Math Problem: A Self Driven Heat Equation PhL 12.17.13

This material has all been installed in new Section 3.1.

1. My motivation is this equation which seems to arise in charge diffusion,

$$D\nabla^2\rho - \partial_t\rho - (\sigma/\varepsilon)\rho = 0 \qquad (1)$$

$$\partial_t\rho = D\nabla^2\rho - (\sigma/\varepsilon)\rho \qquad (2)$$

$$\nabla^2\rho - (1/D)\partial_t\rho - (\sigma/D\varepsilon)\rho = 0 \qquad (3)$$

$$[\nabla^2 - (1/D)\partial_t]\rho = (\sigma/D\varepsilon)\rho \qquad (4)$$

It seems to be a heat equation whose source is its own solution. This is not something that was treated by Stak, he assumed a source q(x) that was prescribed.

2. Write (2) in this form

$$\partial_t\rho = a\nabla^2\rho + b\rho \qquad (5) \qquad a = D \qquad b = -(\sigma/\varepsilon) < 0$$

If we seek a 1D solution, this equation reads

$$\partial_t\rho = a\partial_x^2\rho + b\rho \qquad (5)$$

This matches a Polyanin form

1.1.3. Equation of the Form $\dfrac{\partial w}{\partial t} = a\dfrac{\partial^2 w}{\partial x^2} + bw + \Phi(x,t)$

and P claims this fundy solution

2°. Fundamental solution:

$$\mathscr{E}(x,t) = \frac{1}{2\sqrt{\pi at}}\exp\left(-\frac{x^2}{4at} + bt\right).$$

This gives me a **hint** to perhaps simplify the original equation. Consider

$$\partial_t\rho = a\nabla^2\rho + b\rho$$

and try

$$u = \rho\, e^{-bt}$$

$\partial_t u = \rho(-b\, e^{-bt}) + \partial_t \rho\, e^{-bt} = -bu + \partial_t \rho\, e^{-bt}$

and try

$\rho = e^{bt} u$

$\partial_t \rho = b\, e^{bt} u + e^{bt} \partial_t u = e^{bt}(bu + \partial_t u)$

$\nabla^2 \rho = e^{bt} \nabla^2 u$

Then we have

$\partial_t \rho = a\nabla^2 \rho + b\rho$

or

$e^{bt}(bu + \partial_t u) = a\, e^{bt} \nabla^2 u + b\, e^{bt} u$

or

$(bu + \partial_t u) = a\, \nabla^2 u + b\, u$

or

$\partial_t u = a\, \nabla^2 u$

and I have then successfully obtained the heat equation!

3. If we have a delta function source q(x) for the heat equation, we know how it evolves using the propagator, and that is where P's equation comes from

2°. Fundamental solution:

$$\mathscr{E}(x,t) = \frac{1}{2\sqrt{\pi a t}} \exp\left(-\frac{x^2}{4at} + bt\right).$$

This is the Saxon propagator thing with the extra e^{bt}. The first term describes a packet at x = 0 which gets broader as time increases, since width is $\sqrt{4at}$. The second term must be an exponential decay!

So my solution would be

$\rho(x,t) = 1/[2\sqrt{\pi D t}\,] \exp(-x^2/4Dt)\, e^{-(\sigma/\varepsilon)t}$

This IS the solution to the following equation

$(\partial_t - a\, \nabla^2)u = \delta(x)\delta(t)$ // with some constant.

which I could write as

$(\partial_t - a\, \nabla^2)[\, \rho\, e^{-bt}] = \delta(x)\delta(t)$

$(\partial_t \rho)\, e^{-bt} - b\,\rho\, e^{-bt} - a\, e^{-bt}\nabla^2 \rho = \delta(x)\delta(t)$

$[\partial_t \rho - b\,\rho - a\nabla^2 \rho] = \delta(x)\delta(t)\, e^{bt} = \delta(x)\delta(t)$

So my solution is the propagator for this equation

$[\partial_t - b - a\nabla^2]\rho = \delta(x)\delta(t)$

If we start with a source pulse at x = 0 and t = 0, we get decaying propagation.

Go back to

$\nabla^2\rho - (1/D)\partial_t\rho = (\sigma/D\varepsilon)\rho$

In a good conductor, $(\sigma/D\varepsilon)\rho >> \nabla^2\rho$ so this equation is

$-(1/D)\partial_t\rho \approx (\sigma/D\varepsilon)\rho$

$-\partial_t\rho \approx (\sigma/\varepsilon)\rho$

$\rho(r,t) = \rho(r,0)\, e^{-t/\tau}$ $\qquad\qquad$ $\tau = \varepsilon/\sigma$ = a very short time

In a good dielectric, $(\sigma/D\varepsilon)\rho << \nabla^2\rho$ so the equation is

$\nabla^2\rho - (1/D)\partial_t\rho = 0$

$\partial_t\rho - D\nabla^2\rho = 0$ $\qquad$ $\partial_t = \sec^{-1}$ $\qquad$ $\nabla^2 = m^{-2}$ $\qquad$ $D = m^2/\sec$

which is the diffusion/heat equation. Now **Stak** considers this equation

$\partial_t E - a\nabla^2 E = q\,\delta(x)\delta(t)$ $\qquad\qquad$ 5.133

so the connection is a = D. Stak shows in (5.140) that the solution is

$\rho(r,t) = q\exp(-r^2/4Dt) / (4\pi Dt)^{3/2}$

What about dimensions here??? The factor

$(4\pi Dt)^{-3/2} = (m^2/\sec * \sec)^{-3/2} = m^{-3}$ which is correct.

So in a good dielectric what does this say? As t increases, the distribution spreads out, since it has a radius of about $s = \sqrt{4Dt}$. And the scale at the center decays as $(4\pi Dt)^{-3/2}$. that is

$$\rho(0,t) = q / (4\pi Dt)^{3/2}$$

At t = 0 it is of course infinite since δ(t). So what is the time constant here? Suppose I consider a tiny volume V in which the charge is located, centered at r = 0. then

$$\rho(0,t)V = q\,V / (4\pi Dt)^{3/2}$$

I don't think I am doing this right! **I am really interested in**

$$\partial_t\rho - D\nabla^2\rho = 0 \qquad \rho(r,0) = \rho_o(r)$$

not the causal Green's problem. I have some initial charge distribution, what happens to it? In 3D radial world this equation is

$$\partial_t\rho = D\nabla^2\rho = D\,[r^{-2}\partial_r(r^2\partial_r\rho)\,] = D\,[\,\partial_r^2\rho + (2/r)\,\rho\,] \qquad D = a = m^2/sec$$

This is **Polyanin 1.2.3.** He lists off a ton of solutions. For r in (0,∞) he writes

$$\rho(r,t) = [2r\sqrt{\pi at}\,]^{-1} \int_0^\infty r'dr'\,\rho(r',0)\,\{\,\exp[-(r-r')^2/4at] - \exp[-(r+r')^2/4at]\,\}$$

with a Butkovskiy reference from 1979. I verified that it works at t = 0 based on the fact that only the first term contributes and a little fiddling. **NOW suppose** we use a delta for $\rho(r',0) = q\,\delta(\mathbf{r})$ which has the right dimensions, and we use $\delta(\mathbf{r}) = \delta(r)/4\pi r^2$ so that $\int \delta(\mathbf{r})\,dV = 0$. then

$$\rho(r,t) = [2r\sqrt{\pi at}\,]^{-1} \int_0^\infty r'dr'\,q\,\delta(r')/4\pi r'^2\,\{\,\exp[-(r-r')^2/4at] - \exp[-(r+r')^2/4at]\,\}$$

$$= [2r\sqrt{\pi at}\,]^{-1}\,(q/4\pi) \int_0^\infty r'^{-1}dr'\,\{\,\exp[-(r-r')^2/4at] - \exp[-(r+r')^2/4at]\,\}\,\delta(r')$$

The integrand is supposed to be evaluated at r' = 0, but we have a 0/0 situation, so Hopital?

$$num = \exp[-(r-r')^2/4at] - \exp[-(r+r')^2/4at]$$

$$\partial_{r'}num_1 = \exp[-(r-r')^2/4at] * \partial_{r'}\,[-(r-r')^2/4at]$$

$$= \exp[-(r-r')^2/4at]\;[\,-2(r-r')/4at * (-1)\,]$$

$$= \exp[-(r-r')^2/4at]\;[\,(r-r')/2at\,]$$

$$\partial_{r'}num_2 = \exp[-(r+r')^2/4at] * \partial_{r'}\,[-(r+r')^2/4at]$$

$$= \exp[-(r+r')^2/4at]\;[\,-2(r+r')/4at * (+1)\,]$$

$= \exp[-(r+r')^2/4at]\ \ [\ -(r+r')/2at\ ]$

$\partial_{r'}\text{num} \approx \exp[-(r)^2/4at]\ \{\ \ (r-r')/2at + (r+r')/2at\ ]\ \}$

$= \exp[-(r)^2/4at]\ r/at$

$\partial_{r'}\text{den} = \partial_{r'}r' = 1$

So then we have

$\rho(r,t) = [2r\sqrt{\pi at}\ ]^{-1}\ (q/4\pi)\ \exp[-(r)^2/4at]\ r/at$

$= [2\sqrt{\pi at}\ ]^{-1}\ (q/4\pi)\ \exp[-(r)^2/4at]\ 1/at$

$= [\sqrt{4\pi at}\ ]^{-1}\ (q)\ \exp[-(r)^2/4at]\ 1/(4\pi at)$

$= q\ [4\pi at]^{-3/2}\ \exp[-(r)^2/4at]$

and this is my same solution as before -- this is the fundy solution! How can that be? Here I did not pulse the source only at t = 0, I just said $\rho(\mathbf{r},0) = q\delta(\mathbf{r})$. AHA! The reason is explained in Stak 5.136! I dimly remember this now. So I am treating the right problem here, and the result is then as expected.

I just found this in my Stak support notes,

1. $f_t(x) = \exp(-x^2/(4t))/\ (\sqrt{\pi t}\ )$ $\qquad\qquad$ $\lim_{t\to 0} f_t(x) = 2\ \delta(x)$

so that would be another way to verify the t = 0 limit of the above

Next: try a little narrow Gaussian for $\rho(r',0)$ and see what it does with Maple.

Problem: What I don't like about the delta source at t = 0 is that it is infinite at t = 0 and so I cannot come up with a time constant for it to spread out? The spread radius is $r = \sqrt{4at}$ so that says how big it has become by time t, starting at t = 0. You have to pick a specific distance to get a time constant!

Suppose I pick r = 1 nm = 10^{-9}m, a small but macroscopic distance. Then for germanium

$r^2 = 4at$ $\qquad\qquad$ $t = (1/4a)r^2 = (1/4D)r^2 = (1/4)(r^2/D)$

$D = 100\ \text{cm}^2/\text{sec} \times [1\text{m}^2/10^4\text{cm}^2] = 100 \times 10^{-4}\ \text{m}^2/\text{sec} = 10^{-2}\text{m}^2/\text{sec}$ ok

$r^2/D = 10^{-18}\ \text{m}^2\ /\ [10^{-2}\text{m}^2/\text{sec}\ ] = 10^{-16}\ \text{sec}$

$t = (1/4)(r^2/D) = (1/4)\ 10^{-16}\ \text{sec}$ = very fast

I thought this was going to be slow, not fast?? Polyethylene?

I found a paper that I think does a theoretical study of poly and concludes in its abstract that

$\mu = 2 \times 10^{-3} cm^2/Vs$ = electron mobility in pure amorphous PE

pdfserv.aip.org/JCPSA6/vol_119/iss_5/2669_1.pdf

As I poke around, the idea is that a dielectric doesn't have any free electrons so it really has no free charge at all. The very high σ values I quote in lines ($\sigma \approx 10^{-15}$ mho/m) reflects that fact. I have the equation

$\sigma = (nq^2\tau/m)$ = conductivity

where I think n is supposed to be the density of electrons, and I guess THAT is pretty small in PE. So maybe D doesn't really matter because there are no free electrons to diffuse in the first place. This is true of dielectrics and insulators. So maybe I don't really have to do anything at all on this subject!

Article of Jones says PE really does have a crystalline periodic structure and thus really does have energy bands.

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So maybe Dt = 4 is when the charge is gone, so $\tau \approx$ D/4, What is D for a dielectric??

Room temperature properties of Si, Ge, and GaAs

Quantity	*Symbol*	*Si*	*Ge*	*GaAs*	*(Unit)*
Crystal structure		D	D	Z	–
Gap: Direct (*D*) / Indirect (*I*)		*I*	*I*	*D*	–
Lattice constant	a_0 =	5.43095	5.64613	5.6533	Å
Bandgap energy	E_g =	1.12	0.66	1.42	eV
Intrinsic carrier concentration	n_i =	1.0×10^{10}	2.0×10^{13}	2.0×10^{6}	cm^{-3}
Effective DOS at CB edge	N_c =	2.8×10^{19}	1.0×10^{19}	4.4×10^{17}	cm^{-3}
Effective DOS at VB edge	N_v =	1.0×10^{19}	6.0×10^{18}	7.7×10^{18}	cm^{-3}
Electron mobility	μ_n =	1500	3900	8500	$cm^2/(Vs)$
Hole mobility	μ_p =	450	1900	400	$cm^2/(Vs)$
Electron diffusion constant	D_n =	39	101	220	cm^2/s
Hole diffusion constant	D_p =	12	49	10	cm^2/s
Electron affinity	χ =	4.05	4.0	4.07	V
Minority carrier lifetime	τ =	10^{-6}	10^{-6}	10^{-8}	s
Electron effective mass	m_e^* =	0.98 m_e	1.64 m_e	0.067 m_e	–
Heavy hole effective mass	m_{hh}^* =	0.49 m_e	0.28 m_e	0.45 m_e	–
Relative dielectric constant	ε_r =	11.9	16.0	13.1	–
Refractive index near E_g	$\overline{n}$ =	3.3	4.0	3.4	–
Absorption coefficient near E_g	α =	10^3	10^3	10^4	cm^{-1}

Here I think claim is D = 100 cm^2/sec for Ge, but dimensions seem wrong. No they are right. I found a particle physics paper claiming 35 for Si instead of 39.

http://www.kayelaby.npl.co.uk/toc/

2. R. M. Glaeser and R. S. Berry, "Mobilities of Electrons and Holes in Organic Molecular Solids. Comparison of Band and Hopping Models," J. Chem. Phys. 44, 3797-3810 (1966).

In a symmetric infinite medium the solution is, for D = 1,

$$\rho(r,t) = \theta(t)\,[4\pi(t)]^{-3/2}\exp(-r^2/4t)$$