Homework 4

December 1, 2015

CBE-521, Fall 2015
Homework No. 2 with Prof. Petsev (fourth assignment of year)
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In [1]:
```
from pint import UnitRegistry
ureg = UnitRegistry()
import numpy as np
import math
import scipy as sp
import scipy.special as npsp
np.set_printoptions(precision=4, linewidth = 60)
```

1 Problem 1

1.0.1 Using software of your choice plot both Henry and Ohshima's expressions and comment on the agreement/disagreement between them. Is the Ohshima approximation reasonable to use?

Range of κR to plot

In [2]:
```
kr = np.linspace(0.001,100, 10000)
```

1.1 Henry's Apprdoximation

$$f_1 \kappa R = 1 + \frac{\kappa R^2}{16} - \frac{5\kappa R^3}{48} - \frac{\kappa R^4}{96} + \frac{\kappa R^5}{96} - \left[\frac{\kappa R^4}{8} - \frac{\kappa R^6}{96}\right] exp\left(\kappa R\right) E_1 \tag{1}$$

$$E_1 = \int_{\infty}^{\kappa R} \frac{exp(-t)}{t} dt \implies \text{Exponential Integral} \tag{2}$$

In [3]:
```
E1 = -npsp.exp1(kr) # the exponential integral of order one
f1kr_henry = 1 + 1/16.*kr**2 - 5/48. * kr**3 -1/96.*kr**4 + 1/96.*kr**5 \
    -(kr**4 / 8. - kr**6 / 96.)* np.exp(kr) * E1
```

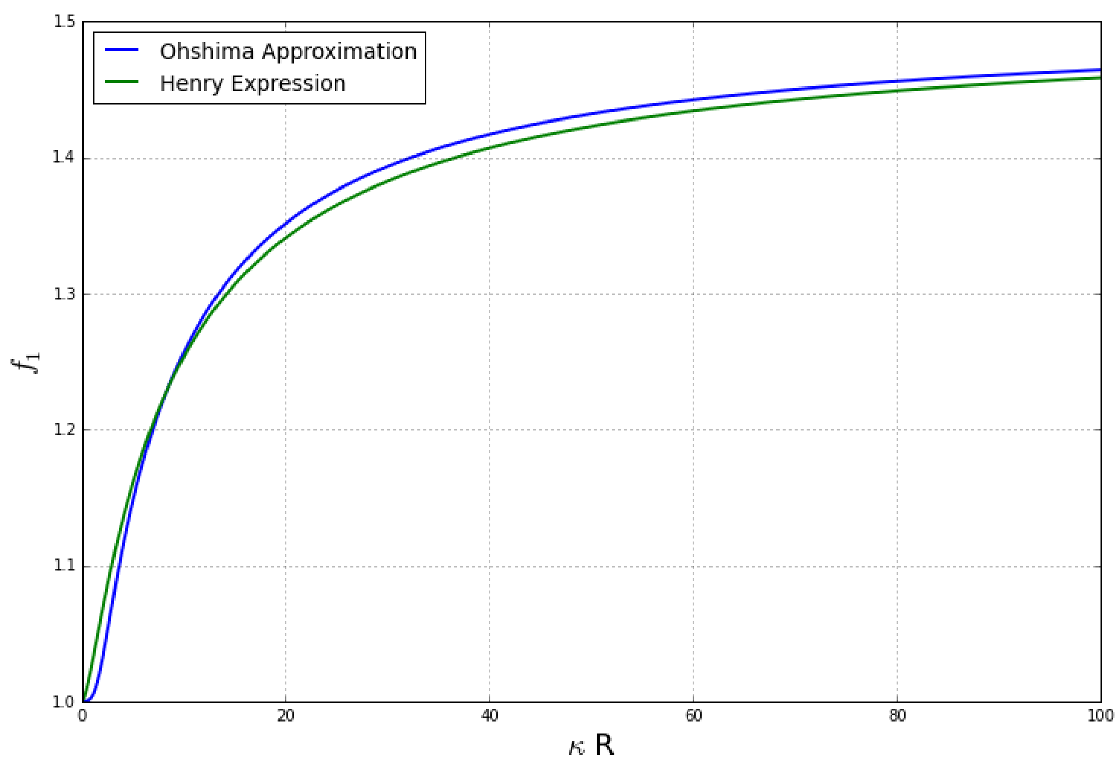
1.2 Ohshima's Approximation

$$f_1 \kappa R = 1 + \frac{1}{2\left[1 + \left(\frac{5}{2\kappa R}\left(1 + 2exp(-\kappa R)\right)\right)\right]^3} \tag{3}$$

In [4]:
```
f1kr_ohshima = 1. + 1. / (2 *(1 + ((5./(2*kr))*(1. + 2. * np.exp(-kr))))**3)
```

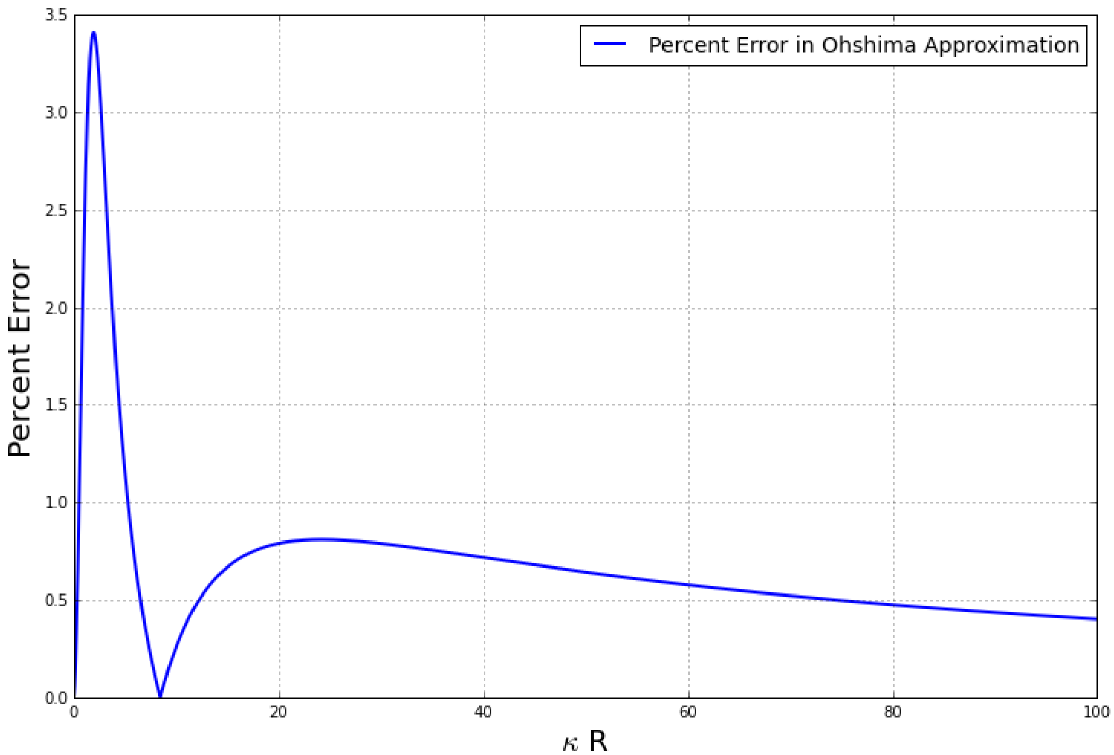
Plot Approximations

In [5]:
```
%matplotlib inline
import matplotlib.pyplot as plt

fig_1, ax = plt.subplots(figsize = (12,8))

# when plotting from arrays, columns from each are plotted against eachother
lbl = ['Ohshima Approximation','Henry Expression']
ax.plot(kr, f1kr_ohshima, kr, f1kr_henry, lw=2)
ax.legend(lbl, frameon=1, framealpha = 1, loc=0, fontsize=14)

ax.set_xlabel(''r'$\kappa$ R', fontsize = 20)
ax.set_ylabel(''r'$f_1$', fontsize = 20)
ax.grid(b = True, which = 'major')
ax.grid(b = True, which = 'major')

fig_name = 'f1_compare.pdf'
path = '/Users/Lampe/Documents/UNM_Courses/CBE-521/HW04/'
fig_1.savefig(path + fig_name)
```



In [6]:
```
fig_2, ax = plt.subplots(figsize = (12,8))

# when plotting from arrays, columns from each are plotted against eachother
lbl = ['Percent Error in Ohshima Approximation']
ax.plot(kr, np.abs(f1kr_ohshima - f1kr_henry)/ f1kr_henry * 100, lw=2)
ax.legend(lbl, frameon=1, framealpha = 1, loc=0, fontsize=14)
```

```python
ax.set_xlabel(''r'$\kappa$ R', fontsize = 20)
ax.set_ylabel(''r'Percent Error', fontsize = 20)
ax.grid(b = True, which = 'major')
ax.grid(b = True, which = 'major')

fig_name = 'f2_error.pdf'
path = '/Users/Lampe/Documents/UNM_Courses/CBE-521/HW04/'
fig_2.savefig(path + fig_name)
```



The maximum error in the Oshima Approximation of Henry's expression is less than 3.5 percent, which is probably in the range of experimental error. Therefore, yes, the Ohshima approximation is reasonable to use.

2 Problem 2

2.0.1 Calculate the average migration conductivity for $\kappa h = 1$ and $\bar{\zeta} = 1$ in a slit-shaped channel.

The electrostatic potential in a slit-shaped channel is:

$$\tilde{\Psi} \approx \tilde{\zeta} \frac{cosh\left(\kappa\left(\frac{h}{2} - x\right)\right)}{cosh\left(\frac{\kappa h}{2}\right)} \tag{4}$$

at the wall, $x = 0$:

$$\tilde{\Psi}(x = 0) \approx \tilde{\zeta} \frac{cosh\left(\kappa \frac{h}{2}\right)}{cosh\left(\frac{\kappa h}{2}\right)} = \tilde{\zeta} \tag{5}$$

at the middle of channel, $x = h/2$:

$$\tilde{\Psi}\left(x = \frac{h}{2}\right) = \tilde{\Psi}_m \approx \tilde{\zeta}\frac{cosh\left(\kappa\left(\frac{h}{2} - \frac{h}{2}\right)\right)}{cosh\left(\frac{\kappa h}{2}\right)} = \frac{\tilde{\zeta}}{cosh\left(\frac{\kappa h}{2}\right)} \tag{6}$$

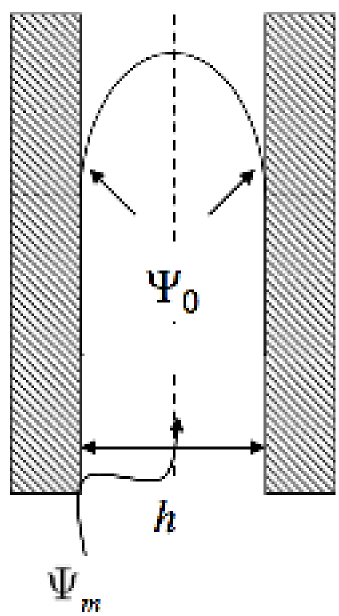
the average migration conductivity in a slit-shaped channel may be calculated via:

$$\bar{K}_{mig} = 1 + \frac{4}{\kappa h}\int_{\tilde{\zeta}}^{\tilde{\Psi}_m}\left(\frac{sinh\left(\tilde{\Psi}\right)}{\sqrt{2\left[cosh\left(\tilde{\zeta}\right) - cosh\left(\tilde{\Psi}_m\right)\right]}}\right)d\tilde{\Psi} \tag{7}$$

The schematic below identifies the physical meaning of parameters in the above equation.

In [7]:
```
from wand.image import Image as WImage
fig_name = 'fig_Sketch.pdf'
img = WImage(filename = path + fig_name)
img
```

Out[7]:



In [8]:
```
import scipy.integrate as spint

kh = 1.
zeta = 1.

psi_m = zeta / np.cosh(kh / 2.)
arg = lambda x: np.sinh(x) / np.sqrt(2*(np.cosh(zeta) - np.cosh(psi_m)))
num_int = spint.quad(arg, psi_m, zeta)
k_mig = 1. + (4./kh)*num_int[0]; k_mig
```

Out[8]: 1.993582535770678

This problem was solved numerically, and the result was:
$\bar{K}_{mig} = 2.0$ in dimensionless form

3 Problem 3

The charge of the ion on a 1:1 electrolyte is 1; therefore, for a 1:1 electrolyte:

$$z = 1 \tag{8}$$
$$m = 0.184, \text{ this value was provided in course notes for KCl} \tag{9}$$
$$M = 1 + \frac{3m}{z^2} \tag{10}$$
$$\tilde{\zeta} = \frac{e\zeta}{kT} \tag{11}$$

The provided equation for electrophoresis mobilities:

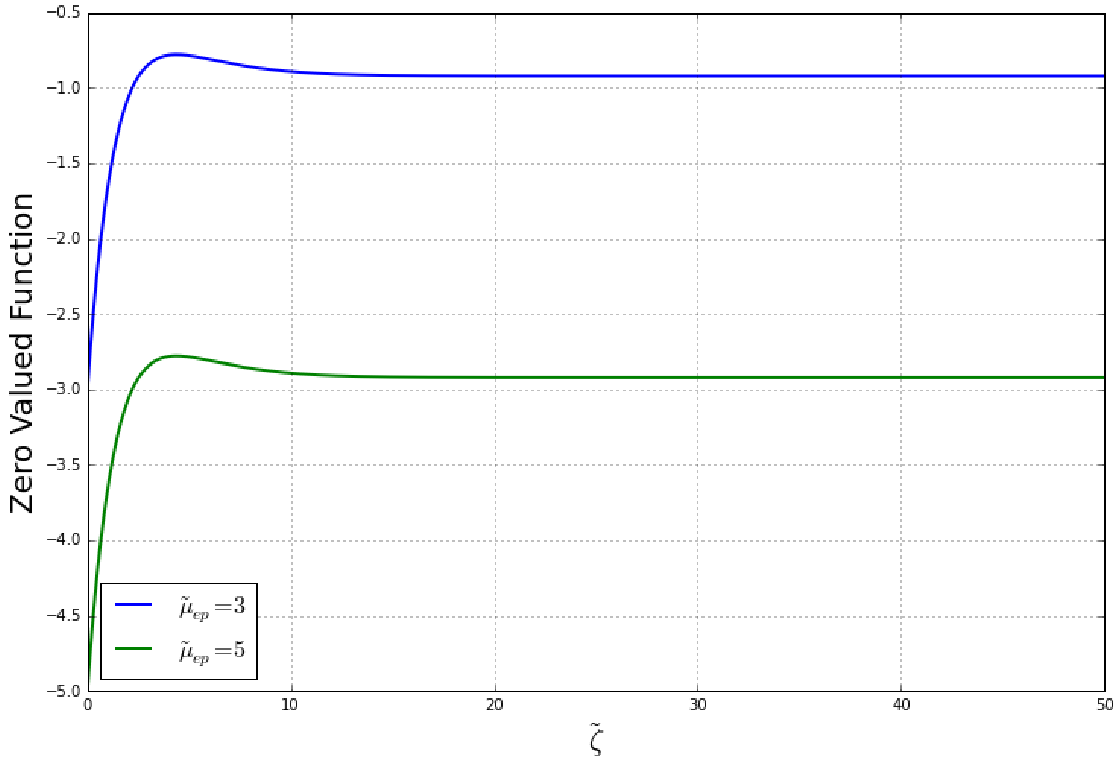
$$\tilde{\mu}_{ep} = \frac{3\tilde{\zeta}}{2} - \frac{6\left[\frac{\tilde{\zeta}}{2} - \frac{ln(2)}{z}\left(1 - exp\left(-z\tilde{\zeta}\right)\right)\right]}{2 + \frac{\kappa R}{M} exp\left(-\frac{z\tilde{\zeta}}{2}\right)} \tag{12}$$

By moving moving all terms onto one side of the equation, the roots may be solved for and $\tilde{\zeta}$ may be determined numericalliy:

$$0 = -\tilde{\mu}_{ep} + \frac{3\tilde{\zeta}}{2} - \frac{6\left[\frac{\tilde{\zeta}}{2} - \frac{ln(2)}{z}\left(1 - exp\left(-z\tilde{\zeta}\right)\right)\right]}{2 + \frac{\kappa R}{M} exp\left(-\frac{z\tilde{\zeta}}{2}\right)} \tag{13}$$

In [48]:
```
zeta = np.linspace(0,50,1000)
z = 1.
mu_1 = 3.
mu_2 = 5.
kr = 1.
z = 1.
m = .184 # for KCL
M = 1. + 3*m/z**2

num = 6*(zeta/2. - np.log(2.)/z*(1-np.exp(-z*zeta)))
den = 2 + kr/M* np.exp(-z*zeta/2.)
arg = 3.*zeta/2. - num / den
eqn_1 = arg - mu_1
eqn_2 = arg - mu_2
```

In [50]:
```
fig_3, ax = plt.subplots(figsize = (12,8))

# when plotting from arrays, columns from each are plotted against eachother
lbl = [''r'$\tilde{\mu}_{ep}= 3$', ''r'$\tilde{\mu}_{ep}= 5$']
ax.plot(zeta, eqn_1, zeta, eqn_2, lw=2)
ax.legend(lbl, frameon=1, framealpha = 1, loc=0, fontsize=16)

ax.set_xlabel(''r'$\tilde{\zeta}$', fontsize = 20)
ax.set_ylabel(''r'Zero Valued Function', fontsize = 20)
ax.grid(b = True, which = 'major')
ax.grid(b = True, which = 'major')

fig_name = 'f3_findZero.pdf'
path = '/Users/Lampe/Documents/UNM_Courses/CBE-521/HW04/'
fig_3.savefig(path + fig_name)
```



The provided equation appear to be incorrect, because I was unable to identify a point where the functions cross the $\tilde{\zeta}$ axis (root). This implies that the provided equation for $\tilde{\mu}_{ep}$ is incorrect. I believe the provided equations or my implementation of them is incorrect.