Fermi statistics in ionic solutions

Bob Eisenberg <bob.eisenberg@gmail.com> Mon, Jan 20, 2014 at 9:08 AM
Reply-To: bob.eisenberg@gmail.com
To: Mark Lundstrom <lundstro@purdue.edu>, Jinn Liang Liu 劉晉良 <jinnliu@mail.nhcue.edu.tw>, Bob Eisenberg <beisenbe@rush.edu>

Dear Mark

I wanted to write you more about the issue of Fermi statistics and Fermi Poisson approach to ions in water and channels.

Let me start with a bald bold possibility so we understand the stakes.

It is possible (but by NO MEANS certain) that a great deal of chemistry in ionic solutions (i.e., all of biochemistry and most of chemistry itself) would fit data much better if it simply replaced its Boltzmann statistics with Fermi statistics.

As I am sure you know, almost all classical chemistry uses Boltzmann statistics reflexively without thought, and I was certainly guilty of that for some 40 years until Jinn Liang Liu showed me otherwise.

The reason that this assumption is inappropriate is that "crowding" phenomena are the dominant (but not the only) source of unpredicted behavior in ionic solutions.

When crowding is introduced one way or the other into traditional chemistry, things get much better.

Specifically, models of ionic solutions that assume ions as spheres

(a) are the best we have although hundreds of higher resolution models have been tried
(b) are not so bad
(c) include saturation phenomena as the first order desciption(s) of what is going on.

So this is a VERY important subject to pursue. Teaching chemists to use pde's and variational approaches is MUCH harder than telling them

to change to Fermi statistics.

Now, a little history

1) Jinn Liang Liu of NCHUE in Taiwan is responsible for this approach. Not me. There is much historical antecedent (see his paper below) but his understanding is MUCH better than those papers in my view.

2) Jinn is a fine analyst and mathematician who knows a lot about pchem. Indeed, he was the one who showed me Laidler's text which (I am embarrassed to say) I did not know about until then. You might want to look at the relevant chapters. They are the best introduction around.

https://dl.dropboxusercontent.com/u/5716448/Laidler%20Chapter%208%20Physical%20Chemistry.pdf

https://dl.dropboxusercontent.com/u/5716448/Laidler%20Physical%20Chemistry%20Chpt.%207.pdf

3) Being a mathematician, Jinn Liang is much more careful with approximations than I, or most physical scientists. Thus, he used field theory (pde's and boundary conditions) in which Fermi statistics were embedded.
I attach the papers. This is both good and bad for obvious reasons.

4) I helped him apply his Fermi Poisson to channels.

5) It was only after doing these two papers that Jinn Liang realized that many channel problems could be "done" (i.e., approximated) with **JUST THE STATISTICS and did not need the pde's.**

6) We do NOT yet know how to parameterize the PURELY statistical models (the pde's are not a problem. everything is pretty clear there) and are starting that in the paper under review. See the abstract based on that paper below.

I do not wish to misquote you, but I believe your intuition that just the statistics themselves might make a great deal of difference is correct.

The problem is to do it!

I am copying this email to Jinn Liang to introduce you two to each other.
Much good would happen if you have a chance to talk to each other.
Jinn will in fact be in San Francisco next month for the Biophysics Meeting.
By any happenstance will you be in that part of the world around then?

As ever
Bob

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Return Address for email: beisenbe@rush.edu or bob.eisenberg@gmail.com

Bob aka RS Eisenberg
Bard Endowed Professor and Chairman

Dept of Molecular Biophysics & Physiology
Rush Medical Center
1653 West Congress Parkway
Chicago IL 60612 USA
Office Location: Room 1291 of
Jelke Building at 1750 West Harrison

Email: beisenbe@rush.edu
Voice: +312-942-6467
FAX: +312-942-8711
FAX to Email: +801-504-8665
Department WebSite: http://www.phys.rush.edu/
Personal WebSite: http://www.phys.rush.edu/RSEisenberg/
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3 attachments

Calcium JPC Oct 2013 AS PUBLISHED.pdf
708K

_ Jinn Liang Liu Poisson Fermi as published.pdf
876K

Jinn Liu Abstract AS SUBMITTED.pdf
649K