3T/4)|^2 = [a_0\psi_0(x)]^2 + [a_2\psi_2(x)]^2 .$$

Below is a plot of the three probability distributions. The light solid (blue) line is for t = 0 and t = T, the heavy solid (green) line for t = T/2, and the dashed line (red) for t = T/4 and 3T/4.



#2·6-1: Oscillations in a Double Square Well

Because of the symmetry of the potential, the energy eigenfunctions must be either even or odd functions about the center of the well.

Nevertheless, the mathematics turns out to be simpler by placing the coordinate origin not at the center of inversion, but at the left wall, as with the single well treated in Sec. 2.2. In the *left-hand* half of the well, all wave functions are then of the form

$$\psi(x) = C \sin kx \quad , \tag{1}$$

with energies given by the general plane-wave energy relation (2·2-3).

The odd-parity states have a null at x = a (see Fig.1), hence their wave number is of the form $k = n\pi/2a$, with even values of n. They are the same as for a simple square well of width L = 2a, with energies given by (2·2-8), not affected by the presence of the barrier at all.

The even-parity states must satisfy the connection rule (1·4-35) at a δ-function barrier, which takes on the form

$$\Delta\psi' \equiv \psi'(a+0) - \psi'(a-0) = -2\psi'(a-0) = +\frac{2MS}{\hbar^2}\psi(a) \quad , \tag{2}$$

where S is the strength of the δ-function. In the second equality in (2) we utilized the symmetry of ψ about the center plane. Evidently, the even-parity eigenfunctions have a kink at the location of the barrier, as shown in Fig.1, which is drawn for a value π/k = 1.1a. The figure also shows the lowest odd-parity state and the superposition ψ_{even} - ψ_{odd} of the two states. The near-cancellation of the two terms in the superposition in the left-hand half of the well is evident.

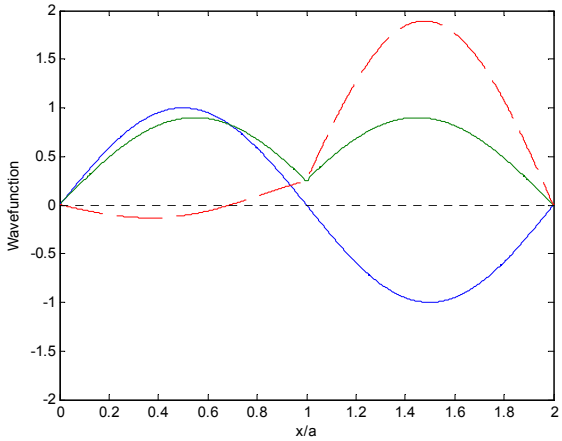


Fig. 1

odd-parity (blue), even-parity(green) and their superposition (red)

This cancellation is even more pronounced in the probability density for t = 0 and t = T/2, both shown in Fig.2, along with that for t = T/4. Note that the probability density for t = T/4 is given by

$$|\psi|^2 = \frac{1}{2}\left[\psi_+^2 + \psi_-^2\right] \quad , \tag{3}$$

which is symmetrical about the center plane. The probability density evidently sloshes back and forth between the two wells, with the density in the center plane staying constant, at a low value.

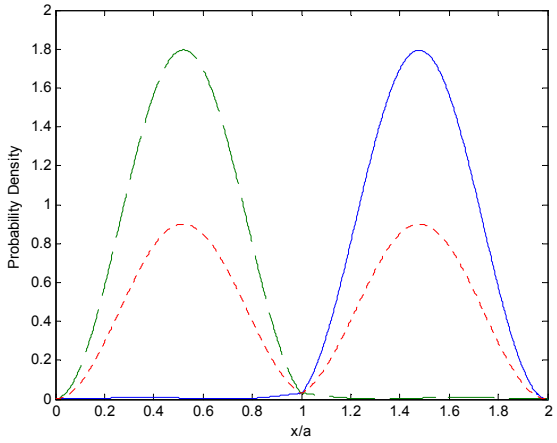


Fig.2

probability density at t = 0(blue), t = T/2(green) and t = T/4(red)

Insertion of (1) into (2) immediately yields the conditions (2·6-9) and (2·6-10) in the text as the condition on *k* for the even-parity states. The condition (2·6-9) may be visualized graphically in terms of the intersection of the trigonometric tangent of *k*a with a straight line (see Fig.3).

With increasing strength S of the δ-function, the coupling parameters c and hence the slope of the straight line in the figure decreases, pushing the intersections with the tangent closer to those values of *k*a that belong to the odd-parity states; that is, each even-parity state gets pushed up closer to the next-higher odd-parity state.

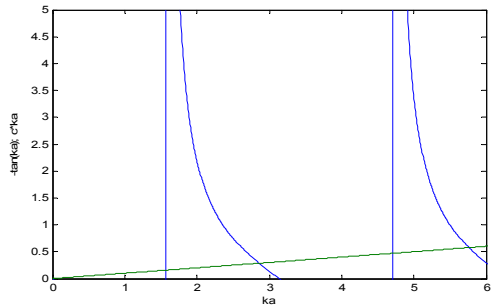


Fig. 3

If we restrict ourselves to the lowest even-parity state, we may write

$$ka = \pi - \alpha \quad , \tag{4}$$

where $0 < \alpha < \frac{\pi}{2}$. With this, (2·6-9) becomes

$$\tan\alpha = c \cdot (\pi - \alpha) \tag{5}.$$

In the limit of sufficiently weak coupling, c<<1, the right-hand side of (5) will be small, which implies that the argument α inside the tangent on the left-hand side must also be small, and that we may replace tanα by α. Solving for α yields

$$\alpha \cong \frac{c\pi}{1+c} \cong c\pi \quad , \tag{6}$$

or, from (4),

$$ka \cong (1-c)\pi \, . \tag{7}$$

Insertion into the general plane-wave energy expression (2·2-3) then yields

$$\boxed{\varepsilon_1 = \frac{\hbar^2 k^2}{2M} = \frac{\hbar^2 (ka)^2}{2Ma^2} \approx \frac{\hbar^2 \pi^2}{2Ma^2}(1-c)^2 \approx \varepsilon_2 - \Delta\varepsilon} \tag{2·6-11}$$

where ε_2 is the energy of the lowest odd-parity state and

$$\varepsilon_2 = \frac{\hbar^2 k_2^2}{2M} = \frac{\hbar^2}{2M}\left(\frac{2\pi}{2a}\right)^2 \approx \frac{\hbar^2 \pi^2}{2Ma^2}$$

As a result,

$$\boxed{\Delta\varepsilon = \varepsilon_2 - \varepsilon_1 = \frac{\hbar^2 \pi^2}{2Ma^2}(2c - c^2) \approx 2c\varepsilon_2 << \varepsilon_2} \tag{2·6-12}$$

We have neglected the c^2 term here since it's too small compared to 2c.