Homework #2 – Solutions

Problem 1:

(a) The function $\hat{G}_0(k)$ is clearly C^∞ for $|k|<1/2$ and $|k|>1/2$. We must only consider $|k|=1/2$. To begin, notice that

$$\frac{d}{dk}\left(\frac{k^2}{k^2-1/4}\right) = \frac{2k(1-k^2)}{(k^2-1/4)^2}$$

is a rational function of k. We use this fact to show, by induction, that

$$\frac{d^n}{dk^n}\exp\left(\frac{k^2}{k^2-1/4}\right) = \exp\left(\frac{k^2}{k^2-1/4}\right)\frac{P_n(k)}{Q_n(k)}$$

for some polynomials $P_n(k)$ and $Q_n(k)$. The case $n=0$ is obvious, with $P_0(k)=Q_0(k)=1$. We use the induction hypothesis to derive

$$\frac{d^{n+1}}{dk^{n+1}}\exp\left(\frac{k^2}{k^2-1/4}\right) = \frac{d}{dk}\left[\exp\left(\frac{k^2}{k^2-1/4}\right)\frac{P_n(k)}{Q_n(k)}\right]$$

$$= \exp\left(\frac{k^2}{k^2-1/4}\right)\cdot\left[\frac{2k(1-k^2)}{(k^2-1/4)^2}\frac{P_n(k)}{Q_n(k)} + \frac{P_n'(k)Q_n(k)-Q_n'(k)P_n(k)}{Q_n^2(k)}\right]$$

$$= \exp\left(\frac{k^2}{k^2-1/4}\right)\cdot\left[\frac{2k(1-k^2)P_n(k)Q_n(k)+P_n'(k)Q_n(k)-Q_n'(k)P_n(k)}{(k^2-1/4)Q_n^2(k)}\right]$$

$$= \exp\left(\frac{k^2}{k^2-1/4}\right)\cdot\frac{P_{n+1}(k)}{Q_{n+1}(k)} \checkmark$$

In fact, it follows from this argument that $Q_{n+1}(k) = (k^2 - 1/4)^2 Q_n^2(k)$ and thus

$$Q_n(k) = \left(k^2 - \frac{1}{4}\right)^{2(2^n - 1)}.$$

We now note that

$$\ln\left[\frac{d^n}{dk^n}\exp\left(\frac{k^2}{k^2 - 1/4}\right)\right]$$

$$= \frac{k^2}{k^2 - 1/4} + \ln P_n(k) - \ln Q_n(k)$$

Taking the limit $k \to 1/2^-$, we see that $\frac{k^2}{k^2 - 1/4} \to -\infty$. The logarithmic terms may also diverge, e.g.

$$\ln Q_n(k) = 2(2^n - 1)\ln\left(k^2 - \frac{1}{4}\right) \longrightarrow -\infty$$

However, this divergence is much slower, at only a logarithmic rate, so that

$$(k^2 - 1/4)\ln P_n(k),\ (k^2 - 1/4)\ln Q_n(k) \longrightarrow 0.$$

Thus,

$$\ln\left[\frac{d^n}{dk^n}\exp\left(\frac{k^2}{k^2 - 1/4}\right)\right] = \frac{1}{k^2 - 1/4} \times$$

$$\left[k^2 + (k^2 - 1/4)\ln P_n(k) - (k^2 - 1/4)\ln Q_n(k)\right]$$

$$\longrightarrow -\infty \times (k^2 + 0) = -\infty$$

as $k \to 1/2^-$.

Equivalently,

$$\frac{d^n}{dk^n} \exp\left(\frac{k^2}{k^2 - 1/4} \right) \longrightarrow 0 \qquad \text{as} \quad k \to 1/2^- .$$

On the other hand, since $\hat{G}_0(k) \equiv 0$ for $k \geq 1/2$, it also follows that

$$\frac{d^n}{dk^n} \hat{G}_0(k) \longrightarrow 0 \qquad \text{as} \quad k \to 1/2^+ .$$

Thus, we ~~have~~

$$\left. \frac{d^n}{dk^n} \hat{G}_0(k) \right|_{k=1/2} = 0$$

to make $\hat{G}_0(k)$ a C^∞ function.

(b) Because $\hat{G}_0(k)$ is even in k, its inverse Fourier transform is given by

$$G_0(x) = \int dk\, \hat{G}_0(k) \cos(kx)$$

which is clearly real, or, equivalently, by

$$G_0(x) = \int dk\, \hat{G}_0(k)\, e^{ikx} .$$

We use the latter formula to prove the rapid decay property. Multiplying both sides by x^p gives

$$x^p\, G_0(x) = \int dk\ \hat{G}_0(k) \left(\frac{1}{i}\frac{\partial}{\partial k}\right)^p e^{ikx}$$

$$= \int dk \left(i \frac{\partial}{\partial k}\right)^p \hat{G}_0(k)\ e^{ikx}$$ by integration by parts

so that

$$|x|^p\, |G_0(x)| \leq \int dk \left| \frac{\partial^p}{\partial k^p} \hat{G}_0(k) \right| \cdot \underbrace{\left| e^{ikx} \right|}_{=1}$$

$$= \underbrace{\int_{-1/2}^{1/2} dk \left| \frac{\partial^p}{\partial k^p} \hat{G}_0(k) \right|}_{\equiv C_p} < +\infty$$

Thus,

$$|G_0(x)| \leq \frac{C_p}{|x|^p},$$

for some constant C_p, for all integers p.

To show analyticity of $G_0(x)$, we substitute

$$\cos(kx) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} k^{2n} x^{2n},$$

to obtain

$$G_0(x) = \sum_{n=0}^{\infty} c_{2n}\, x^{2n}$$

with

$$c_{2n} = \frac{(-1)^n}{(2n)!} \int dk\ \hat{G}_0(k)\, k^{2n}.$$

We shall show that this power series for $G_0(x)$ converges absolutely and, thus, that $G_0(x)$ is analytic. Note that

$$|c_{2n}| \leq \frac{1}{(2n)!} \int_{-1/2}^{1/2} dk\, \hat{G}_0(k)\, k^{2n}$$

$$\leq \frac{1}{(2n)!} \left(\frac{1}{2}\right)^{2n} \int_{-1/2}^{1/2} dk\, \hat{G}_0(k) = \frac{C}{(2n)!} \left(\frac{1}{2}\right)^{2n}$$

Thus,

$$\sum_{n=0}^{\infty} |c_{2n}| \cdot |x|^{2n} \leq C \sum_{n=0}^{\infty} \frac{1}{(2n)!} \left|\frac{x}{2}\right|^{2n}$$

$$= C \cosh\left(\frac{x}{2}\right) < +\infty .$$

(c) Although real, $G_0(x)$ need not be everywhere positive. However,

$$G(x) = [G_0(x)]^2 \geq 0 .$$

Furthermore, since $G_0(x)$ is C^∞, so is $G(x)$ (by the product-rule of differentiation). Also, $G(x)$ decays faster than any power law, since

$$|x|^p G(x) = \left[|x|^{p/2} G_0(x)\right]^2 \longrightarrow 0$$

as $|x| \longrightarrow \infty$.

(d) By the convolution theorem

$$\hat{G}(k) = (\widehat{G_0^2})(k) = \int đp\ \hat{G}_0(p)\,\hat{G}_0(k-p).$$

Since $\hat{G}_0(p) \geq 0$, we see that $\hat{G}(k) \geq 0$. Also,

$$\frac{d^n}{dk^n}\hat{G}(k) = \int đp\ \hat{G}_0(p) \cdot \frac{d^n}{dk^n}\hat{G}_0(k-p),$$

which is well-defined, since $\hat{G}_0$ is C^∞. Thus, $\hat{G}$ is C^∞, too.
Finally, we note that the above integral vanishes unless

$$|p| \leq \tfrac{1}{2} \quad \underline{\text{and}} \quad |k-p| \leq \tfrac{1}{2}.$$

In that case,

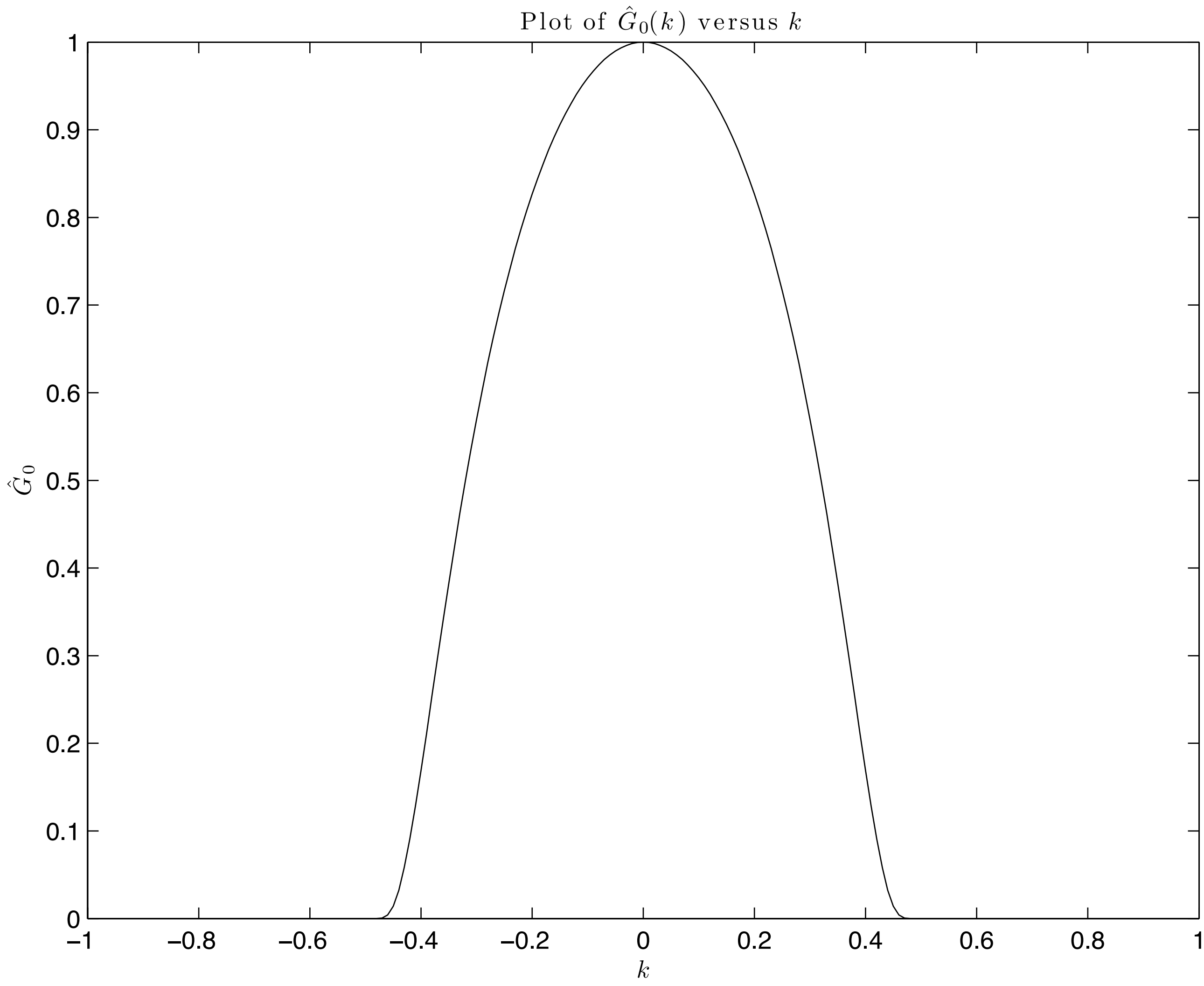
$$|k| = |(k-p) + p| \leq |k-p| + |p| \leq \tfrac{1}{2} + \tfrac{1}{2} = 1.$$

Thus,

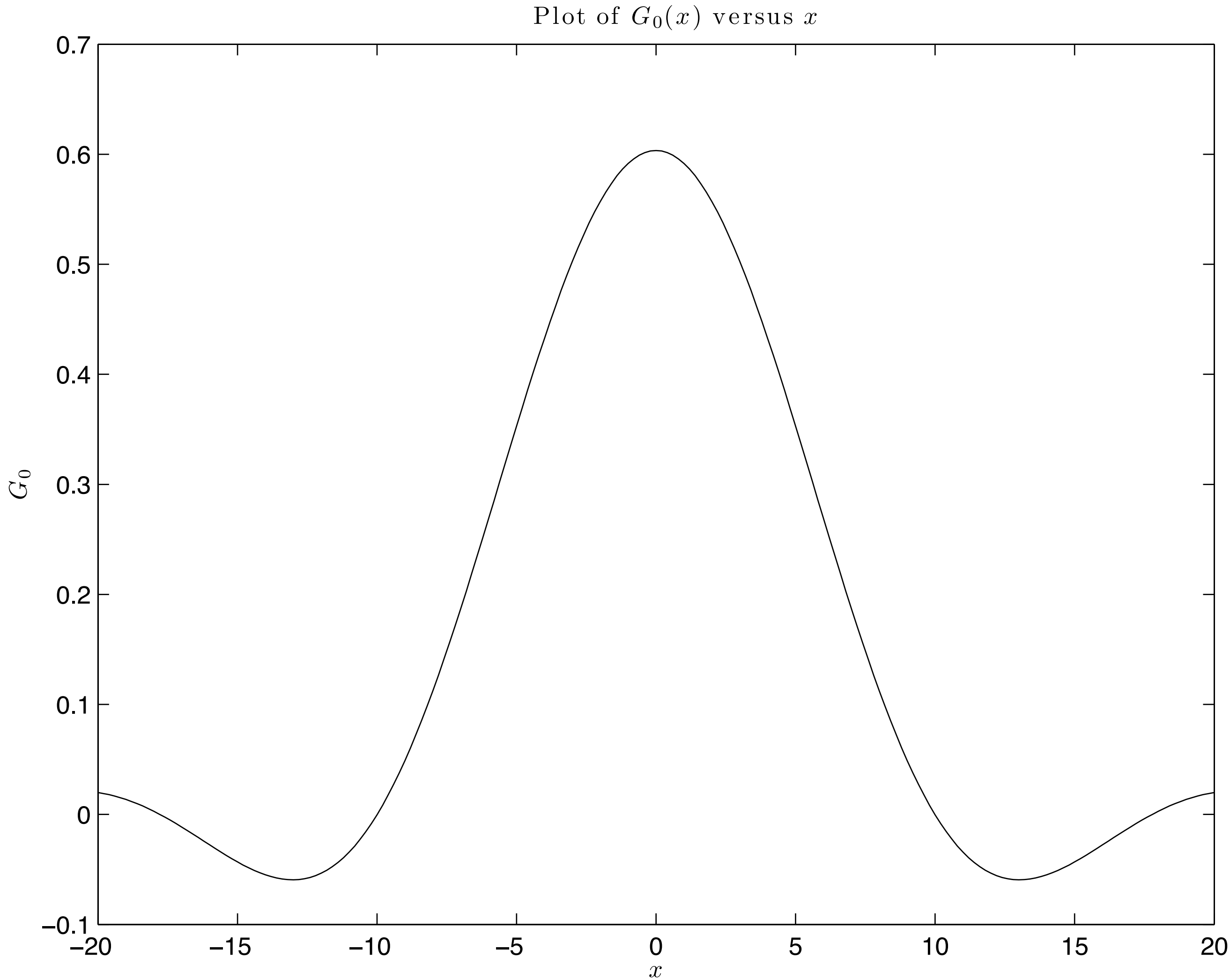
$$\hat{G}(k) \equiv 0$$

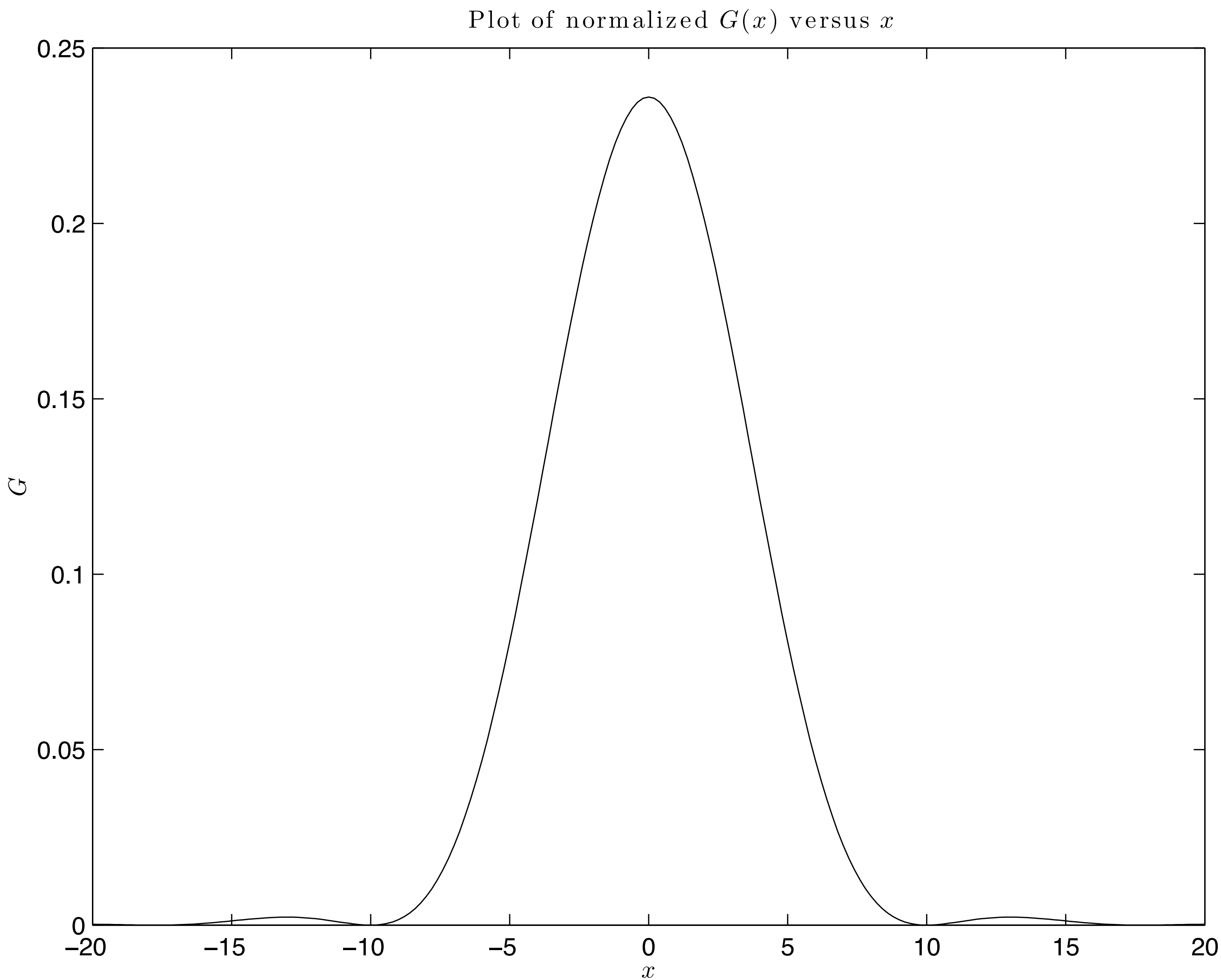
unless $|k| \leq 1$, so that $\hat{G}$ is compactly supported in the interval $[-1, 1]$.

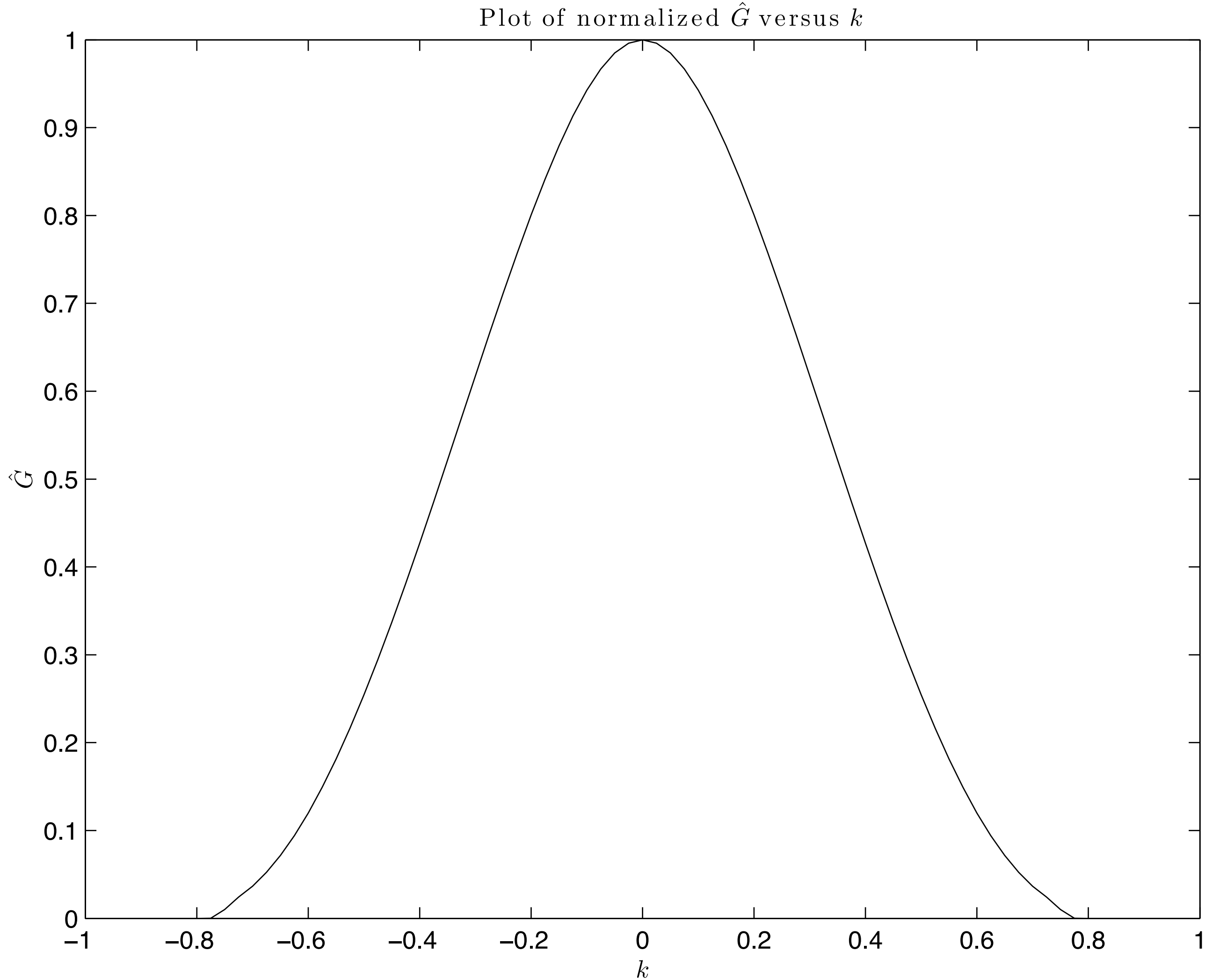
<u>QED</u>



Plot of $\hat{G}_0(k)$ versus k
$\hat{G}_0$
k
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
−1
−0.8
−0.6
−0.4
−0.2
0
0.2
0.4
0.6
0.8
1


Plot of $G_0(x)$ versus x
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
−0.1
G_0
−20
−15
−10
−5
0
5
10
15
20
x


Plot of normalized $G(x)$ versus x
0.25
0.2
0.15
0.1
0.05
0
G
−20
−15
−10
−5
0
5
10
15
20
x



Plot of normalized Ĝ versus k
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Ĝ
–1
–0.8
–0.6
–0.4
–0.2
0
0.2
0.4
0.6
0.8
1
k

Problem 2: (a) Starting with

$$\mathbf{j}(\mathbf{x},t) = \sum_{n=1}^{N} \mathbf{p}_n(t)\, \delta^3(\mathbf{x}-\mathbf{r}_n(t)))$$

we get that

$$\partial_t \mathbf{j}(\mathbf{x},t) = \left.\sum_{n=1}^{N} \dot{\mathbf{p}}_n(t)\, \delta^3(\mathbf{x}-\mathbf{r}_n(t))\ \right\} (\mathrm{I})$$
$$\left. + \sum_{n=1}^{N} \mathbf{p}_n(t)\, (-\dot{\mathbf{r}}_n(t)\cdot\nabla_x)\, \delta^3(\mathbf{x}-\mathbf{r}_n(t))\ \right\} (\mathrm{II})$$

by the product rule and the chain rule.

Since $\dot{\mathbf{r}}_n(t) = \mathbf{p}_n(t)/m$, the second term (II) becomes

$$(\mathrm{II}) = -\sum_{n=1}^{N} \frac{\mathbf{p}_n(t)\,\mathbf{p}_n(t)}{m}\cdot\nabla_x\, \delta^3(\mathbf{x}-\mathbf{r}_n(t))$$

$$= -\nabla_x \cdot \left[\sum_{n=1}^{N} \frac{\mathbf{p}_n(t)\,\mathbf{p}_n(t)}{m}\, \delta^3(\mathbf{x}-\mathbf{r}_n(t)) \right]$$

Since $\dot{\mathbf{p}}_n(t) = \sum_{m\neq n} \mathbf{F}_{nm}$, the first term (I) becomes

$$(\mathrm{I}) = \sum_{\substack{n,m \\ n\neq m}} \mathbf{F}_{n,m}\, \delta^3(\mathbf{x}-\mathbf{r}_n(t)).$$

By Newton's third law,

$$\mathbf{F}_{n,m} = -\mathbf{F}_{n,m}.$$

Thus, we may write by symmetrization

$$(\mathrm{I}) = -\frac{1}{2} \sum_{\substack{n,m \\ n\neq m}} \mathbf{F}_{n,m} \left[\delta^3(\mathbf{x}-\mathbf{r}_m(t)) - \delta^3(\mathbf{x}-\mathbf{r}_n(t)) \right) \Big].$$

Note next by the fundamental theorem of calculus that

$$\delta^3(\mathbf{x}-\mathbf{r}_m) - \delta^3(\mathbf{x}-\mathbf{r}_n) = \int_0^1 ds \, \frac{d}{ds} \delta^3(\mathbf{x}-\mathbf{r}_n + s\mathbf{r}_{nm})$$

w/ $\mathbf{r}_{nm} = \mathbf{r}_n - \mathbf{r}_m$

$$= (\mathbf{r}_{nm} \cdot \nabla_x) \int_0^1 ds \, \delta^3(\mathbf{x}-\mathbf{r}_n + s\mathbf{r}_{nm})$$

by the chain rule.

Substituting gives

$$(\mathrm{I}) = -\nabla_x \cdot \Big\{ \frac{1}{2} \sum_{\substack{n,m \\ n\neq m}} \mathbf{F}_{n,m} \mathbf{r}_{n,m} \int_0^1 ds \, \delta^3(\mathbf{x}-\mathbf{r}_n + s\mathbf{r}_{nm}) \Big].$$

Combining the two results gives $\partial_t \mathbf{j}(\mathbf{x},t) + \nabla \cdot \mathbf{T}(\mathbf{x},t) = 0$, with

$$\mathbf{T}(\mathbf{x},t) = \sum_{n=1}^{N} \frac{\mathbf{p}_n(t)\mathbf{p}_n(t)}{m} \delta^3(\mathbf{x}-\mathbf{r}_n(t)))$$

$$+ \frac{1}{2} \sum_{\substack{n,m \\ n\neq m}} \mathbf{F}_{n,m} \mathbf{r}_{nm} \int_0^1 ds \, \delta^3(\mathbf{x}-\mathbf{r}_n + s\mathbf{r}_{nm}).$$

(b) We now make a similar argument for energy conservation, starting with

$$e(x,t) = \sum_{n=1}^{N} \left(\frac{p_n^2(t)}{2m} + \frac{1}{2} \sum_{m \neq n} U(r_{nm}(t)) \right) \delta^3(x - r_n(t))$$

so that

$$\left.\partial_t e(x,t) = \sum_{n=1}^{N} \frac{d}{dt} \left(\frac{p_n^2(t)}{2m} + \frac{1}{2} \sum_{m \neq n} U(r_{nm}(t)) \right) \delta^3(x - r_n(t)) \right\} (\mathrm{II})$$

$$\left. + \sum_{n=1}^{N} \left(\frac{p_n^2}{2m} + \frac{1}{2} \sum_{m \neq n} U(r_{nm}(t)) \right) \frac{d}{dt} \delta^3(x - r_n(t)) \right\} (\mathrm{I})$$

by the product rule.

For the term (I), we use as before that $\frac{d}{dt} \delta^3(x - r_n(t)) = -\frac{p_n(t)}{m} \cdot \nabla_x \delta^3(x - r_n(t))$, which gives

$$(\mathrm{I}) = -\nabla_x \cdot \left[\sum_{n=1}^{N} \left(\frac{p_n^2}{2m} + \frac{1}{2} \sum_{m \neq n} U(r_{nm}) \right) \frac{p_n}{m} \delta^3(x - r_n) \right].$$

The time-derivative of the second term (II) gives two contributions:

$$(\mathrm{II}) = \sum_{n=1}^{N} \frac{p_n(t)\cdot \dot{p}_n(t)}{m}\delta^3(x-r_n(t)) + \frac{1}{2}\sum_{\substack{n,m\\ n\neq m}} \dot{r}_{nm}(t)\cdot \overbrace{\nabla U(r_{nm})}^{-F_{nm}}\delta^3(x-r_{nm}(t)))$$

by the product & chain rule

$$= \sum_n \frac{p_n}{m}\Big(\sum_{m\neq n} F_{nm}\Big)\delta^3(x-r_n) - \frac{1}{2m}\sum_{\substack{n,m\\ n\neq m}} (p_n - p_m)\cdot F_{nm}\,\delta^3(x-r_n)$$

by the equations of motion

$$= \sum_{\substack{n,m\\ n\neq m}} \frac{1}{2m}(p_n + p_m)\cdot F_{nm}\,\delta^3(x-r_n)$$ by combining the terms

$$= \sum_{\substack{n,m\\ n\neq m}} \frac{1}{4m}(p_n+p_m)\cdot F_{n,m}\Big[\delta^3(x-r_n) - \delta^3(x-r_m)\Big]$$ using $F_{nm} = -F_{mn}$

$$= -\nabla_x\cdot\left[\sum_{\substack{n,m\\ n\neq m}} \frac{1}{4m}\Big((p_n+p_m)\cdot F_{nm}\Big) r_{nm}\int_0^1 ds\, \delta^3(x-r_n+sr_{nm})\right]$$

using the same identity for the difference of delta functions as before. Finally, we obtain $\partial_t e(x,t) + \nabla\cdot s(x,t) = 0$, with

$$s(x,t) = \sum_{n=1}^{N}\Big(\frac{p_n^2}{2m} + \frac{1}{2}\sum_{m\neq n} U(r_{nm})\Big)\frac{p_n}{m}\delta^3(x-r_n)$$

$$+ \sum_{\substack{n,m\\ n\neq m}} \frac{1}{4m}\Big((p_n+p_m)\cdot F_{nm}\Big) r_{nm}\int_0^1 ds\,\delta^3(x-r_n+sr_{nm})$$

Problem 3. (a) The formal integral solution of the y-equation is

$$y(t) = \int_{-\infty}^{t} ds \; e^{D(t-s)} \left[C\,x(s) + g(s) \right].$$

This may be verified by explicit differentiation

$$\frac{d}{dt} y(t) = \int_{-\infty}^{t} ds \; D e^{D(t-s)} \left[Cx(s) + g(s) \right] + e^{D(t-s)} \left[Cx(s) + g(s) \right] \Big|_{s=t}$$

$$= D\,y(t) + C\,x(t) + g(t) \quad \checkmark$$

Substituting the result into the x-equation gives

$$\dot{x} = Ax + By + f(t)$$

$$= Ax + B \cdot \int_{-\infty}^{t} ds \; e^{D(t-s)} \left[Cx(s) + g(s) \right] + f(t)$$

$$= Ax + \int_{-\infty}^{t} ds \; K(t-s)\, x(s) + f^*(t) + f(t),$$

with

$$K(\tau) \equiv B e^{D\tau} C$$

and

$$f^*(t) = \int_{-\infty}^{t} ds \; B e^{D(t-s)} g(s).$$

Using the result for the $\mathbf{g}$-covariance

$$\langle \mathbf{g}(t)\, \mathbf{g}^T(t') \rangle = \mathbf{G}\, \delta(t-t'),$$

we then get

$$\mathbf{F}^*(t,t') \equiv \langle \mathbf{f}^*(t) [\mathbf{f}^*(t')]^T \rangle$$

$$= \int_{-\infty}^{t} ds \int_{-\infty}^{t'} ds'\; \mathbf{B}\, e^{\mathbf{D}(t-s)} \underbrace{\langle \mathbf{g}(s)\, \mathbf{g}^T(s') \rangle}_{\mathbf{G}\,\delta(s-s')} e^{\mathbf{D}^T(t-s')} \mathbf{B}^T$$

$$= \int_{-\infty}^{t\wedge t'} ds\; \mathbf{B}\, e^{\mathbf{D}(t-s)}\, \mathbf{G}\, e^{\mathbf{D}^T(t-s)}\, \mathbf{B}^T$$

(b) As an application of the above general result, we see that

$$\dot{x}(t) = -x(t) + \int_{-\infty}^{t} ds\; e^{-(t-s)} x(s) + 4\,\delta(t) + f^*(t)$$

with

$$f^*(t) = \int_{-\infty}^{t} ds\; e^{-(t-s)}\, 2\,\delta(s) = 2e^{-t}$$

and

$$\int_{-\infty}^{t} ds\; e^{-(t-s)} x(s) = \int_{0}^{t} ds\; e^{-(t-s)} x(s)$$

$$= \int_{0}^{t} d\tau\; e^{-\tau}\, x(t-\tau), \qquad \begin{aligned}\tau &= t-s\\ d\tau &= -ds\end{aligned}$$

which gives the stated integro-differential equation.

The exact solution of the coupled ODE's

$$\begin{cases} \dot{x} = -x + y, & x(0) = 4 \\ \dot{y} = x - y, & y(0) = 2 \end{cases}$$

is easily checked to be

$$x(t) = 3 + e^{-2t}, \quad y(t) = 3 - e^{-2t}.$$

This solution may be approximated with standard numerical software to solve ODE's, e.g. the Runge-Kutta-Fehlberg algorithm ode45 in MATLAB. This code gave an approximate solution with relative error $O(10^{-4})$ in a wall clock time of 0.4183 secs.

Another approach is to approximate the integral in the integro-differential equation as a discrete sum. For example, with an imposed finite memory T, we set

$$\dot{x}(t) \cong -x(t) + \int_0^T d\tau \, e^{-\tau} x(t-\tau) + 2e^{-t}$$

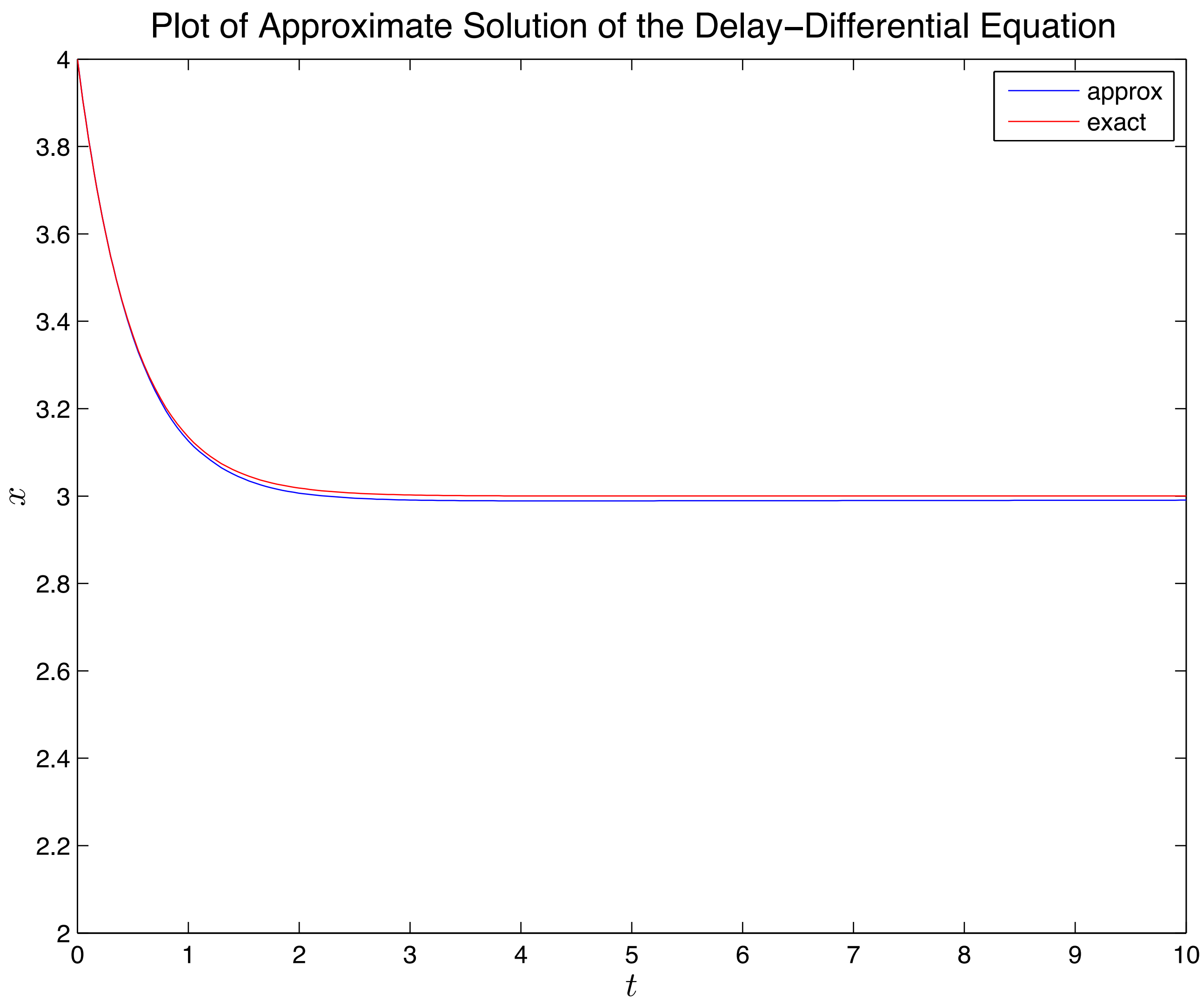
$$\cong -x(t) + \frac{\Delta t}{2} x(t) + \sum_{i=1}^{M-1} \Delta t \, e^{-i\Delta t} x(t - i\Delta t) + \frac{\Delta t}{2} x(t-T) + 2e^{-t}$$

with $T = M\Delta t$, using the composite trapezoid rule to approximate the integral.

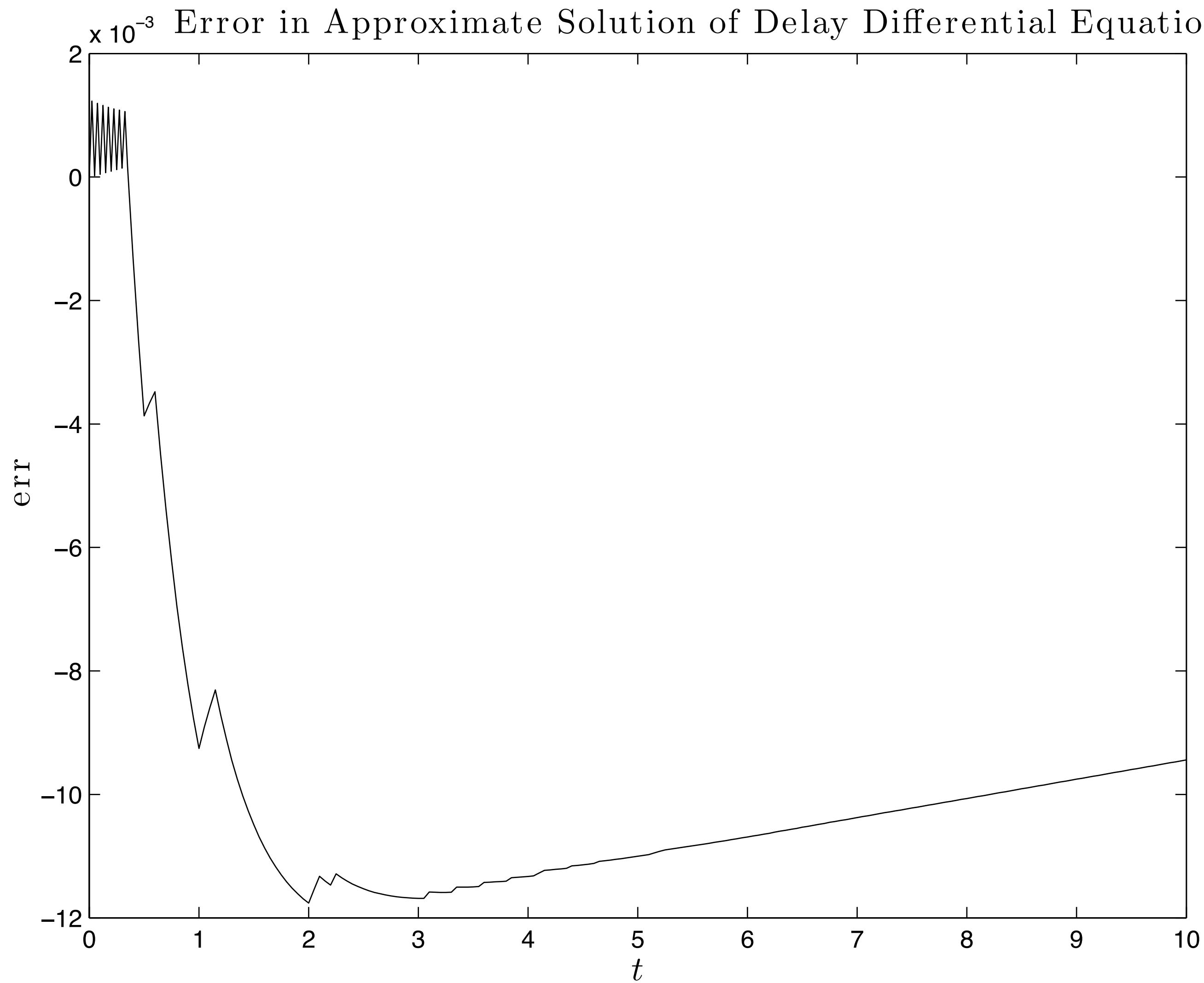
We employ the above discretization scheme with $T=10$ and $\Delta t = 0.05$. We then employ MATLAB's Runge-Kutta integrator for delay-differential equations, dde23, to approximate the solution of the discretized equation. This approach gave an approximate solution with relative error $O(10^{-3})$ in a wall clock time of 424.6 secs.

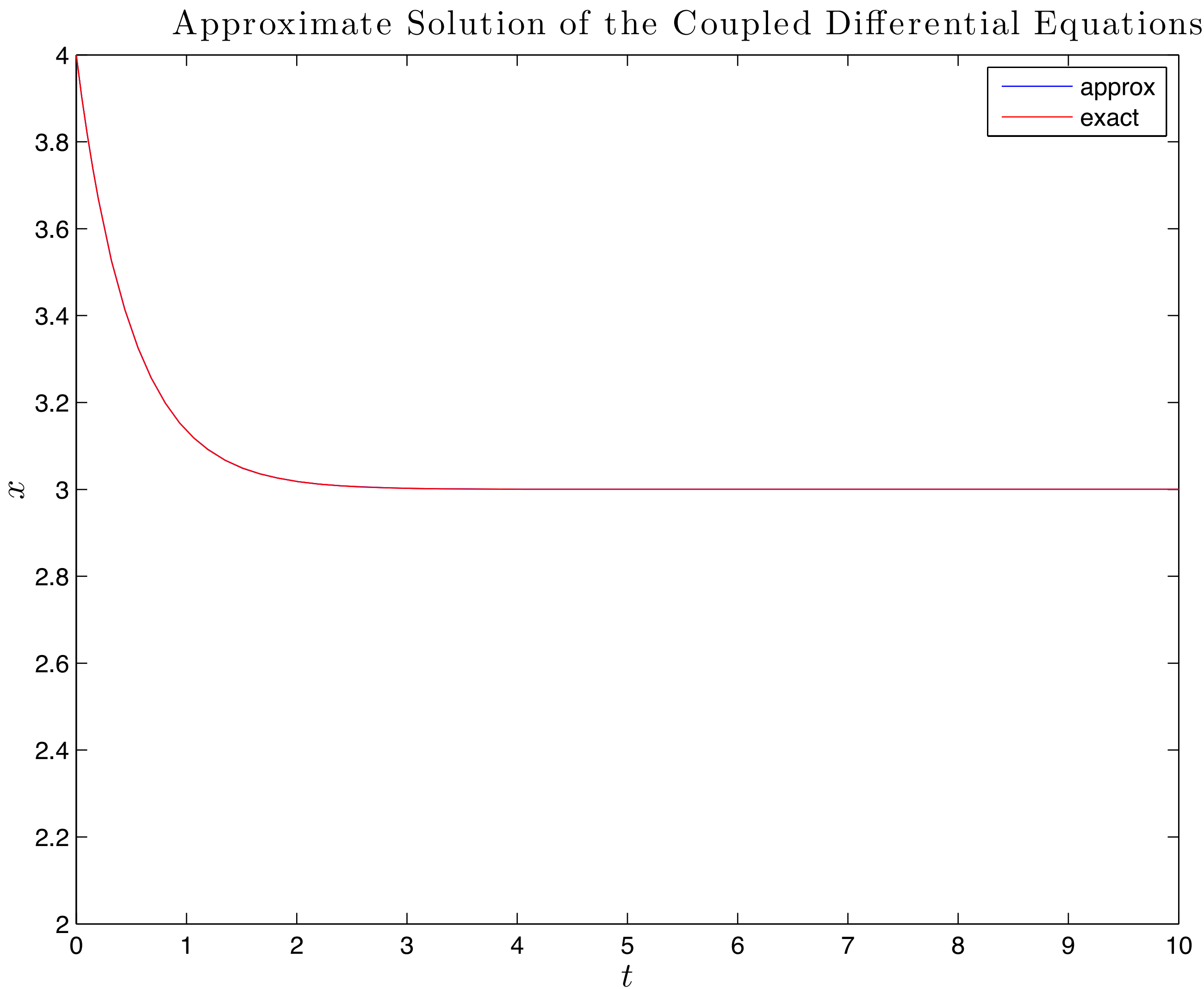
In conclusion, solving the integro-differential equation gave an approximate solution with errors 10 times larger than solving the original system of coupled differential equations and in a total amount of time 1000 times longer!!!
Clearly, the "reduction" of the system from two equations for $(x(t), y(t))$ to one equation with memory for $x(t)$ is not computational useful.

```
tic

dt=.05;
mem=10;
lags=dt:dt:mem;
fac=exp(-lags).';
nn=length(lags);
hist=inline('4*(1+sign(t))','t');
ddef=inline('-y+2*exp(-t)+(z*fac+y/2-z(1,nn)*fac(nn,1)/2)↙
*dt','t','y','z','fac','dt','nn');
tspan=[0, 10];

sol=dde23(@(t,y,z) ddef(t,y,z,fac,dt,nn),lags,hist,tspan);

toc

plot(sol.x,sol.y,'-b',sol.x,3+exp(-2*sol.x),'-r');

figure
plot(sol.x,sol.y-3-exp(-2*sol.x));
pause

tic

f=inline('[-x(1)+x(2);x(1)-x(2)]','t','x');
[t,x]=ode45(@(t,x) f(t,x),[0 10],[4 2]);

toc

figure
plot(t,x(:,1),'-b',t,3+exp(-2*t),'-r')

figure
plot(t,x(:,1)-3-exp(-2*t))
```

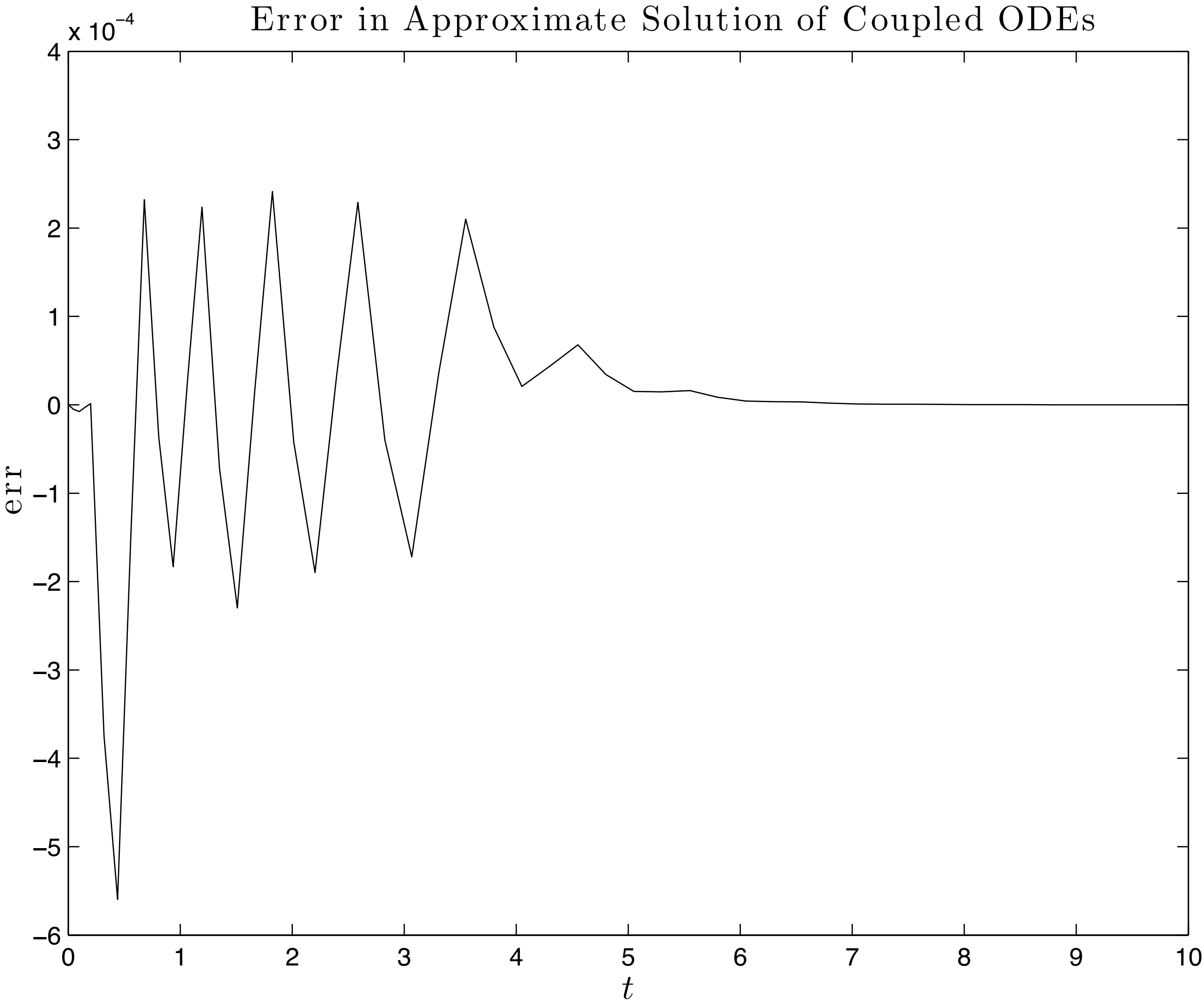


Plot of Approximate Solution of the Delay−Differential Equation
approx
exact
x
t
4
3.8
3.6
3.4
3.2
3
2.8
2.6
2.4
2.2
2
0
1
2
3
4
5
6
7
8
9
10


Error in Approximate Solution of Delay Differential Equation
x 10^-3
2
0
−2
−4
−6
−8
−10
−12
err
0
1
2
3
4
5
6
7
8
9
10
t



Approximate Solution of the Coupled Differential Equations
approx
exact
4
3.8
3.6
3.4
3.2
3
2.8
2.6
2.4
2.2
2
0
1
2
3
4
5
6
7
8
9
10
x
t


Error in Approximate Solution of Coupled ODEs
x 10^-4
4
3
2
1
0
−1
−2
−3
−4
−5
−6
err
0
1
2
3
4
5
6
7
8
9
10
t