Chemistry 243 Winter Quarter 2017.
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Problem Set #5

1. Frumkin Isotherm – Electrochemical Applications
In class, we used the Nernst Equation to model the CV of a monolayer of a reversible redox reaction:

Red → Ox + e

$\Gamma_{tot} = \Gamma_{ox} + \Gamma_{red}$; $\theta = \Gamma_{ox} / \Gamma_{tot}$G

where q is the relative surface coverage.

$$\frac{\Gamma_{ox}}{\Gamma_{red}} = \frac{\theta}{(1-\theta)} = exp\left[\frac{-F}{RT}(E - E^0)\right]$$

a) Assuming we scan the potential linearly in the positive direction, make plots of θ and reversible current as a function of potential using the Nernst equation. Assume E^0 = 1.0V. What is the FWHM of the current peak?

b) The Frumkin isotherm assumes a free energy of adsorption that varies linearly with surface coverage:

$$\Delta G^0 = \Delta G^0_{\theta=0} + g\theta$$

Use this Frumkin isotherm to make plots of θ and reversible current as a function of potential. What value of g is required to create a current peak with half the FWHM of the Nernstian case?

2) Ordered monolayers

Iodine is purported to form three different ordered monolayers on a Pt(111) surface: (i) (√3×√3)R30° iodine monolayer, (ii) (√7×√7)R19.1° iodine monolayer, and (iii) (3×3) iodine monolayer. Using a computer graphic program (e.g. Powerpoint, Keynote, Adobe Illustrator), please make accurate drawings of these three structures, with Iodine-Iodine distances. State the surface coverage (ratio of Iodine to Platinum surface atoms) for each structure.

3) Resonator circuits and Q factor.

a) Consider a damped SHO:

$$m\frac{d^2x}{dt^2} + 2m\Gamma\frac{dx}{dt} + m\omega_0^2 x = 0$$

What is the Q factor of this system in terms of gamma and omega? Create Bode Nyquist Plots for Q-factors of 10^x where x = 1, 2, 3.

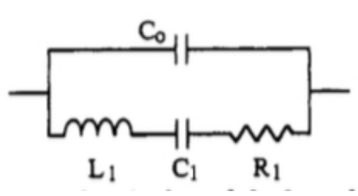
b) Create Bode and Nyquist plots for Q-factors of 10^x where x = 1, 2, 3 for the following resonator circuits:

Filter type (2nd order)	Transfer function[13]
Lowpass	$H(s) = \frac{\omega_0^2}{s^2 + \frac{\omega_0}{Q}s + \omega_0^2}$
Bandpass	$H(s) = \frac{\frac{\omega_0}{Q}s}{s^2 + \frac{\omega_0}{Q}s + \omega_0^2}$
Notch (Bandstop)	$H(s) = \frac{s^2 + \omega_0^2}{s^2 + \frac{\omega_0}{Q}s + \omega_0^2}$
Highpass	$H(s) = \frac{s^2}{s^2 + \frac{\omega_0}{Q}s + \omega_0^2}$

Can you write down the circuit corresponding to the bandpass filter?

4) QCM Measurements.

The Quartz Crystal Microbalance is often used to monitor adsorption onto surfaces. The QCM uses an AT cut quartz crystal that is driven piezoelectrically. The electrical response of the QCM can be modeled by a simple LCR circuit:



a) Consider a system where where R1=100 ohms, C0 = 1.00 picofarad, C1= 0.01 picofarads, and L1 = 75 milliHenrys. What is the resonance frequency of this system (in rad sec^{-1}) and the Q factor?

b) Please create Bode plots for the Magnitude and Phase of the total admittance (Y), and a Nyquist plot (ImY vs ReY) for the system.