

Partial Differential Equations and Difference Differential Equations: Exercises

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2 Partial Differential Equations

1. Prove that the solution Φ of the equation

$$-\frac{d^2}{dx^2}\Phi(x) = n_D(x) - \int_{\mathbb{R}} \frac{dk}{1 + \exp(\epsilon(k) - \Phi(x))}$$

with $\int_{\mathbb{R}^2} \frac{dkdx}{1 + \exp(\epsilon(k) - \Phi(x))} = a$ fixed and $\frac{d\Phi}{dx} \in L^2$ is unique.

Taken from [21]. Assume that there are two solutions Φ_1 and Φ_2 satisfying such conditions. Set $U = \Phi_1 - \Phi_2$. Then, $\frac{dU}{dx} \in L^2$ and

$$\frac{d^2U}{dx^2} = \int_{\mathbb{R}} \frac{dk}{1 + \exp(\epsilon(k) - \Phi_1(x))} - \int_{\mathbb{R}} \frac{dk}{1 + \exp(\epsilon(k) - \Phi_2(x))}.$$

Let us assume first that $U(x) > 0$ everywhere. Then

$$a = \int_{\mathbb{R}^2} \frac{dkdx}{1 + \exp(\epsilon(k) - \Phi_1(x))} > \int_{\mathbb{R}^2} \frac{dkdx}{1 + \exp(\epsilon(k) - \Phi_2(x))} = a,$$

which is impossible.

Let us assume now that there is a unique point x_0 at which $U(x_0) = 0$.

We take $U(x) < 0$ for $x < x_0$ and $U(x) > 0$ for $x > x_0$. Thus, $\frac{d^2U}{dx^2} < 0$ if $x < x_0$ and $\frac{d^2U}{dx^2} < 0$ if $x > x_0$. Then, $\frac{dU}{dx}$ is decreasing if $x < x_0$ and $\frac{dU}{dx}$ is increasing if $x > x_0$. On the other hand,

$$\int_{\mathbb{R}} \left(\frac{dU}{dx}\right)^2 dx = \int_{-\infty}^{x^*} \left(\frac{dU}{dx}\right)^2 dx + \int_{x^*}^{\infty} \left(\frac{dU}{dx}\right)^2 dx$$

is finite. If there exists x^* such that $\frac{dU(x^*)}{dx} > 0$ and $x^* < x_0$ then $\int_{-\infty}^{x^*} \left(\frac{dU}{dx}\right)^2 dx > \left(\frac{dU(x^*)}{dx}\right)^2 \int_{-\infty}^{x^*} dx = \infty$. This is impossible, so that $\frac{dU}{dx} \leq 0$ for all x and U is decreasing. This contradicts our assumption on x_0 . Therefore, we should have at least two points x_0 and x_1 at which U vanishes.

Let x_0 and x_1 be such that $U(x_0) = U(x_1) = 0$. If x_M is such that $U(x_M) = \max\{U(x), x_0 \leq x \leq x_1\} > 0$, then $\frac{d^2U(x_M)}{dx^2} \leq 0$ because the maximum is attained at an interior point. However,

$$0 \geq \frac{d^2U(x_M)}{dx^2} = \int_{\mathbb{R}} \frac{dk}{1 + \exp(\epsilon(k) - \Phi_1(x_M))} - \int_{\mathbb{R}} \frac{dk}{1 + \exp(\epsilon(k) - \Phi_2(x_M))} > 0,$$

since $U(x_M) > 0$. Hence, $\max\{U(x), x_0 \leq x \leq x_1\} = 0$. In an analogous way, we conclude that $U(x_m) = \min\{U(x), x_0 \leq x \leq x_1\} = 0$. Therefore, $U = 0$ on $[x_0, x_1]$.

Now we set $x_0 = \min\{x | U(x) = 0\}$ and $x_1 = \max\{x | U(x) = 0\}$. Then, $U(x) < 0$ for $x < x_0$ and $U(x) > 0$ for $x > x_1$. Repeating the above arguments, we would obtain $x' \notin [x_0, x_1]$ such that $U(x') = 0$. This contradicts the definition of x_0 and x_1 . Therefore, $U = 0$ everywhere and $\Phi_1 = \Phi_2$.

2. Consider balls $B_\varepsilon = B(\mathbf{x}, \varepsilon)$ centered at a point \mathbf{x} of small radius ε . Given a smooth function $u(\mathbf{x})$, let v_ε be the solution of

$$\begin{cases} \Delta v_\varepsilon + k^2 v_\varepsilon = 0, & \text{in } \mathbb{R}^2 \setminus \overline{B_\varepsilon}, \\ v_\varepsilon = -u(\mathbf{x}), & \text{on } \partial B_\varepsilon, \\ \lim_{r \rightarrow \infty} r^{1/2} \left(\frac{\partial v_\varepsilon}{\partial r} - ikv_\varepsilon \right) = 0. \end{cases}$$

What is the behavior of $\frac{\partial v_\varepsilon}{\partial \mathbf{n}}$ as $\varepsilon \rightarrow 0$?

Taken from [47]. The Dirichlet-to-Neumann provides an expression for the normal derivative of v_ε on Γ_ε :

$$\begin{aligned} \partial_{\mathbf{n}} v_\varepsilon(\mathbf{x} + \varepsilon(\cos \theta, \sin \theta)) \\ = \frac{k}{2\pi} \sum_{n=-\infty}^{\infty} \frac{(H_{|n|}^{(1)})'(k\varepsilon)}{H_{|n|}^{(1)}(k\varepsilon)} \int_0^{2\pi} e^{in(\theta-\Theta)} u(\mathbf{x} + \varepsilon(\cos \Theta, \sin \Theta)) d\Theta \end{aligned}$$

in polar coordinates. Here $H_{|n|}^{(1)}$ denotes the Hankel function of the first kind of order $|n|$. We choose the normal vector \mathbf{n} pointing into B_ε . For sufficiently small $\varepsilon > 0$,

$$\frac{\partial v_\varepsilon}{\partial \mathbf{n}}(\mathbf{x} + \varepsilon(\cos \theta, \sin \theta)) = k \frac{(H_0^{(1)})'(k\varepsilon)}{H_0^{(1)}(k\varepsilon)} u(\mathbf{x}) + O(\varepsilon).$$

For small $\varepsilon > 0$, the Hankel functions have the following leading parts:

$$H_0^{(1)}(k\varepsilon) \sim \frac{-2 \log(k\varepsilon)}{\pi i}, \quad (H_0^{(1)})'(k\varepsilon) = -H_1^{(1)}(k\varepsilon) \sim \frac{-2}{\pi i k\varepsilon}.$$

Thus,

$$\frac{(H_0^{(1)})'(k\varepsilon)}{H_0^{(1)}(k\varepsilon)} \sim \frac{1}{k\varepsilon \log(k\varepsilon)},$$

and $\frac{\partial v_\varepsilon}{\partial \mathbf{n}}(\mathbf{x} + \varepsilon(\cos \theta, \sin \theta)) \sim \frac{1}{\varepsilon \log(k\varepsilon)} u(\mathbf{x})$.

3. Given a bounded open set $\Omega \subset \mathbb{R}^N$, we consider the problem: Find $u > 0$ such that

$$\begin{aligned} -\Delta u &= u^p & \mathbf{x} \in \Omega, \\ u &= 0 & \mathbf{x} \in \partial\Omega, \\ u &> 0 & \mathbf{x} \in \Omega. \end{aligned}$$

Prove that there is a solution when $1 < p+1 < p^*$, where $p^* = \infty$ if $N \leq 2$ and $p^* < \frac{2N}{N-2}$ when $N > 2$.

Consider the minimization problem

$$I = \operatorname{Min}_{u \in H_0^1(\Omega)} \frac{\int_{\Omega} |\nabla u|^2 d\mathbf{x}}{\int_{\Omega} |u|^{p+1} d\mathbf{x}} = \operatorname{Min}_{u \in H_0^1(\Omega)} J(u).$$

The functional $J(u)$ to be minimized is positive, thus, bounded from below. Consider a minimizing sequence $u_n \in H_0^1(\Omega)$, such that $J(u_n) \rightarrow I$ as $n \rightarrow \infty$. The sequence $v_n = \frac{u_n}{\|u_n\|_{L^{p+1}}}$ is a minimizing sequence satisfying also $\|v_n\|_{L^{p+1}} = 1$. Then, $\int_{\Omega} |\nabla v_n|^2 d\mathbf{x} \rightarrow I$ implies that v_n is bounded in $H_0^1(\Omega)$ and v_n tends weakly in H_0^1 to a limit $v \in H_0^1(\Omega)$. By Sobolev injections, v_n is compact in L^{p+1} , $p+1 < p^*$, thus $v \in L^{p+1}(\Omega)$ and $\|v_n\|_{L^{p+1}} = 1 \rightarrow \|v\|_{L^{p+1}} = 1$. By lower semicontinuity of weak convergence, we have $J(v) \leq \lim_{n \rightarrow \infty} J(v_n) = I$. Since $v \in H_0^1(\Omega)$, we have $I \leq J(v)$. Therefore, $I = J(v)$ and the minimum is attained at v . Moreover, we can replace v by $|v|$ and $J(|v|) \leq I(v)$, so that $w = |v| \geq 0$ is a minimizer too and $I = J(w)$. $w \neq 0$ because $\|w\|_{L^{p+1}} = 1$.

Now, $J(w) \leq J(w + tr)$, $r \in H_0^1(\Omega)$ for real t . An asymptotic expansion first for $t > 0$ then for $t < 0$ leads to

$$\int_{\Omega} \nabla w \nabla r d\mathbf{x} = c \int_{\Omega} w^p r d\mathbf{x}$$

for all $r \in H_0^1(\Omega)$ and some $c > 0$. This implies $-\Delta w = c w^p$. Setting $u = c^{-1/(p-1)} w$, we get $-\Delta u = u^p$ and $u \geq 0$, $u \neq 0$. By the strong maximum principle, $u > 0$.

If $p+1 = p^* = \frac{2N}{N-2}$ and $N > 2$ existence depends on the geometry of Ω , see [1].

4. Prove that the function $v(\mathbf{x}, t) = |t|^{\frac{p}{p-1}} \phi(\mathbf{x})$, $1 < p < p^* - 1$, where

$$\begin{aligned} -\Delta \phi &= \left(\frac{p}{p-1} \right)^p |\phi|^{p-1} \phi & \mathbf{x} \in \Omega, \\ \phi &= 0 & \mathbf{x} \in \partial\Omega, \end{aligned}$$

is a solution of the backward parabolic problem

$$\begin{aligned} -\Delta v + |v_t|^{p-1} v_t &= 0 & \mathbf{x} \in \Omega \times (-\infty, 0], \\ v &= 0 & \mathbf{x} \in \partial\Omega \times (-\infty, 0]. \end{aligned}$$

Proof taken from [3, 8]. We see that

$$\begin{aligned} v_t &= -\frac{p}{p-1} |t|^{\frac{1}{p-1}} \phi(\mathbf{x}), \\ |v_t|^{p-1} v_t &= -\left(\frac{p}{p-1} \right)^p |t|^{\frac{p}{p-1}} |\phi(\mathbf{x})|^{p-1} \phi(\mathbf{x}), \\ -\Delta v &= -|t|^{\frac{p}{p-1}} \Delta \phi(\mathbf{x}) = |t|^{\frac{p}{p-1}} \left(\frac{p}{p-1} \right)^p |\phi(\mathbf{x})|^{p-1} \phi(\mathbf{x}), \end{aligned}$$

so that the equation is fulfilled. Existence of ϕ follows from critical point theory.

5. Given a solution $u \in W_{\text{loc}}^{1,\infty}(\mathbb{R}^+, H_0^1(\Omega)) \cap W_{\text{loc}}^{2,\infty}(\mathbb{R}^+, L^2(\Omega))$ of

$$u_{tt} - \Delta u + \alpha |u_t|^{p-1} u_t = 0 \quad \text{in } L^\infty(\mathbb{R}^+, H^{-1}(\Omega))$$

with $\alpha > 0$, $1 < p$ and $p+1 < p^*$, we set

$$E(t) = \frac{1}{2} \int_{\Omega} |\nabla u(\mathbf{x}, t)|^2 d\mathbf{x} + \frac{1}{2} \int_{\Omega} |u_t(\mathbf{x}, t)|^2 d\mathbf{x}.$$

Then, for some positive constant $C(E(0))$, we have

$$E(t) \leq C(E(0))t^{-2/(p-1)}, \quad t > 0.$$

Proof taken from [2]. We set $\phi(t) = E^{(p-1)/2} \int_{\Omega} uu_t d\mathbf{x}$. Next, we differentiate with respect to t to get

$$\begin{aligned} E'(t) &= -\alpha \int_{\Omega} |u_t|^{p+1} d\mathbf{x} \leq 0, \\ \phi'(t) &= E(t)^{(p-1)/2} \left(\int_{\Omega} |u_t|^2 d\mathbf{x} - \int_{\Omega} |\nabla u|^2 d\mathbf{x} - \alpha \int_{\Omega} |u_t|^{p-1} u_t u d\mathbf{x} \right) \\ &\quad + \frac{p-1}{2} E(t)^{(p-3)/2} E'(t) \int_{\Omega} uu_t d\mathbf{x} \end{aligned}$$

First, notice that $E(t) \leq E(0)$ and $-\int_{\Omega} |\nabla u|^2 d\mathbf{x} = -2E(t) + \int_{\Omega} |u_t|^2 d\mathbf{x}$. Moreover,

$$E(t)^{-1} \left| \int_{\Omega} uu_t d\mathbf{x} \right| \leq E(t)^{-1} \left(\frac{1}{2} \int_{\Omega} |u|^2 d\mathbf{x} + \frac{1}{2} \int_{\Omega} |u_t|^2 d\mathbf{x} \right) \leq C(\Omega)$$

for some positive constant $C(\Omega)$ because Poincaré's inequality implies $\frac{1}{2} \int_{\Omega} |u|^2 d\mathbf{x} \leq \frac{\lambda(\Omega)}{2} \int_{\Omega} |\nabla u|^2 d\mathbf{x}$. As a consequence, we get

$$\begin{aligned} \phi'(t) &\leq 2E(t)^{(p-1)/2} \int_{\Omega} |u_t|^2 d\mathbf{x} - \alpha E(t)^{(p-1)/2} \int_{\Omega} |u_t|^{p-1} u_t u d\mathbf{x} \\ &\quad - 2E(t)^{(p+1)/2} - \frac{p-1}{2} C(\Omega) E(0)^{(p-1)/2} E'(t). \end{aligned}$$

Now we set $\psi_\varepsilon(t) = (1 + K_1 \varepsilon)E(t) + \varepsilon \phi(t)$ with $K_1 = \frac{p-1}{2} C(\Omega) E(0)^{(p-1)/2}$. We get

$$\begin{aligned} \psi'_\varepsilon(t) &\leq 2\varepsilon E(t)^{(p-1)/2} \int_{\Omega} |u_t|^2 d\mathbf{x} - \alpha \varepsilon E(t)^{(p-1)/2} \int_{\Omega} |u_t|^{p+1} d\mathbf{x} \\ &\quad - 2\varepsilon E(t)^{(p+1)/2} - \alpha \int_{\Omega} |u_t|^{p+1} d\mathbf{x} \end{aligned}$$

Notice that $\|u_t\|_{L^2}^2 \leq \text{meas}(\Omega)^{(p-1)/(p+1)} (\int_{\Omega} |u_t|^{p+1})^{2/(p+1)}$. By Young's inequality

$$\begin{aligned} 2\varepsilon E(t)^{\frac{p-1}{2}} \int_{\Omega} |u_t|^2 dx &\leq 2\varepsilon \text{meas}(\Omega)^{\frac{p-1}{p+1}} E(t)^{\frac{p-1}{2}} \left(\int_{\Omega} |u_t|^{p+1} \right)^{\frac{2}{p+1}} \\ &\leq \varepsilon E(t)^{\frac{p+1}{2}} + \varepsilon \delta \int_{\Omega} |u_t|^{p+1} \end{aligned}$$

for some positive δ depending on Ω .

Using Sobolev injections for $p+1 < p^*$ we find

$$\int_{\Omega} |u_t|^{p-1} u_t u dx \leq \left(\int_{\Omega} |u_t|^{p+1} dx \right)^{\frac{p}{p+1}} \|u\|_{L^{p+1}} \leq S(\Omega) \|u_t\|_{L^{p+1}}^p \|\nabla u\|_{L^2}.$$

Notice that $\|\nabla u\|_{L^2} \leq 2E(t)$. By Young's inequality again

$$\begin{aligned} \varepsilon \alpha E(t)^{(p-1)/2} \int_{\Omega} |u_t|^{p-1} u_t u dx &\leq \varepsilon \alpha E(t)^{(p-1)/2} S(\Omega) \|u_t\|_{L^{p+1}}^p \|\nabla u\|_{L^2} \\ &\leq \frac{\alpha}{2} \int_{\Omega} |u_t|^{p+1} + \varepsilon \eta(\varepsilon) E(t)^{(p+1)/2} \end{aligned}$$

where $\eta > 0$ depends on $E(0)$, Ω , α and ε , and tends to zero as ε tends to zero. Adding up, we get

$$\psi'_\varepsilon(t) \leq \left(-\frac{\alpha}{2} + \varepsilon \delta\right) \int_{\Omega} |u_t|^{p+1} + \varepsilon(-1 + \eta(\varepsilon)) E(t)^{(p+1)/2}.$$

On the other hand, for ε small enough,

$$\frac{1}{\varepsilon} E(t) \leq (1 - K_2 \varepsilon) E(t) \leq \psi_\varepsilon(t) \leq (1 + K_2 \varepsilon) \leq 2E(t).$$

Choosing ε small enough, we find

$$\psi'_\varepsilon(t) \leq -\frac{\varepsilon}{4} E^{(p+1)/2} \leq -\frac{\varepsilon K_3}{4} \psi_\varepsilon(t)^{(p+1)/2}.$$

Integrating the inequality we find $E(t) \leq C(E(0))t^{-2/(p-1)}$ for $t > 0$.

6. Consider the vorticity equation in two dimensions. Let $v = \text{curl } \mathbf{u} \in C((0, \infty); W^{1,p}(\mathbb{R}^2))$, $1 \leq p \leq \infty$, be the solution of

$$\begin{aligned} v_t - \Delta v + \mathbf{u} \cdot \nabla v &= 0, & \mathbf{x} \in \mathbb{R}^2 \times \mathbb{R}^+ \\ v(\mathbf{x}, 0) &= v_0, & \mathbf{x} \in \mathbb{R}^2, \end{aligned}$$

for a divergence free velocity field u and an initial datum $v_0 \in L^1(\mathbb{R}^2)$. Prove 1) that the mass $\int_{\mathbb{R}^2} v_0 dx$ does not change with time and 2) that $\|v(t)\|_{L^p(\mathbb{R}^2)} \leq Ct^{-1+\frac{1}{p}}$ for $t > 0$.

Proof taken from [4, 5]. Notice that $\mathbf{u} \cdot \nabla v = \operatorname{div}(\mathbf{u}v) = 0$. Integrating the equation, using the divergence theorem, and the fact that v vanishes at infinity we get

$$\frac{d}{dt} \int_{\mathbb{R}^2} v_0 \, d\mathbf{x} = 0.$$

The velocity vector is given by

$$\mathbf{u}(\mathbf{x}, t) = K * v(\mathbf{x}, t) = \frac{1}{2\pi} \int_{\mathbb{R}^2} \frac{(-y_2, y_1)}{|\mathbf{y}|^2} v(\mathbf{x} - \mathbf{y}, t) d\mathbf{y}$$

where the kernel $K \in L^{2,\infty}$ and $\|K * v\|_{L^r} \leq \|K\|_{L^{2,\infty}} \|v\|_{L^p}$ for $r > 2$, $1 < p < 2$, $1/r = 1/p - 1/2$.

Writing down the integral expression for the solution

$$v(t) = G(t) * v_0 + \int_0^t \nabla G(t-s) * [v(s) \mathbf{K} * v(s)] ds,$$

where $G(t)$ stands for the heat kernel, and taking norms we find

$$\|v(t)\|_{L^p} = \|G(t) * v_0\|_{L^p} + \int_0^t \|\nabla G(t-s) * [v(s) \mathbf{K} * v(s)]\|_{L^p} ds.$$

The integral terms decays faster than the rest, therefore

$$\|v(t)\|_{L^p} \sim \|G(t) * v_0\|_{L^p} \leq Ct^{-1+\frac{1}{p}}.$$

Recall that $G(t) * v_0$ is a solution of the heat equation with datum v_0 and it belongs to L^p for all $1 \leq p \leq \infty$ for any $t > 0$ if $v_0 \in L^1$. Moreover, $\|G(t) * v_0\|_{L^p} \leq \|G(t)\|_{L^p} \|v_0\|_{L^1}$ and $\|G(t)\|_{L^p} = Ct^{-1+\frac{1}{p}}$.

7. Let \mathbf{u} be a solution of the incompressible Navier-Stokes equations in two dimensions with initial datum $\mathbf{u}_0 \in L^1 \cap L^2(\mathbb{R}^2)$ such that $\operatorname{div}(\mathbf{u}_0) = 0$. Then $\mathbf{u}(t) \in L^p(\mathbb{R}^2)$ for $1 \leq p \leq 2$ and $t > 0$.

Proof taken from [6, 10]. The theory of classical solutions with L^2 data, that is, $\mathbf{u}_0 \in L^2(\mathbb{R}^2)$ guarantees that $\mathbf{u}(t) \in L^\infty([0, \infty); L^2(\mathbb{R}^2))$ and is bounded by $\|\mathbf{u}_0\|_{L^2}$. By taking the divergence of Navier-Stokes equations

$$\mathbf{u}_t - \Delta \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = \nabla p, \quad \operatorname{div}(\mathbf{u}) = 0,$$

we get an equation for the pressure

$$-\Delta p = \operatorname{div}(\mathbf{u} \cdot \nabla \mathbf{u}).$$

The pressure is then the convolution $p = E_2 * \operatorname{div}(\mathbf{u} \cdot \nabla \mathbf{u})$, where E_2 is the fundamental solution of $-\Delta$ in \mathbb{R}^2 , up to a function of time. Then \mathbf{u} satisfies the integral equation

$$\begin{aligned} \mathbf{u}(t) &= G(t) * \mathbf{u}_0 + \int_0^t \partial_i G(t-s) * u_i \mathbf{u}(s) ds \\ &\quad + \int_0^t \partial_i G(t-s) * \partial_j \nabla E_2 * u_i u_j(s) ds, \end{aligned}$$

where ∂_i denotes partial derivative with respect to x_i , u_i are components of \mathbf{u} and summation with respect to repeated indices is intended. Since $u \in L^1$, $G(t) * u_0 \in L^q$ for all $q > 1$ and $t > 0$. On the other hand, $u(s) \in L^2$ implies that $u_i u_j(s) \in L^1$. Moreover,

$$\left\| \int_0^t \partial_i G(t-s) * u_i u_j(s) ds \right\|_{L^q} \leq C \int_0^t (t-s)^{-1+\frac{1}{q}-\frac{1}{2}} \|\mathbf{u}\|_{L^2}^2 ds \leq C t^{\frac{1}{q}-\frac{1}{2}}$$

for $1 \leq q < 2$. Thus, the first integral belongs to L^q for $1 \leq q < 2$. Let us consider now the second integral. Since $\partial_i G(t)$ belongs to the Hardy space $\mathcal{H}^1(\mathbb{R}^2)$ and $\partial_j \nabla E_2$ is a Calderon-Zygmund kernel, we conclude that $\partial_i G(t-s) * \partial_j \nabla E_2 \in L^1$ and

$$\|\partial_i G(t-s) * \partial_j \nabla E_2\|_{L^1} \leq C \|\partial_i G(t-s)\|_{\mathcal{H}^1} < C(t-s)^{-\frac{1}{2}}.$$

Thus,

$$\left\| \int_0^t \partial_i G(t-s) * \partial_j \nabla E_2 * u_i u_j(s) ds \right\|_{L^1} \leq \int_0^t C(t-s)^{-\frac{1}{2}} \|\mathbf{u}(s)\|_{L^2}^2 ds \leq C t^{\frac{1}{2}}.$$

In an analogous way, since $\partial_j \nabla E_2$ is a Calderon-Zygmund kernel, we conclude that $\partial_i G(t-s) * \partial_j \nabla E_2 \in L^q$, $1 < q < \infty$ and

$$\|\partial_i G(t-s) * \partial_j \nabla E_2\|_{L^q} \leq C \|\partial_i G(t-s)\|_{L^q} < C(t-s)^{-1+\frac{1}{q}-\frac{1}{2}}.$$

Thus,

$$\begin{aligned} \left\| \int_0^t \partial_i G(t-s) * \partial_j \nabla E_2 * u_i u_j(s) ds \right\|_{L^q} &\leq \int_0^t C(t-s)^{-1+\frac{1}{q}-\frac{1}{2}} \|\mathbf{u}(s)\|_{L^2}^2 ds \\ &\leq C t^{\frac{1}{q}-\frac{1}{2}} \end{aligned}$$

for $1 < q \leq 2$.

8. *A line vortex lying along a curve Γ in an incompressible inviscid and irrotational fluid is a solution of the following equations*

$$\operatorname{div}(\mathbf{u}) = 0, \quad \operatorname{curl}(\mathbf{u}) = \omega_0 \delta_\Gamma(\mathbf{x}),$$

where \mathbf{u} is the fluid velocity, $\omega_0 = 2\pi\gamma$ is the circulation around the vortex and γ is the vortex strength. δ_Γ is a Dirac function supported at the curve Γ . Express this solution in terms of a vector stream function.

Taken from [11]. We define a vector stream function \mathbf{U} in \mathbb{R}^3 as the solution of $\operatorname{div}(\mathbf{U}) = 0$, $\operatorname{curl}(\mathbf{U}) = \mathbf{u}$. Then $-\Delta \mathbf{U} = \omega_0 \delta_\Gamma(\mathbf{x})$. Using the Green function for the Laplacian in \mathbb{R}^3 we get $\mathbf{U} = \frac{\omega_0}{4\pi} \int_\Gamma \frac{1}{|\mathbf{x}-\mathbf{x}'|} d\mathbf{x}'$.

9. *Consider the convection diffusion equation*

$$u_t - \Delta u + \partial_y(|u|^{q-1}u) = 0$$

set in $\mathbb{R}^{n-1} \times \mathbb{R} \times \mathbb{R}^+$, with $\mathbf{x} = (x_1, \dots, x_{n-1}, y)$. Assume that V is a solution with initial datum $V_0 \in (L^1 \cap L^\infty)(\mathbb{R}^n)$ and v is a solution with initial datum $v_0 \in (L^1 \cap L^\infty)(\mathbb{R}^n)$. Assume that

$$v, V \in C^1([0, T]; L^2(\mathbb{R}^2)) \cap L^\infty([0, T]; H^2(\mathbb{R}^2)) \cap L^\infty((0, T) \times \mathbb{R}^2)$$

for every $T > 0$. Then, $v \leq V$.

Proof taken from [7, 9]. The function $w = v - V$ satisfies

$$w_t - \Delta w + \partial_y(|v|^{q-1}v) - \partial_y(|V|^{q-1}V) \leq 0$$

and $w(0) \leq 0$. Multiplying the inequality by w^+ and integrating by parts, we obtain

$$\frac{d}{dt} \int \frac{|w^+(t)|^2}{2} d\mathbf{x} + \int |\nabla w^+(t)|^2 d\mathbf{x} \leq \int a w^+(t) \partial_y w^+(t) d\mathbf{x}$$

where $a(\mathbf{x}, t) = \frac{|v|^{q-1}v - |V|^{q-1}V}{v - V}$ is a bounded function. Integrating in t and applying Young's inequality we get

$$\frac{\|w^+(t)\|_2^2}{2} + \int_0^t \|\nabla w^+(s)\|_2^2 ds \leq K_1 \int_0^t \|w^+(s)\|_2^2 ds + \varepsilon \int_0^t \|\nabla w^+(s)\|_2^2 ds$$

for ε as small as needed. Notice that $w^+(0) = 0$. Gronwall's inequality for

$$\|w^+(t)\|_2^2 \leq 2K_1 \int_0^t \|w^+(s)\|_2^2 ds$$

implies $w^+(t) = 0$.

10. Prove that the solution of

$$z_t - \Delta z = \mathbf{d} \cdot \nabla(G^q), \quad z(0) = 0$$

can be calculated in terms of heat kernels.

Taken from [19]. Set $z = \mathbf{d} \cdot \nabla g$ where $g_t - \Delta g = G^q$, $g(0) = 0$, that is,

$$g(t) = \int_0^t G(t-s) * G^q(s) ds.$$

11. Express the solution of the transmission heat problem

$$\begin{cases} U_t - \kappa_e \Delta U = 0, & \text{in } \mathbb{R}^N \setminus \overline{\Omega}_i \times (0, \infty), \\ U_t - \alpha_i \kappa_i \Delta U = 0, & \text{in } \Omega_i \times (0, \infty), \\ U^- - U^+ = U_{\text{inc}}, & \text{on } \partial\Omega_i \times (0, \infty), \\ \alpha_i \frac{\partial}{\partial \mathbf{n}} U^- - \frac{\partial}{\partial \mathbf{n}} U^+ = \frac{\partial}{\partial \mathbf{n}} U_{\text{inc}}, & \text{on } \partial\Omega_i \times (0, \infty), \\ U(\cdot, 0) = 0, & \text{in } \mathbb{R}^N, \end{cases}$$

in terms of Helmholtz problems using Laplace transforms.

Taken from [41]. We define u_{inc} and u as the Laplace transforms in time of U_{inc} and U :

$$u_{\text{inc}}(\mathbf{x}, s) = \int_0^\infty e^{-st} U_{\text{inc}}(\mathbf{x}, t) dt, \quad u(\mathbf{x}, s) = \int_0^\infty e^{-st} U(\mathbf{x}, t) dt, \quad \mathbf{x} \in \mathbb{R}^N.$$

For each value of s , the function $u_s(\mathbf{x}) := u(\mathbf{x}, s)$ solves

$$\begin{cases} \Delta u_s + \lambda_{s,e}^2 u_s = 0, & \text{in } \mathbb{R}^N \setminus \overline{\Omega_i}, \\ \alpha_i \Delta u_s + \lambda_{s,i}^2 u_s = 0, & \text{in } \Omega_i, \\ u_s^- - u_s^+ = u_{\text{inc},s}, & \text{on } \Gamma, \\ \alpha_i \partial_{\mathbf{n}} u_s^- - \partial_{\mathbf{n}} u_s^+ = \partial_{\mathbf{n}} u_{\text{inc},s}, & \text{on } \Gamma, \end{cases}$$

where $\lambda_{s,e}^2 := -s/\kappa_e$, $\lambda_{s,i}^2 := -s/\kappa_i$ and $u_{\text{inc},s}(\mathbf{x}) := u_{\text{inc}}(\mathbf{x}, s)$. We set $\Gamma = \partial\Omega_i$. This problem has a unique solution satisfying the Sommerfeld radiation condition at infinity,

$$\lim_{r \rightarrow \infty} r^{(N-1)/2} (\partial_r u_s - i\lambda_{s,e} u_s) = 0, \quad r = |\mathbf{x}|,$$

for all $s \in \mathbb{C} \setminus (-\infty, 0]$. This characterization of $u_s(\mathbf{x})$ can be used to define and compute $u(\cdot, s)$ for all $s \in \mathbb{C} \setminus (-\infty, 0]$.

The solution of the time-dependent problem is recovered by inverting the Laplace transform:

$$U(\mathbf{x}, t) = \frac{1}{2\pi i} \int_{\mathcal{C}} e^{st} u(\mathbf{x}, s) ds.$$

Since $u(\cdot, s)$ exists for all $s \in \mathbb{C} \setminus (-\infty, 0]$ and depends holomorphically on s , many different choices for the inversion path \mathcal{C} are possible.

12. *We know that the problem*

$$\begin{aligned} g_t - \Delta_{\mathbf{v}} g + \mathbf{v} \cdot \nabla_{\mathbf{x}} g + \mathbf{E}(\mathbf{x}, t) \cdot \nabla_{\mathbf{v}} g &= 0, & \mathbf{x} \in \mathbb{R}^3, \mathbf{v} \in \mathbb{R}^3, t \in \mathbb{R}^+, \\ g(\mathbf{x}, \mathbf{v}, 0) &= g_0(\mathbf{x}, \mathbf{v}), & \mathbf{x} \in \mathbb{R}^3, \mathbf{v} \in \mathbb{R}^3, \end{aligned}$$

with $g_0 \in L^1(\mathbb{R}^3 \times \mathbb{R}^3)$ and bounded and Lipschitz \mathbf{E} admits fundamental solutions $\Gamma_{\mathbf{E}}$. The solution of the initial value problem can be expressed as

$$g(\mathbf{x}, \mathbf{v}, t) = \int \Gamma_{\mathbf{E}}(\mathbf{x}, \mathbf{v}, t; \mathbf{x}', \mathbf{v}', 0) d\mathbf{x}' d\mathbf{v}'$$

and $\Gamma_{\mathbf{E}}$ satisfies the estimates

$$\begin{aligned} |\Gamma_{\mathbf{E}}(\mathbf{x}, \mathbf{v}, t; \mathbf{x}', \mathbf{v}', t')| &\leq C(\|\mathbf{E}\|_{L_{\mathbf{x},t}^\infty}, T) G(\mathbf{x}/2, \mathbf{v}/2, t; \mathbf{x}'/2, \mathbf{v}'/2, t'), \\ |\partial_{v_i} \Gamma_{\mathbf{E}}(\mathbf{x}, \mathbf{v}, t; \mathbf{x}', \mathbf{v}', t')| &\leq C(\|\mathbf{E}\|_{L_{\mathbf{x},t}^\infty}, T) \frac{G(\mathbf{x}/2, \mathbf{v}/2, t; \mathbf{x}'/2, \mathbf{v}'/2, t')}{(t-t')^{1/2}}, \end{aligned}$$

where G is the fundamental solution for the problem with $\mathbf{E} = 0$. Extend these results to problems for which \mathbf{E} is just bounded.

Taken from [12]. We regularize \mathbf{E} by convolution and consider $\mathbf{E}_\delta = \mathbf{E} * \eta_\delta$ where η_δ is a mollifying family of functions. Then \mathbf{E}_δ are bounded and Lipschitz, so for each of them we can construct solutions g_δ of the initial value problem and have estimates on the fundamental solutions Γ_δ . Moreover, $\|\mathbf{E}_\delta\|_{L_{x,t}^\infty} \leq \|\mathbf{E}\|_{L_{x,t}^\infty}$ and $\mathbf{E}_\delta \rightarrow \mathbf{E}$ as $\delta \rightarrow 0$.

Since Γ_δ is bounded (locally in t) in any L_{xvt}^p space, a subsequence converges weakly (locally in t) in any L_{xvt}^p (weakly * if $p = \infty$) to a function $\Gamma_{\mathbf{E}}$ and we can pass to the limit in the right-hand side of the integral expressions for the solutions g_δ in terms of Γ_δ .

Moreover, the integral expressions imply that g_δ are uniformly bounded in any space L_{xvt}^p with respect to δ and locally in t. Therefore, g_δ converges weakly (locally in t) in any L_{xvt}^p space to a function g and their derivatives also converge in the sense of distributions.

In the distribution sense, the derivatives of Γ_δ with respect to \mathbf{v} converge weakly to the derivatives of $\Gamma_{\mathbf{E}}$. We can also pass to the limit in the inequalities satisfied by Γ_δ and establish similar inequalities for $\Gamma_{\mathbf{E}}$ because $\|\mathbf{E}_\delta\|_{L_{x,t}^\infty} \leq \|\mathbf{E}\|_{L_{x,t}^\infty}$.

Now, multiplying the differential equation satisfied by g_δ by g_δ we get a uniform L_{xvt}^2 bound on $\nabla_v g_\delta$. If we multiply the equation by $|\mathbf{v}|^2$ we get a uniform L_{xvt}^1 bound on $|\mathbf{v}|^2 g_\delta$.

Multiplying the differential equations satisfied by g_δ by test functions, we can pass to the limit in all the terms of the weak formulation of the equation except in $\mathbf{E}_\delta \nabla_v g_\delta$ with the convergences already established. The passage to the limit in this term is technical, see details in [12]. Finally, g is a solution for the initial value problem with bounded \mathbf{E} and $\Gamma_{\mathbf{E}}$ an associated fundamental solution.

13. *Calculate the equilibrium solution of the Liouville-master equation*

$$\begin{aligned} \partial_t \mathcal{P}(x, p, \boldsymbol{\sigma}, t) + \frac{p}{m} \partial_x \mathcal{P}(x, p, \boldsymbol{\sigma}, t) + \left(-m\omega_0^2 x + \mu \sum_{i=1}^n \sigma_i \sigma_{i+1} \right) \partial_p \mathcal{P}(x, p, \boldsymbol{\sigma}, t) \\ = \sum_{i=1}^N [W_i(R_i \boldsymbol{\sigma} | x, p) \mathcal{P}(x, p, R_i \boldsymbol{\sigma}, t) - W_i(\boldsymbol{\sigma} | x, p) \mathcal{P}(x, p, \boldsymbol{\sigma}, t)]. \end{aligned}$$

Taken from [49]. The equilibrium solution of this equation is the canonical distribution

$$\mathcal{P}_{\text{eq}}(x, p, \boldsymbol{\sigma}) = \frac{1}{Z} e^{-\beta \mathcal{H}(x, p, \boldsymbol{\sigma})},$$

where Z is the partition function

$$Z = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dp \sum_{\boldsymbol{\sigma}} e^{-\beta \mathcal{H}(x, p, \boldsymbol{\sigma})},$$

and $\beta = (k_B T)^{-1}$. For a study of nonequilibrium behavior see [50].

14. Construct solutions of the scalar conservation law $w_t + (c(x)w)_x = x$ with $w(0) = w_0$.

Taken from [17]. We set $v = cw$. Then, $v_t + cv_x = 0$. Thus, v is constant along the characteristic curves $x(t)$ solution of $x'(t) = c(x(t))$, $x(0) = x_0$, because

$$\frac{d}{dt}v(x(t), t) = v_x(x(t), t)x'(t) + v_t(x(t), t) = 0.$$

Given (x, t) we may be able to calculate $x_0(x, t)$ such that the characteristic curve with initial value $x_0(x, t)$ satisfies $x(t) = x$. Then $v(x, t) = v(x(t), t) = v_0(x_0(x, t))$ and $w(x, t) = \frac{v_0(x_0(x, t))}{c(x_0(x, t))}$. The feasibility of this procedure will depend on the function c .

15. Solve the problem

$$\begin{aligned} \frac{\partial r}{\partial s} + \frac{\partial}{\partial k}(k^{1/3}r) &= 0, \\ \int_0^\infty kr(s, k)dk &= t, \\ \lim_{k \rightarrow 0} k^{1/3}r(s, k) &= 2c. \end{aligned}$$

Taken from [34]. Integrating the equation over $k > 0$ we find

$$\frac{d}{ds} \int_0^\infty r(s, k)dk = \lim_{k \rightarrow 0} k^{1/3}r(s, k) = 2c(s).$$

Arguing as in the previous exercise, the method of characteristics yields

$$\begin{aligned} k^{1/3}r(s, k) &= 2c(s - a(k))H(s - a(k)), \\ a(k) &= \frac{3}{2}k^{2/3}, \end{aligned}$$

in which $H(x)$ is the Heaviside function (1 for positive x , 0 otherwise).

3 Differential-Difference Equations

1. Consider the differential difference equation $u'_n(t) = u_{n+1} - 2u_n + u_{n-1} - A \sin(u_n)$, where A is a positive parameter. Prove that there is a monotone solution such that $u_{-\infty} = 0$ and $u_\infty = 2\pi$ with $u_0 = \pi$ and $u_n - \pi = \pi - u_{-n}$ for all n .

Taken from [14]. We set $u_0 = \pi$ and vary u_1 in the interval $(\pi, 2\pi)$ to find the desired solution. The condition $u_0 = \pi$ ensures that $u_n - \pi$ is an odd function of n . We first choose $\epsilon > 0$ so that $-A \sin(u) > \epsilon(u - \pi)$ for $\pi < u \leq \frac{3}{2}\pi$. Then, we choose N large so that $\epsilon(N - 1) > 1$. Next, we choose $u_1 - \pi$ small so that $u_j \leq \frac{3}{2}\pi$ for $1 \leq j \leq N$. We wish to

show that under these conditions, the finite sequence $\{u_1, \dots, u_N\}$ is not monotone increasing. It is convenient to let $U_n = u_n - \pi$. If $\{U_1, \dots, U_N\}$ is monotone increasing, then $2 \leq j \leq N$ and $U_j \leq (2 - \epsilon)U_{j-1} - U_{j-2}$. Adding these inequalities results in $U_N - U_{N-1} \leq \epsilon \sum_{i=2}^{N-1} U_i + (1 - \epsilon)U_1$. Since we assumed that $U_i \geq U_1$ for $2 \leq i \leq N$, our lower bound on N then shows that $U_N < U_{N-1}$, a contradiction. Therefore, we have shown that for sufficiently small U_1 , the sequence starts to decrease before crossing π . On the other hand, we have simply to choose $U_1 > \pi$ to have the sequence cross π before decreasing. Note that if the sequence increases until some first N such that $U_N = \pi$, then $U_{N+1} > \pi$. If, finally, there is an N such that the sequence increases up to $n = N$, with $U_N < \pi$, and $U_N = U_{N+1}$, then $U_{N+2} < U_{N+1}$ so that the sequence decreases before reaching π .

2. Let $U_i(t)$ and $L_i(t)$, $i \in \mathbb{Z}$ be differentiable sequences such that

$$U'_i(t) - d_1(U_i)(U_{i+1} - U_i) - d_2(U_i)(U_{i-1} - U_i) - f(U_i) \geq \\ L'_i(t) - d_1(L_i)(L_{i+1} - L_i) - d_2(L_i)(L_{i-1} - L_i) - f(L_i)$$

and $U_i(0) < L_i(0)$ for all i , where f , $d_1 > 0$ and $d_2 > 0$ are Lipschitz continuous functions. Then, $U_i(t) > L_i(t)$ for all $t > 0$ and $i \in \mathbb{Z}$.

Taken from [15]. By contradiction, set $W_i(t) = U_i(t) - L_i(t)$. At $t = 0$, $W_i(0) > 0$ for all i . Let us assume that W_i changes sign after a certain minimum time $t_1 > 0$, at some value of i , $i = k$. Thus $W_k(t_1) = 0$ and $W'_k(t) \leq 0$, as $t \rightarrow t_1$. We shall show that this is contradictory. At $t = t_1$, there must be an index m (equal or different from k) such that $W_m(t_1) = 0$, while its next neighbor $W_{m+j}(t_1) > 0$ (j is either 1 or -1), and $W_i(t_1) = 0$ for all indices between k and m . For otherwise W_k should be identically 0 for all k . The differential inequality implies

$$W'_m(t_1) \geq d_1(U_m(t_1))W_{m+1}(t_1) + d_2(U_m(t_1))W_{m-1}(t_1) > 0.$$

This contradicts the fact that $W'_m(t)$ should have been nonpositive as $t \rightarrow t_1$, for $W_m(t_1)$ to have become zero in the first place.

3. Consider the equation

$$U'(t) = z_1(F/A) + z_3(F/A) - 2U(t) - A \sin(U(t)) + F,$$

for $|F| < A$, $A \gg 1$ where $z_1(F/A) < z_2(F/A) < z_3(F/A)$ are three consecutive solutions of the equation $\sin(z) = F/A$ in one period. Prove that there is a critical value F_c such that this equation has three stable constant solutions if $0 \leq F < F_c$ but one if $F > F_c$. Characterize F_c .

Taken from [18]. When $F = 0$, $z_1(0) = 0$, $z_2(0) = \pi$ and $z_3(0) = 2\pi$. We need to solve

$$2z + A \sin(z) = F + 2\arcsin(F/A) + 2\pi.$$

As we increase F from 0, we keep on finding three solutions $z_1(F/A) < z_2(F/A) < z_3(F/A)$ continuing these branches until $F + 2\arcsin(F/A) + 2\pi$ hits the first local maximum of $2z + A\sin(z)$ (remember that A is large). The value F_c at which this happens is characterized by the existence of a double zero, a value u_0 such that $2 + A\cos(u_0) = 0$ and $2u_0 + A\sin(u_0) = F_c + 2\arcsin(F_c/A) + 2\pi$. Then, $u_0 = \arccos(-2/A)$ and F_c is the solution of $2u_0(A) + A\sin(u_0(A)) = F_c + 2\arcsin(F_c/A) + 2\pi$. Below F_c we have three zeroes, at F_c two collapse, above F_c the collapsing ones, $z_1(F/A)$ and $z_2(F/A)$ are lost.

$z_1(F/A)$ and $z_3(F/A)$ are stable while they exist. This picture corresponds to a saddle node bifurcation in the system, see [18].

4. The system of equations

$$\frac{dE_i}{dt} + \frac{v(E_i)}{\nu}(E_i - E_{i-1}) - \frac{D(E_i)}{\nu}(E_{i+1} - 2E_i + E_{i-1}) = J - v(E_i),$$

for $i \in \mathbb{Z}$ admits traveling wave solutions of the form $E_i(t) = E(i - ct)$ propagating at constant velocity c when the parameter J is large enough. Here, v, D are positive functions and $\nu > 0$ is large. v is a cubic, it grows from 0 to a local maximum, decreases to a positive minimum, and increases to infinity later. Justify that the wavefront velocity scales as $(J - J_c)^{1/2}$ where J_c is the threshold for existence of travelling waves.

Taken from [20]. For ν large, we can construct stationary solutions, which can be approximated by

$$E_i \sim z_1(J) \quad i < 0, \quad E_i \sim z_3(J) \quad i > 0,$$

for $|J| < J_c$, while E_0 solves

$$J - v(E_0) - \frac{v(E_0)}{\nu}(E_0 - z_1(J)) + \frac{D(E_0)}{\nu}(z_3(J) - 2E_0 + z_1(J)) = 0,$$

where $z_1(J) < z_2(J) < z_3(J)$ are solutions of $J = v(z)$. At a value J_c , $z_1(J_c) = z_2(J_c)$ and these roots are lost for $J > J_c$, only $z_3(J)$ remains. The reduced equation

$$\frac{dE_0}{dt} = J - v(E_0) - \frac{v(E_0)}{\nu}(E_0 - z_1(J)) + \frac{D(E_0)}{\nu}(z_3(J) - 2E_0 + z_1(J)),$$

for the middle point undergoes a saddle node bifurcation at J_c with normal form

$$\phi' = \alpha(J_c)(J - J_c) + \beta(J_c)\phi^2,$$

which has solutions of the form $\sqrt{\frac{\alpha}{\beta}(J - J_c)} \tan(\sqrt{\alpha\beta(J - J_c)}(t - t_0))$, blowing up when the argument of the tangent approaches $\pm\pi/2$, over a time $t - t_0 \sim \pi/\sqrt{\alpha\beta(J - J_c)}$. This value J_c separates the regime for which

we have stationary (pinned) wave front solutions and travelling wave front solutions. It marks the depinning transition.

Now, for $J > J_c$ but close to J_c , simulations show staircase like wave profiles, in which a point stays near the vanished equilibrium $E_0(J_c)$ until it moves following the tangent path given by the normal form and is replaced at position $E_0(J_c)$ by a neighbouring one, once and again. The wave velocity is the reciprocal of the time this transition takes $c(J, \nu) \sim \frac{\sqrt{\alpha\beta(J-J_c)}}{\pi}$, see [20] for details.

5. *We consider a problem with noise*

$$\frac{du_i}{dt} = u_{i+1} - 2u_i + u_{i-1} + F - A \sin(u_i) + \gamma \xi_i,$$

where $A > 0$ is large and $\gamma > 0$ characterizes the disorder strength and ξ_i is a zero mean random variable taking values on an interval $(-1, 1)$ with equal probability. Show that the speed of the wavefronts for F larger than the critical value F_c^* scales as $(F - F_c^*)^{3/2}$.

Taken from [22]. Setting $\gamma = 0$, we can repeat with this equation the study done in the previous exercise and obtain a velocity that scales like $(F - F_c)^{1/2}$. However, when we add noise, for each realization of the noise, the threshold F_c is shifted slightly up or down by the noise. The observed velocity will be the average of the velocities observed for a large number of realizations. If

$$|c_R| \sim \frac{1}{\pi} \sqrt{\alpha(F_c)\beta(F_c)(F - F_c) + \gamma\beta(F_c)\xi_0}$$

the average

$$\bar{c} = \frac{1}{N} \sum_{R=1}^N |c_R| = \frac{1}{2\pi} \int_{-1}^1 (\alpha\beta(F - F_c) + \gamma\beta\xi)^{1/2} d\xi \sim (F - F_c^*)^{3/2}$$

where the new critical field is $F_c^* = F_c - \frac{\gamma}{\alpha}$.

6. *Consider the problem*

$$\frac{du_i}{dt} = u_{i+1} - 2u_i + u_{i-1} + F - A \sin(u_i),$$

with A large. Let $z_1(F/A) < z_2(F/A) < z_3(F/A)$ be the three consecutive branches of zeros of $F - A \sin(z) = 0$ which start at $z_1(0) = 0$, $z_2(0) = \pi$, $z_3(0) = 2\pi$. We know that for $|F| < F_c(A)$ the problem admits stationary solutions increasing from $z_1(F/A)$ at $-\infty$ to $z_3(F/A)$ at ∞ . When F surpasses that threshold, we have travelling wave solutions. Write the equation for such travelling wave solutions and find a formula for the velocity.

Taken from [24]. Travelling wave solutions have the form $u_i(t) = u(i - ct)$, where c is a constant wave speed and $u(z)$, $z = i - ct$ is a wave profile, which solve

$$-cu_z(z) = u(z+1) - 2u(z) + u(z-1) + F - A \sin(u(z)), \quad z \in \mathbb{R}$$

with $u(-\infty) = z_1(F/A)$ and $u(\infty) = z_3(F/A)$. These type of travelling wave solutions are called fronts. Multiplying the equation by u_z and integrating, we find

$$-c \int_{-\infty}^{\infty} u_z^2 dz = F [z_3(F/A) - z_1(F/A)].$$

7. *The discrete Fitz Hugh-Nagumo system is a typical model for pulse propagation*

$$\begin{aligned} \epsilon u'_i &= d(u_{i+1} - 2u_i + u_{i-1}) + u_i(2 - u_i)(u_i - a) - v_i, \\ v'_i &= u_i - Bv_i. \end{aligned}$$

when the parameter values $\epsilon, d > 0$ and a are such that $(0, 0)$ is the only constant solution. ϵ is small and a is such that $z(2 - z)(z - a)$ has three roots $z_1(a) < z_2(a) < z_3(a)$. Explain how to describe the evolution of pulse solutions in terms of front solutions for Nagumo type equations

$$\epsilon u'_i = d(u_{i+1} - 2u_i + u_{i-1}) + u_i(2 - u_i)(u_i - a) - w.$$

Taken from [25]. Pulse-like solutions take the form $u_i(t) = u(z)$, $v_i(t) = v(z)$, $z = i - ct \in \mathbb{R}$, with

$$\begin{aligned} -\epsilon u_z(z) &= d(u(z+1) - 2u(z) + u(z-1)) + u(z)(2 - u(z))(a - u(z)) - v, \\ -cv_z(z) &= 0, \end{aligned}$$

for $z \in \mathbb{R}$. For small enough v , we denote by $z_1(a, v) < z_2(a, v) < z_3(a, v)$ the three roots of $u(z)(2 - u(z))(a - u(z)) - v = 0$. Since ϵ is small, u_i and v_i evolve in different time scales. We distinguish 5 regions in a pulse like solution

- Pulse front: $u_i = z_1(a, v_i)$ and $v'_i = z_1(a, v_i) - Bv_i$, which evolves to $(0, 0)$ as i grows.
- Pulse leading edge: Described by a traveling solution of $\epsilon u'_i = d(u_{i+1} - 2u_i + u_{i-1}) + u_i(2 - u_i)(u_i - a) - 0$ which decreases from 2 to 0, with $v_i \sim 0$. It travels at speed c .
- Pulse peak: $u_i = z_2(a, v_i)$ and $v'_i = z_3(a, v_i) - Bv_i$.
- Pulse trailing edge: Described by a traveling solution of $\epsilon u'_i = d(u_{i+1} - 2u_i + u_{i-1}) + u_i(2 - u_i)(u_i - a) - w$ which increases from 0 to 2, with $v_i \sim w$, w selected in such a way that it travels with speed c too.

- Pulse tail: $u_i = z_1(a, v_i)$ and $v_i' = z_1(a, v_i) - Bv_i$, which evolves to $(0, 0)$ as i decreases.

See [25] for a visualization. See [32] for an application of these ideas to Hodgkin-Huxley models for myelinated nerves. Pulse solutions fail to propagate when the leading pulse cannot move because for the parameters we use the reduced from equation has only stationary front solutions, they are pinned.

8. Consider the system

$$\begin{aligned} v_j' &= d(v_{j+1} - 2v_j + v_{j-1}) + f(v_j, w_j), \\ w_j' &= \lambda g(v_j, w_j), \end{aligned}$$

with $d, \lambda > 0$ and λ is small, for the two variables to evolve in different scales. For w fixed, $f(v, w)$ is a 'bistable cubic', that is, it has three zeros, two of which are stable. When $f(v, w) = 0 = g(v, w)$ has a unique solution, which is stable, we have pulse like solutions for the differential system, as for Fitz Hugh-Nagumo. When it is unstable, show that oscillating solutions appear.

Taken from [33]. When g and f intersect at a stable zero, we have an excitable system displaying pulse like solutions. When they intersect at an unstable zero, limit cycle solutions $(V(t), W(t))$ with period T , $T > 0$ of

$$v' = f(v, w), \quad w' = \lambda g(v, w),$$

for λ small, play a role. The trajectories of the system behave like $v_j(t) = V(t + \phi_j)$ and $w_j(t) = W(t + \phi_j)$, for a slowly varying phase ϕ_j which may become independent of t as $t \rightarrow \infty$. All the trajectories are then synchronized.

9. Let $u_{i,j}(t)$ be a solution to

$$\frac{\partial u_{i,j}}{\partial t} = u_{i-1,j} - 2u_{i,j} + u_{i+1,j} + A(\sin(u_{i,j-1} - u_{i,j}) \sin(u_{i,j+1} - u_{i,j}))$$

for $i, j \in \mathbb{Z}$ and $u_{i,j}(0) = \alpha_{i,j}$ satisfying $\alpha_{i+1,j} - 2\alpha_{i,j} + \alpha_{i-1,j} \in l^2$, $\sin(\alpha_{i,j-1} - \alpha_{i,j}) \sin(\alpha_{i,j+1} - \alpha_{i,j}) \in l^2$ and $\alpha_{i,j} \in l_{\text{loc}}^\infty$. If $(u_{i,j+1} - u_{i,j})(t) \in \cap_{n \in \mathbb{Z}} [-\frac{\pi}{2} + 2n\pi, \frac{\pi}{2} + 2n\pi]$ holds for all i, j, t , then $u_{i,j}(t)$ tends to a limit $s_{i,j}$ as $t \rightarrow \infty$ which is a stationary solution of the problem.

Taken from [23]. Define $w_{i,j}(t) = u_{i,j}(t + \tau) - u_{i,j}(t)$ for some $\tau > 0$. Then

$$\begin{aligned} \frac{d}{dt} \left(\frac{1}{2} \sum_{i,j} |w_{i,j}(t)|^2 \right) &= - \sum_{i,j} ((w_{i+1,j} - w_{i,j})(t))^2 - \sum_{i,j} (\sin((u_{i,j+1} - u_{i,j})(t + \tau)) \\ &\quad - \sin((u_{i,j+1} - u_{i,j})(t))) ((u_{i,j+1} - u_{i,j})(t + \tau) - (u_{i,j+1} - u_{i,j})(t)) \leq 0. \end{aligned}$$

This implies $w_{i,j}(t) \rightarrow 0$ as $t \rightarrow \infty$ for every i, j . In conclusion, $u_{i,j}(t)$ tends to a limit $s_{i,j}$ which is a stationary solution of the problem.

10. We solve

$$\frac{\partial u_{i,j}}{\partial t} = u_{i-1,j} - 2u_{i,j} + u_{i+1,j} + A(\sin(u_{i,j-1} - u_{i,j}) \sin(u_{i,j+1} - u_{i,j}))$$

with boundary conditions $s_{i,j} = \theta(i, j/\sqrt{A}) + Fj$ where θ is the angle function from 0 to 2π and $F > 0$ is a control parameter. For $F = 0$, the previous exercise ensures existence of stationary solutions. Can you expect a change as F grows?

Taken from [26]. As F grows, the condition

$$(u_{i,j+1} - u_{i,j})(t) \in \cap_{n \in \mathbb{Z}} \left[-\frac{\pi}{2} + 2n\pi, \frac{\pi}{2} + 2n\pi \right]$$

will fail. Stationary solutions will disappear and travelling patterns will be observed. Notice that if we linearize the spatial operator about $s_{i,j}$, we have a discrete elliptic problem for F small but it changes type as F grows.

11. We construct numerically solutions of

$$m \frac{\partial^2 u_{i,j}}{\partial t^2} + \alpha \frac{\partial u_{i,j}}{\partial t} = u_{i-1,j} - 2u_{i,j} + u_{i+1,j} + A(\sin(u_{i,j-1} - u_{i,j}) \sin(u_{i,j+1} - u_{i,j}))$$

in a square lattice $i = 1, \dots, N_x$, $j = 1, \dots, N_y$, with boundary conditions $u_{i,j} = F(j - (N_y + 1)/2)$. This is equivalent to 'shearing' the lattice. As F grows, we observe that the initial zero solution for $F = 0$ changes into slowly varying stationary solutions until we reach a point F_c past which the lattice structure is distorted in two main different ways. Linearizing the problem at $F = F_c$ we find a zero eigenvalue for the resulting matrix, while all the eigenvalues are negative for $F < F_c$. How do you explain this?

Taken from [36]. The branch of stationary solutions $s_{i,j}(F)$ seems stable. At $F = F_c$ and two new branches appear. The system undergoes a pitchfork bifurcation.

12. We construct numerically solutions of

$$m \frac{\partial^2 v_{i,j}}{\partial t^2} + \alpha \frac{\partial v_{i,j}}{\partial t} = v_{i-1,j} - 2v_{i,j} + v_{i+1,j} + A(\sin(v_{i,j-1} - v_{i,j}) \sin(v_{i,j+1} - v_{i,j}))$$

in a square lattice $i = 1, \dots, N_x$, $j = 1, \dots, N_y$. We set the boundary conditions representing a 'push down' from the central top part:

- Left-hand side: $v_{1,j} = v_{0,j}$.
- Right-hand side: $v_{N_x,j} = v_{N_x+1,j}$.

- *Left-hand-side of the top layer* ($1 \leq i < p_1$): $v_{i,N_y} = v_{i,N_y+1}$.
- *Right-hand-side of the top layer* ($p_2 < i \leq N_x$): $v_{i,N_y} = v_{i,N_y+1}$.
- *Bottom layer of the domain*: $v_{i,0} = 0$.
- *Central atoms* ($p_1 \leq i \leq p_2$) are pushed downwards according to: $v_{i,N_y+1} - v_{i,N_y} = -f(i)$, where f has a triangular profile, pointing downwards, with magnitude $F > 0$.

As F grows, we observe that the initial zero solution for $F = 0$ develops localized lattice distortions that travel downwards. As we decrease F to zero the distortions travel upwards and may disappear. How do you explain that?

Taken from [45]. The branch of stationary solutions that starts at $F = 0$ develops bifurcations at specific values of F at which lattice with different distortions are created. Such new branches are stable for some ranges of F , while the defects simply travel. The configuration bifurcates at new F values, new distortions are created, that travel for while, and the process is repeated as F grows. When we decrease F , the process is reversed. Created distortions travel upwards, and disappear.

13. Consider the problem

$$u_j'' + \alpha u_j' = u_{j+1} - 2u_j + u_{j-1} + F - Ag(u_j),$$

where $g(u) = u + 1$ if $u < 0$ and $g(u) = u - 1$ if $u > 0$. Construct traveling wave front solutions.

Taken from [27]. A traveling wave front solution takes the form $u_i(t) = u(i - ct)$, $z = i - ct$. The profile $v(z) = u(z) + 1$ satisfies

$$\begin{aligned} c^2 v_{zz}(z) - \alpha c v_z(z) - (v(z+1) - 2v(z) + v(z-1)) + Av(z) \\ = F + 2AH(-\text{sign}(cF)z), \quad z \in \mathbb{R}, \end{aligned}$$

with $v(-\infty) = 0$ and $v(\infty) = 2$. We have written $g(u) = u + 1 - 2H(u)$, where u is the Heaviside function. Using the complex contour integral expression for the Heaviside function

$$H(-z) = -\frac{1}{2\pi i} \int_C \frac{e^{ikx}}{k} dk.$$

C is a contour formed by a closed semicircle in the upper complex plane oriented counterclockwise and another one oriented clockwise in the lower half plane, which includes zero inside and forms a small semicircle around it. The profile we seek admits the expression

$$v(z) = \frac{F}{A} - \frac{A}{\pi i} \int_C \frac{\exp(ik \text{sign}(cF)z) dk}{k A + 4 \sin^2(k/2) - k^2 c^2 - ik|c|\alpha \text{sign}(F)}.$$

Imposing $v(0) = 1$ we obtain a relation between the velocity c and the applied force F . Once we know $c(F)$, the above expression provides the profiles v . Unlike previous exercises, such profiles are not monotonic, but display oscillations, see [27].

14. Show that the initial value problem

$$\begin{aligned} u_j'' + \alpha u_j' &= d(u_{j+1} - 2u_j + u_{j-1}) - u_j + F, \\ u_j(0) &= u_j^0, \quad u_j'(0) = u_j^1, \end{aligned}$$

$d > 0$, $\alpha \geq 0$, admits solutions of the form

$$u_j(t) = \sum_k [G_{j,k}^0(t)u_k'(0) + G_{j,k}^1(t)u_k(0)] + \int_0^t \sum_k G_{j,k}^0(t-s)f_k(s)ds$$

for adequate Green functions $G_{j,k}^0$ and $G_{j,k}^1$.

Taken from [28]. Firstly, we get rid of the difference operator by using the generating functions $p(\theta, t)$ and $f(\theta, t)$

$$p(\theta, t) = \sum_j u_j(t)e^{-ij\theta}, \quad f(\theta, t) = \sum_j f_j(t)e^{-ij\theta}.$$

Differentiating p with respect to t and using the equation, we see that p solves the ordinary differential equation

$$p''(\theta, t) + \alpha p'(\theta, t) + \omega(\theta)^2 p(\theta, t) = f(\theta, t)$$

with $\omega(\theta)^2 = 1 + 4d \sin^2(\theta/2)$ and initial conditions for p from those for u_j . Fixed θ we know how to calculate explicit solutions of this linear second order equation with constant coefficients to get

$$p(\theta, t) = p(\theta, 0)g^0(\theta, t) + p'(\theta, 0)g^1(\theta, t) + \int_0^t g^1(\theta, t-s)f(\theta, s)ds,$$

for

$$g^0(\theta, t) = \begin{cases} \frac{e^{r_+(\theta)t} - e^{r_-(\theta)t}}{r_+(\theta) - r_-(\theta)}, & \alpha^2/4 > \omega^2(\theta), \\ te^{-\alpha t/2}, & \alpha^2/4 = \omega^2(\theta), \\ e^{-\alpha t/2} \frac{\sin(I(\theta)t)}{I(\theta)}, & \alpha^2/4 < \omega^2(\theta), \end{cases}$$

$$g^1(\theta, t) = \begin{cases} \frac{e^{r_+(\theta)t} r_+(\theta) - e^{r_-(\theta)t} r_-(\theta)}{r_+(\theta) - r_-(\theta)}, & \alpha^2/4 > \omega^2(\theta), \\ te^{-\alpha t/2} \left(1 + \frac{\alpha}{2}t\right), & \alpha^2/4 = \omega^2(\theta), \\ e^{-\alpha t/2} \left(\cos(I(\theta)t) + \frac{\alpha \sin(I(\theta)t)}{2I(\theta)}\right), & \alpha^2/4 < \omega^2(\theta). \end{cases}$$

We recover u_j as

$$u_j(t) = \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} e^{ij\theta} p(\theta, t),$$

and find

$$G_{jk}^0(t) = \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} e^{i(j-k)\theta} g^0(\theta, t), \quad G_{jk}^1(t) = \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} e^{i(j-k)\theta} g^1(\theta, t).$$

15. Use the expression of the solutions of the initial value problem established before to define a nonreflecting boundary condition at $n = 0$ for truncated problems set in $n \geq 0$, so that the solution we obtain is the same we would obtain solving the system for all n .

Taken from [48]. We place an artificial boundary at $n = 0$ and restrict the computational domain to the region $n \geq 0$. Thus, we need a boundary condition to compute $u_0(t)$ and close the system. In principle,

$$\frac{d^2 u_0}{dt^2} = d(u_1 - 2u_0 + u_{-1}) + f_0,$$

but $u_{-1}(t)$ is unknown unless we solve also for $n \leq 0$. The equation at $n = -1$ can be rewritten as:

$$\frac{d^2 u_{-1}}{dt^2} = d(0 - 2u_{-1} + u_{-2}) + f_{-1} + du_0.$$

Assuming we know $u_0(t)$, the problem for $n \leq 0$ with boundary condition $u_0(t)$ can be seen as a problem with zero boundary condition at the wall and a modified source term: $f_n + d\delta_{n,-1}u_0$ for $n < 0$. We can extend this problem to the whole space setting:

$$v_n = \begin{cases} u_n & n < 0 \\ 0 & n = 0 \\ -u_{-n} & n > 0 \end{cases}$$

The extension v_n solves:

$$\frac{d^2 v_n}{dt^2} = d(v_{n+1} - 2v_n + v_{n-1}) + g_n, \\ v_n(0) = v_n^0, \quad \frac{dv_n}{dt}(0) = v_n^1,$$

for all n , where v_n^0 and v_n^1 are odd extensions of u_n^0 and u_n^1 . The source g_n is obtained extending $f_n + \delta_{n,-1}u_0$. We have included the boundary condition u_0 as a force acting on u_{-1} to allow for an odd extension with $v_0 = 0$. Using the symmetry of the data:

$$u_n(t) = v_n(t) = \sum_{n' < 0} [\mathcal{G}_{n,n'}^0(t) \frac{du_{n'}}{dt}(0) + \frac{d\mathcal{G}_{n,n'}^0}{dt}(t) u_{n'}(0)] \\ + \int_0^t \sum_{n' < 0} \mathcal{G}_{n,n'}^0(t-s) (f_{n'}(s) + d\delta_{n',-1}u_0(s)) ds, \quad n < 0$$

where $\mathcal{G}_{n,n'}^0 = G_{n,n'}^0 - G_{n,-n'}^0$ is the Green function for the half space $n < 0$ with zero boundary condition at $n = 0$. In this way, we obtain the desired formula for u_{-1} :

$$\begin{aligned} u_{-1}(t) &= r_{-1}(t) + d \int_0^t \mathcal{G}_{-1-1}^0(t-s)u_0(s)ds, \\ r_{-1}(t) &= \sum_{n' < 0} [\mathcal{G}_{-1,n'}^0(t) \frac{du_{n'}}{dt}(0) + \frac{d\mathcal{G}_{-1,n'}^0}{dt}(t)u_{n'}(0) \\ &\quad + \int_0^t \mathcal{G}_{-1,n'}^0(t-s)f_{n'}(s)ds]. \end{aligned}$$

The term $r_{-1}(t)$ represents the contribution of the data in the outer region. Our boundary condition at $n = 0$ takes the form:

$$\frac{d^2 u_0}{dt^2} = d \left(u_1 - 2u_0 + d \int_0^t \mathcal{G}_{-1-1}^0(t-s)u_0(s)ds \right) + dr_{-1} + f_0,$$

where the kernel is:

$$\mathcal{G}_{-1-1}^0(t) = \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} \frac{1 - e^{-2i\theta}}{\omega(\theta)} \sin(\omega(\theta)t).$$

In a similar way, we can set no reflecting boundary conditions in finite intervals $-N \leq n \leq N$, see [48].

16. *Consider the initial value problem*

$$\begin{aligned} u_j'' &= d(u_{j+1} - (2+r)u_j + u_{j-1}) + f(u_j), \quad j = 1, \dots, N \\ u_j(0) &= u_j^0, \quad u_j'(0) = u_j^1, \quad j = 1, \dots, N \\ u_0(t) &= u_{N+1}(t) = 0, \end{aligned}$$

for a continuous function f . Set $V(u) = -\int_0^u f(s)ds$. Assume $uf(u) + 2(2\sigma + 1)V(u) \geq 0$ for $\sigma > 0$. Define the energy

$$E(t) = \frac{1}{2} \sum_{j=-\infty}^{\infty} u_j'^2(t) + \frac{d}{2} \sum_{j=-\infty}^{j=\infty} [(u_{j+1} - u_j)^2(t) + ru_j^2(t)] + \sum_{j=-\infty}^{j=\infty} V(u_j(t)).$$

If $E(0) < 0$, then $\sum_{j=1}^N |u_j(t)|^2 \rightarrow \infty$ as $t \rightarrow T$ for some finite $T > 0$.

Taken from [29]. We define $H(t) = \sum_{j=1}^N |u_j(t)|^2 + \rho(t + \tau)^2$, $\rho, \sigma > 0$ to be selected so that $(H^{-\sigma})'' = \sigma H^{-\sigma-2}((\sigma+1)(H')^2 - HH'') \leq 0$. When $H(0) \neq 0$ we have

$$H^\sigma(t) \geq H^{\sigma+1}(0)(H(0) - \sigma t H'(0))^{-1}$$

and $H(t)$ blows up at some time $T \leq H(0)/\sigma H'(0)$ provided $H'(0) > 0$.

Let us explain how to do this. We calculate H' and H'' , and use the

equation to get

$$HH'' - (\sigma + 1)(H')^2 = 4(\sigma + 1)Q + 2HG,$$

$$Q = \left(\sum_{j=1}^N |u_j|^2 + \rho(t + \tau)^2 \right) \left(\sum_{j=1}^N |u'_j|^2 + \rho \right) - \left(\sum_{j=1}^N u_j u'_j + \rho(t + \tau) \right)^2,$$

$$G = \sum_{j=1}^N u_j f(u_j) - \sum_{i,j} u_i a_{i,j} u_j - (2\sigma + 1) \left(\sum_{j=1}^N |u'_j|^2 + \rho \right),$$

where $\mathbf{A} = (a_{ij})$ is the matrix defining the linear part of the system. We have $Q \geq 0$. We estimate $G'(t)$ to find $G(t) \geq \sigma(2\sigma + 1) \left(-\frac{\rho}{2} - E(0) \right) \geq 0$ for $\rho = -2E(0) > 0$.

We have $(H^{-\sigma})'' \leq 0$ and $H(0) \neq 0$. Moreover, $H'(0) = 2 \sum_{j=1}^N u_j^0 u_j^1 + 2\rho\tau > 0$ if $\tau > -\rho^{-1} \sum_{j=1}^N u_j^0 u_j^1$.

17. Let $u_n(t)$ be a solution of

$$u'_n = d(u_n)(u_{n+1} - 2u_n + u_{n-1}) + v(u_n)(u_{n-1} - u_n) + f(u_n),$$

with non negative initial data and a strong reactive source f , such that $f(u) > Cu^p$, with $p > 1$, $C > 0$, when $u > 0$ large. We set $a(u) = -(2d(u) + v(u))u + f(u)$ and assume that $d(u) > 0$, $d(u) + v(u) > 0$ grow slower than u^p for u large. For any component k such that $a(u_k(0)) > 0$ and $a'(u) > 0$ when $u > u_k(0)$

$$u_k(t) \rightarrow \infty \quad \text{as} \quad t \rightarrow T \leq T_b = \int_{u_k(0)}^{\infty} \frac{ds}{a(s)} < \infty.$$

Taken from [44]. In all cases, a maximum principle ensures the positivity of $u_n(t)$ everywhere. Using $u_{k+1}, u_{k-1} \geq 0$, we obtain the differential inequality $u'_k(t) \geq a(u_k)$. By hypothesis, $a(u) > a(u_k(0)) > 0$ for $u \geq u_k(0)$. Then $u_k(t)$ is increasing and it is bounded from below by the solution $y(t)$ of $y'(t) = g(y)$, $y(0) = u_k(0)$, which is given implicitly by:

$$t = \int_{u_k(0)}^{y(t)} \frac{ds}{a(s)}.$$

The integral $\int_{u_k(0)}^{\infty} \frac{ds}{a(s)} < \infty$ due to the growth condition $a(s) \gg s^p$, $p > 1$ for s large, since $a(u) > 0$ for $u \geq u_k(0)$. When $t \rightarrow T_b = \int_{u_k(0)}^{\infty} \frac{ds}{a(s)} < \infty$, $y(t) \rightarrow \infty$.

18. Consider the Becker-Döring equations

$$\sum_{k=1}^{\infty} k\rho_k = \rho > 0,$$

$$\rho'_k = j_{k-1} - j_k, \quad k \geq 2,$$

$$j_k = d_k(e^{aD+\epsilon_k} \rho_1 \rho_k - \rho_{k+1})$$

for a given sequence $\epsilon_k > 0$ with $D_+\epsilon_k = \epsilon_{k+1} - \epsilon_k$, with a and ρ positive constants. Calculate the equilibrium distributions.

Taken from [30]. We set $j_k = 0$. Then $\rho_k = \rho_1^k e^{a\epsilon_k}$. This system admits traveling wavefront solutions, see [30].

19. Consider the kinetic system

$$\begin{aligned}\frac{dr_k}{ds} &= (k-1)^{1/3}D(k-1)r_{k-1} - k^{1/3}D(k)r_k, \quad k \geq 3, \\ \frac{dr_2}{ds} &= 2cD(1) - 2^{1/3}D(2)r_2, \\ c\frac{dc}{ds} + 4c^2D(1) + cM_{\frac{1}{3}} &= 1, \\ \frac{dt}{ds} &= \frac{1}{c}.\end{aligned}$$

Find an expression for r_k in terms of the parameter problems.

Taken from [51]. Notice that the equations for s and c start from a singularity at $s = 0$. Laplace transforming the equations:

$$\begin{aligned}\frac{dr_2}{ds} &= 2cD(1) - 2^{1/3}D(2)r_2, \\ \frac{dr_k}{ds} &= (k-1)^{1/3}D(k-1)r_{k-1} - k^{1/3}D(k)r_k, \quad k \geq 3.\end{aligned}$$

we find:

$$\begin{aligned}\hat{r}_2(\sigma) &= \frac{2D(1)}{\sigma + 2^{\frac{1}{3}}D(2)}\hat{c}, \\ \hat{r}_k(\sigma) &= \frac{(k-1)^{\frac{1}{3}}D(k-1)}{\sigma + k^{\frac{1}{3}}D(k)}\hat{r}_{k-1}, \quad k \geq 3.\end{aligned}$$

Therefore,

$$\begin{aligned}2^{\frac{1}{3}}D(2)\hat{r}_2(\sigma) &= \frac{2D(1)}{1 + \sigma 2^{\frac{-1}{3}}D(2)^{-1}}\hat{c}, \\ k^{\frac{1}{3}}D(k)\hat{r}_k(\sigma) &= \frac{(k-1)^{\frac{1}{3}}D(k-1)}{1 + \sigma k^{\frac{-1}{3}}D(k)^{-1}}\hat{r}_{k-1}, \quad k \geq 3.\end{aligned}$$

By iteration,

$$k^{\frac{1}{3}}D(k)\hat{r}_k = 2\hat{c}D(1)\hat{R}_k,$$

where

$$\hat{R}_k(\sigma) = \prod_{j=2}^k \frac{1}{1 + \sigma j^{\frac{-1}{3}}D(j)^{-1}}.$$

Using the inversion formula

$$f(t) = \frac{1}{2\pi i} \int_{\mathcal{C}} e^{st} \hat{f}(s) ds = \frac{1}{2\pi i} \int_{s_1+i\infty}^{s_1-\iota\infty} e^{st} \hat{f}(s) ds,$$

we find r_k as a function of the inverse transforms R_k of \hat{R}_k :

$$r_k(s) = \frac{2D(1)}{k^{\frac{1}{3}}D(k)} \int_0^s R_k(s-s')c(s')ds', \quad k \geq 2,$$

with

$$R_k(t) = \frac{1}{2\pi i} \int_{\mathcal{C}} e^{st} \hat{R}_k(s) ds = \frac{1}{2\pi i} \int_{s_1+i\infty}^{s_1-i\infty} e^{st} \hat{f}(s) ds = \lim_{L \rightarrow \infty} \frac{1}{2\pi} \int_{-L}^L e^{its} \hat{R}_k(is) ds,$$

where \mathcal{C} is an inversion contour. A classical choice for inversion paths are Bromwich contours $s_1 - is$, parallel to the imaginary axis and located to the right of the singularities of $\hat{R}_k(s)$. In this case, we may select the imaginary axis $s_1 = 0$. For numerical purposes, the best choices of the inversion contour are those along which this inversion formula can be approximated by a quadrature formula involving a few points. We may resort instead to deformations of Bromwich contours, such as Talbot paths or hyperbolic paths.

4 Numerical methods

1. Given a profile $c_e > 0$, functions $\rho(x) > 0$, $n(x) > 0$, $u(x)$ and constants $a, R > 0$, we consider the following free boundary problem. We must find x^* such that

$$\begin{aligned} c''(x) + au(x)c'(x) &= R\rho(x)n(x)^{1/3}(c(x) - c_e(x)), & 0 < x < x_*, \\ c''(x) + au(x)c'(x) &= 0, & x > x_*, \\ c(x_*) &= c_e(x_*) = c_*, \quad c'(x_*^-) = c'(x_*^+), \quad c(\infty) = 1, \quad c(0) = c_e(0). \end{aligned}$$

Taken from [42]. We write $c(x) = 1 + \frac{c_*-1}{\phi(x_*)}\phi(x)$ where

$$\begin{aligned} \phi''(x) + au(x)\phi'(x) &= 0, & x \geq 0, \\ \phi(0) &= 1, \quad \phi(\infty) = 0, \end{aligned}$$

that is,

$$\phi(x) = \int_x^\infty e^{-a \int_0^y u(x') dx'} dy \left(\int_0^\infty e^{-a \int_0^y u(x') dx'} dy \right)^{-1}.$$

To calculate x_* , we start from a trial value x_* . Next, we define $c(x)$ for $x > x_*$ as explained above for a trial value of x_* . Then, we solve $c''(x) + au(x)c'(x) = R\rho(x)n(x)^{1/3}(c(x) - c_e(x))$, $0 < x < x_*$ with $c(x_*) = c_*$ and $c'(x_*) = (c_* - 1) \frac{\phi'(x_*)}{\phi(x_*)}$. Finally, we compare $c(0)$ with $c_e(0)$. Depending on whether it is larger or smaller we increase or decrease x_* until the difference is small enough.

2. Consider the hyperbolic problem

$$\begin{aligned} \frac{\partial^2 E}{\partial x \partial t} + A \frac{\partial E}{\partial t} + B \frac{\partial E}{\partial x} + C \frac{\partial J}{\partial t} + D &= 0, & x \in (0, L), t > 0, \\ E(x, 0) &= 0, & x \in (0, L), \\ E(0, t) &= \rho J(t), & t \geq 0, \\ \int_0^L E(x, t) dx &= \phi, & t \geq 0, \end{aligned}$$

where ρ, ϕ, L are positive and A, B, C, D are bounded functions, A and B positive, while C is negative. What would be an adequate numerical scheme to solve this problem?

Hyperbolic problems are typically discretized in explicit ways. However, in this case i) we have an integral constraint which couples all the values at each time level, ii) the hyperbolic operator is given in non characteristic form. We use forward finite differences of first order for first order time derivatives of E and J . We use a second order backward approximation scheme for the space derivative of E because the use of central differences leads to instabilities. The second order derivative E_{xt} is approximated combining the space and time derivative approximation just described. At the left end we use for the first order spatial derivative of E a first order backward difference formula. The integral constraint is discretized by means of a composite trapezoidal rule. For a proof of the convergence and stability properties of the scheme see [16].

3. Consider the Navier equations for crystals with cubic symmetry in two dimensional situations, defined by three positive constants c_{11}, c_{22}, c_{44} :

$$\begin{aligned} Mu_1'' &= C_{11} \frac{\partial^2 u_1}{\partial x_1^2} + C_{12} \frac{\partial^2 u_2}{\partial x_1 \partial x_2} + C_{44} \frac{\partial^2 u_1}{\partial x_2^2} + C_{44} \frac{\partial^2 u_2}{\partial x_1 \partial x_2}, \\ Mu_2'' &= C_{11} \frac{\partial^2 u_2}{\partial x_2^2} + C_{12} \frac{\partial^2 u_1}{\partial x_1 \partial x_2} + C_{44} \frac{\partial^2 u_2}{\partial x_1^2} + C_{44} \frac{\partial^2 u_1}{\partial x_1 \partial x_2}, \end{aligned}$$

where $M > 0$. Propose a stable finite difference discretization.

Taken from [31]. Let us construct a rectangular mesh. We denote by D_i^+ and D_i^- the first order progressive and regressive finite difference equations in the direction i , that is,

$$\begin{aligned} D_1^+ u_j(\ell, m) &= \frac{u_j(\ell + \delta x_1, m) - u_j(\ell, m)}{\delta x_1}, \\ D_1^- u_j(\ell, m) &= \frac{u_j(\ell, m) - u_j(\ell - \delta x_1, m)}{\delta x_1}, \end{aligned}$$

for $i = 1$ and analogous expressions for $i = 2$. In view of the presence of

cross terms, we choose

$$\begin{aligned} Mu_1'' &= C_{11} \frac{D_1^- D_1^+ u_1}{\delta x_1^2} + C_{12} \frac{D_1^- D_2^+ u_2}{\delta x_1 \delta x_2} + C_{44} \frac{D_2^- D_2^+ u_1}{\delta x_2^2} + C_{44} \frac{D_2^- D_1^+ u_2}{\delta x_1 \delta x_2}, \\ Mu_2'' &= C_{11} \frac{D_2^- D_2^+ u_2}{\delta x_2^2} + C_{12} \frac{D_2^- D_1^+ u_1}{\delta x_1 \delta x_2} + C_{44} \frac{D_1^- D_1^+ u_2}{\delta x_1^2} + C_{44} \frac{D_1^- D_2^+ u_1}{\delta x_1 \delta x_2}. \end{aligned}$$

See [35] for extensions to three dimensional crystals and lattices with two bases.

4. Consider a planar hexagonal graphene lattice and ignore possible vertical deflections. In the continuum limit, in-plane deformations are described by the Navier equations of linear elasticity for the two-dimensional (2D) displacement vector (u, v) ,

$$\begin{aligned} \rho_2 \frac{\partial^2 u}{\partial t^2} &= (\lambda + 2\mu) \frac{\partial^2 u}{\partial x^2} + \mu \frac{\partial^2 u}{\partial y^2} + (\lambda + \mu) \frac{\partial^2 v}{\partial x \partial y}, \\ \rho_2 \frac{\partial^2 v}{\partial t^2} &= \mu \frac{\partial^2 v}{\partial x^2} + (\lambda + 2\mu) \frac{\partial^2 v}{\partial y^2} + (\lambda + \mu) \frac{\partial^2 u}{\partial x \partial y}, \end{aligned}$$

where ρ_2 is the 2D mass density and λ and μ are the 2D Lamé coefficients ($\lambda = C_{12}$, $\mu = C_{66}$, $\lambda + 2\mu = C_{11}$). Propose a finite difference discretization in a hexagonal lattice of constant a .

Taken from [40]. Consider a point A in the hexagonal lattice with coordinates (x, y) . Its 9 (3+6) closest neighbours have coordinates

$$\begin{aligned} n_1 &= \left(x - \frac{a}{2}, y - \frac{a}{2\sqrt{3}} \right), n_2 = \left(x + \frac{a}{2}, y - \frac{a}{2\sqrt{3}} \right), n_3 = \left(x, y + \frac{a}{\sqrt{3}} \right), \\ n_4 &= \left(x - \frac{a}{2}, y + \frac{a\sqrt{3}}{2} \right), n_5 = \left(x + \frac{a}{2}, y + \frac{a\sqrt{3}}{2} \right), n_6 = (x - a, y), \\ n_7 &= (x + a, y), n_8 = \left(x - \frac{a}{2}, y + \frac{a\sqrt{3}}{2} \right), n_9 = \left(x + \frac{a}{2}, y + \frac{a\sqrt{3}}{2} \right). \end{aligned}$$

Let us define the following operators acting on functions of the coordinates (x, y) of node A :

$$\begin{aligned} Tu &= [u(n_1) - u(A)] + [u(n_2) - u(A)] + [u(n_3) - u(A)], \\ Hu &= [u(n_6) - u(A)] + [u(n_7) - u(A)], \\ D_1 u &= [u(n_4) - u(A)] + [u(n_9) - u(A)], \\ D_2 u &= [u(n_5) - u(A)] + [u(n_8) - u(A)], \end{aligned}$$

Taylor expansions of these finite difference combinations about (x, y) yield

$$\begin{aligned} Tu &\sim (\partial_x^2 u + \partial_y^2 u) \frac{a^2}{4}, \\ Hu &\sim (\partial_x^2 u) a^2, \\ D_1 u &\sim \left(\frac{1}{4} \partial_x^2 u + \frac{\sqrt{3}}{2} \partial_x \partial_y u + \frac{3}{4} \partial_y^2 u \right) a^2, \\ D_2 u &\sim \left(\frac{1}{4} \partial_x^2 u - \frac{\sqrt{3}}{2} \partial_x \partial_y u + \frac{3}{4} \partial_y^2 u \right) a^2, \end{aligned}$$

as $a \rightarrow 0$. Now we replace in the motion equations Hu/a^2 , $(4T - H)u/a^2$ and $(D_1 - D_2)u/(\sqrt{3}a^2)$ instead of $\partial_x^2 u$, $\partial_y^2 u$ and $\partial_x \partial_y u$, respectively, with similar substitutions for the derivatives of v , thereby obtaining the following equations at each point of the lattice:

$$\begin{aligned} \rho_2 a^2 \frac{\partial^2 u}{\partial t^2} &= 4\mu Tu + (\lambda + \mu) Hu + \frac{\lambda + \mu}{\sqrt{3}} (D_1 - D_2)v, \\ \rho_2 a^2 \frac{\partial^2 v}{\partial t^2} &= 4(\lambda + 2\mu) Tv - (\lambda + \mu) Hv + \frac{\lambda + \mu}{\sqrt{3}} (D_1 - D_2)u. \end{aligned}$$

5. Consider a planar hexagonal lattice of lattice constant a . The isotropic Navier equations have singular solutions such as

$$\begin{aligned} u &= \frac{a}{2\pi} \left[\tan^{-1} \left(\frac{y}{x} \right) + \frac{xy}{2(1-\nu)(x^2 + y^2)} \right], \\ v &= \frac{a}{2\pi} \left[-\frac{1-2\nu}{4(1-\nu)} \ln \left(\frac{x^2 + y^2}{b^2} \right) + \frac{y^2}{2(1-\nu)(x^2 + y^2)} \right], \end{aligned}$$

where $\nu = \lambda/[2(\lambda + \mu)]$ for any a . We choose (x_0, y_0) different from a lattice point and solve a damped version of the discrete Navier equations formulated in the previous exercise. How would you expect the system to evolve starting from $(u(x - x_0, y - y_0), v(x - x_0, y - y_0))$?

Taken from [38]. The damped equations take the form

$$\begin{aligned} \rho_2 a^2 \frac{\partial^2 u}{\partial t^2} + \gamma \frac{\partial u}{\partial t} &= 4\mu Tu + (\lambda + \mu) Hu + \frac{\lambda + \mu}{\sqrt{3}} (D_1 - D_2)v, \\ \rho_2 a^2 \frac{\partial^2 v}{\partial t^2} + \gamma \frac{\partial v}{\partial t} &= 4(\lambda + 2\mu) Tv - (\lambda + \mu) Hv + \frac{\lambda + \mu}{\sqrt{3}} (D_1 - D_2)u, \end{aligned}$$

with $\gamma > 0$. We expect the system to relax to a stationary configuration behaving like $(u(x - x_0, y - y_0), v(x - x_0, y - y_0))$ at a distance of (x_0, y_0) . Such solutions represent lattice defects with the chosen elastic far fields.

6. Write the Helmholtz equation set in the whole space

$$\begin{aligned} \Delta u + k^2 u &= 0, \quad \mathbf{x} \in \mathbb{R}^N, \\ \lim_{r=|\mathbf{x}| \rightarrow \infty} |\mathbf{x}|^{\frac{N-1}{2}} \left(\frac{\partial}{\partial r} (u - u_{\text{inc}}) - ik(u - u_{\text{inc}}) \right) &= 0, \end{aligned}$$

in an equivalent variational form set in a bounded domain by means of the Dirichlet-to-Neumann operator.

Taken from [37]. Let B_R be a sphere of radius R and Γ_R its boundary. The Dirichlet-to-Neumann (also called Steklov-Poincaré) operator associates to any Dirichlet data on Γ_R the normal derivative of the solution of the exterior Dirichlet problem:

$$\begin{aligned} L : H^{1/2}(\Gamma_R) &\longrightarrow H^{-1/2}(\Gamma_R) \\ f &\longmapsto \frac{\partial w}{\partial \mathbf{n}} \end{aligned}$$

where $w \in H_{loc}^1(\mathbb{R}^N \setminus \overline{B_R})$, $B_R := B(\mathbf{0}, R)$, is the unique solution of

$$\begin{cases} \Delta w + k^2 w = 0, & \text{in } \mathbb{R}^N \setminus \overline{B_R}, \\ w = f, & \text{on } \Gamma_R, \\ \lim_{r \rightarrow \infty} r^{N-1/2} \left(\frac{\partial w}{\partial r} - ikw \right) = 0. \end{cases}$$

$H^{1/2}(\Gamma_R)$ and $H^{-1/2}(\Gamma_R)$ are standard trace spaces. One can study an equivalent boundary value problem in B_R with a non-reflecting boundary condition on its boundary Γ_R :

$$\begin{cases} \Delta u + k^2 u = 0, & \text{in } B_R, \\ \frac{\partial}{\partial \mathbf{n}}(u - u_{\text{inc}}) = L(u - u_{\text{inc}}), & \text{on } \Gamma_R. \end{cases}$$

The solution u also solves the variational equation

$$\begin{cases} u \in H^1(B_R), \\ b(u, v) = \ell(v), \quad \forall v \in H^1(B_R), \end{cases}$$

where

$$\begin{aligned} b(u, v) &= \int_{B_R} (\nabla u \nabla \bar{v} - k^2 u \bar{v}) d\mathbf{x} - \int_{\Gamma_R} Lu \bar{v} dl, \quad \forall u, v \in H^1(B_R), \\ \ell(v) &= \int_{\Gamma_R} \left(\frac{\partial u_{\text{inc}}}{\partial \mathbf{n}} - Lu_{\text{inc}} \right) \bar{v} dl, \quad \forall v \in H^1(B_R). \end{aligned}$$

7. Write the transmission Helmholtz problem

$$\begin{cases} \nabla \cdot (\alpha_e \nabla u) + \lambda_e^2 u = 0, & \text{in } \mathbb{R}^2 \setminus \overline{\Omega}_i, \\ \nabla \cdot (\alpha_i \nabla u) + \lambda_i(k)^2 u = 0, & \text{in } \Omega_i, \\ u^- - u^+ = 0, & \text{on } \partial\Omega_i, \\ \alpha_i \frac{\partial u^-}{\partial \mathbf{n}} - \alpha_e \frac{\partial u^+}{\partial \mathbf{n}} = 0, & \text{on } \partial\Omega_i, \\ \lim_{r \rightarrow \infty} r^{1/2} \left(\frac{\partial}{\partial r} (u - u_{\text{inc}}) - i\lambda_e (u - u_{\text{inc}}) \right) = 0, & r = |\mathbf{x}|, \end{cases}$$

in variational form and calculate the derivative of $J(k) = \int_{\Gamma} |u(k) - d|^2 dl$ with respect to k .

Taken from [39]. Arguing as in the previous exercise we have

$$\begin{cases} u \in H^1(B_R), \\ S(\Omega_i; u, v) = \ell(v), \quad \forall v \in H^1(B_R), \end{cases}$$

where

$$\begin{aligned} S(\Omega_i; u, v) &:= \int_{B_R \setminus \overline{\Omega}_i} (\alpha_e \nabla u \nabla \bar{v} - \lambda_e^2 u \bar{v}) d\mathbf{x} + \int_{\Omega_i} (\alpha_i \nabla u \nabla \bar{v} - \lambda_i^2 u \bar{v}) d\mathbf{x} \\ &\quad - \int_{\Gamma_R} \alpha_e L u \bar{v} dl, \quad \forall u, v \in H^1(B_R), \\ \ell(v) &:= \int_{\Gamma_R} \alpha_e \left(\frac{\partial u_{\text{inc}}}{\partial \mathbf{n}} - L u_{\text{inc}} \right) \bar{v} dl, \quad \forall v \in H^1(B_R). \end{aligned}$$

where L denotes the Dirichlet-to-Neumann operator defined by

$$\begin{cases} \nabla \cdot (\alpha_e \nabla w) + \lambda^2 w = 0, & \text{in } \mathbb{R}^2 \setminus \overline{B}_R, \\ w = f, & \text{on } \Gamma_R, \\ \lim_{r \rightarrow \infty} r^{1/2} \left(\frac{\partial w}{\partial r} - i \lambda_e w \right) = 0. \end{cases}$$

Differentiating J with respect to k we see that

$$\frac{dJ}{dk} = 2 \int_{\Gamma} \overline{(u(k) - d)} u_k(k) dl,$$

where the derivative $u_k(k) = \frac{du(k)}{dk} \in H^1(B_R)$ is a solution of

$$\begin{aligned} \int_{B_R \setminus \overline{\Omega}_i} (\alpha_e \nabla u_k(k) \nabla \bar{v} - \lambda_e^2 u_k(k) \bar{v}) d\mathbf{x} + \int_{\Omega_i} (\alpha_i \nabla u_k(k) \nabla \bar{v} - \lambda_i(k)^2 u_k(k) \bar{v}) d\mathbf{x} \\ - \int_{\Gamma_R} \alpha_e L u_k(k) \bar{v} dl = 2 \int_{\Omega_i} \lambda_i(k) \lambda_i'(k) u(k) \bar{v} d\mathbf{x}, \end{aligned}$$

for all $v \in H^1(B_R)$ and $u(k)$ the solution of the Helmholtz problem for $\lambda_i(k)$.

8. Consider the cost $J(a, k) = \sum_{m=1}^M \int_{\Gamma} |u_m - d_m|^2$, where u_m solves

$$\begin{cases} \operatorname{div}(a_e \nabla u) + k_e^2 u = 0, & \text{in } \mathbb{R}^N \setminus \overline{\Omega}_i, & \operatorname{div}(a \nabla u) + k^2 u = 0, & \text{in } \Omega_i, \\ u^- = u^+, & a \frac{\partial u^-}{\partial \mathbf{n}} = a_e \frac{\partial u^+}{\partial \mathbf{n}}, & \text{on } \partial \Omega_i, \\ r^{(N-1)/2} \left(\frac{\partial(u - u_{\text{inc}}^m)}{\partial r} - i k_e (u - u_{\text{inc}}^m) \right) \rightarrow 0, & \text{as } r := |\mathbf{x}| \rightarrow \infty. \end{cases}$$

Given a_j, k_j , find descent directions for

$$J(\delta) := J(a_j + \delta\phi, k_j + \delta\psi),$$

where $\delta > 0$, in order to implement an optimization procedure.

Taken from [46]. We seek δ , ϕ and ψ such that $\frac{dJ(\delta)}{d\delta} < 0$. Differentiating we find

$$\left. \frac{dJ}{d\delta} \right|_{\delta=0} = - \sum_{m=1}^M \operatorname{Re} \left[\int_{\Omega_j} [\phi \nabla u_m \nabla \bar{w}_m - 2\psi k_j u_m \bar{w}_m] dz \right],$$

where u_m solves the forward problem with $a = a_j$, and $k = k_j$. The adjoint fields w_m solve

$$\begin{cases} \operatorname{div}(a_e \nabla w_m) + k_e^2 w_m = (d_m - u_m) \delta_{\Gamma_{meas}}, & \text{in } \mathbb{R}^N \setminus \bar{\Omega}_i, \\ \operatorname{div}(a_j \nabla w_m) + k_j^2 w_m = 0, & \text{in } \Omega_i, \\ w_m^- = w_m^+, \quad a_i \frac{\partial w_m^-}{\partial \mathbf{n}} = a_e \frac{\partial w_m^+}{\partial \mathbf{n}}, & \text{on } \partial \Omega_i, \\ r^{(N-1)/2} \left(\frac{\partial w_m}{\partial r} + \iota \kappa_e w_m \right) \rightarrow 0, & \text{as } r \rightarrow \infty. \end{cases}$$

Setting

$$\phi(\mathbf{x}) = \sum_{m=1}^M \operatorname{Re} (\nabla u_m(\mathbf{x}) \nabla \bar{w}_m(\mathbf{x})), \quad \psi(\mathbf{x}) = - \sum_{m=1}^M \operatorname{Re} (u_m(\mathbf{x}) \bar{w}_m(\mathbf{x})), \quad \mathbf{x} \in \Omega_j,$$

and

$$a_{j+1} = a_j + \delta \phi, \quad k_{j+1} = k_j + \delta \psi,$$

we guarantee $J(a_{j+1}, k_{j+1}) < J(a_j, k_j)$ for δ small.

9. Explain how to solve the following equations using the deterministic particle method:

$$\begin{aligned} \partial_t f + \frac{\Delta l}{2\hbar v_M} \sin(k) \partial_x f + \frac{\tau_e}{\eta} F \partial_k f = \\ \frac{1}{\eta} \left[f^{FDa}(k; \mu(n)) - \left(1 + \frac{\nu_{imp}}{2\nu_{en}} \right) f + \frac{\nu_{imp}}{2\nu_{en}} f(x, -k, t) \right], \end{aligned}$$

$$\partial_x^2 V = \partial_x F = n - 1$$

$$n = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x, k, t) dk = \frac{1}{2\pi} \int_{-\pi}^{\pi} f^{FDa}(k; \mu(n)) dk$$

$$f^{FDa}(k; \mu) = \alpha \ln [1 + \exp(\mu - \delta + \delta \cos(k))]$$

$$\eta = \frac{v_M}{\nu_{en} x_0} \quad \delta = \frac{\Delta}{2k_B T}.$$

The boundary conditions are, for $x = 0$:

$$f^+ = \beta F - \frac{f^{(0)}}{\int_0^\pi \sin(k) f^{(0)} dk} \int_{-\pi}^0 \sin(k) f^- dk$$

with

$$\beta = \frac{2\pi\hbar\sigma F_M}{e\Delta N_D}$$

and for $x = L/x_0$:

$$f^- = \frac{f^{(0)}}{(1/(2\pi)) \int_{-\pi}^0 f^{(0)} dk} \left(1 - \frac{1}{2\pi} \int_0^\pi f^+ dk \right)$$

The boundary conditions for the electric potential V are

$$V(0, t) = 0, \quad V(L, t) = \phi_L \sim \frac{\phi}{F_M} \frac{L}{x_0}.$$

The initial condition is

$$f^{(0)}(k; n) = \sum_{j=-\infty}^{\infty} \exp(ijk) \frac{1 - i j F / \tau_e}{1 + j^2 (F)^2} f_j^{FD}(n)$$

$$f_j^{FD}(n) = \frac{1}{\pi} \int_0^\pi f^{FD}(k; \mu(n)) \cos(jk) dk$$

with $x \in [0, L = L/x_0]$ and f periodic in k with period 2π . The average energy E is defined as

$$E = \frac{E}{k_B T} = \frac{\int_{-\pi/l}^{\pi/l} \varepsilon(k) f(x, k, t) dk}{k_B T \int_{-\pi/l}^{\pi/l} f(x, k, t) dk} = \delta \frac{\int_{-\pi}^{\pi} (1 - \cos k) f(x, k, t) dk}{\int_{-\pi}^{\pi} f(x, k, t) dk}.$$

Taken from [43]. We rely on particle description of the distribution function, which means that $f(x, k, t)$ is written as a sum of delta functions

$$f(x, k, t) \approx \sum_{i=1}^N \omega_i f_i(t) \delta(x - x_i(t)) \otimes \delta(k - k_i(t))$$

where ω_i , $f_i(t)$, $x_i(t)$ and $k_i(t)$ are, respectively, the (constant) control volume, the weight, the position and the wave vector of the i th particle. N is the number of numerical particles. The motion of particles is governed by collisionless dynamics, whereas the collisions are accounted for by the variation of weights. Large gradients in the solution profile arise from appropriate particles acquiring large weights, not by accumulating many particles in the large gradient regions. The evolution of the particles is determined by their positions and wave vectors which are the characteristic curves of the convective part of the equation. Their equations are:

$$\frac{d}{dt} k = \frac{\tau_e}{\eta} F, \quad \frac{d}{dt} x = \frac{\Delta l}{2\hbar v_M} \sin(k).$$

The evolution of the distribution function over these characteristic curves is given by the ordinary differential equation:

$$\frac{d}{dt}f = \frac{1}{\eta} \left[- \left(1 + \frac{\nu_{imp}}{2\nu_{en}} \right) f + \frac{\nu_{imp}}{2\nu_{en}} f(-k) + f^{FD} \right].$$

The system of ordinary differential equations is now discretized by using a modified Euler method:

$$f_i^n = f_i^{n-1} + dt \frac{1}{\eta} \left[- \left(1 + \frac{\nu_{imp}}{2\nu_{en}} \right) f_i^{n-1} + \frac{\nu_{imp}}{2\nu_{en}} f_i^{(-k)} + f_i^{FD,n-1} \right]$$

with $f_i^{(-k)} = f(x_i^{n-1}, -k_i^{n-1}, t^{n-1})$,

$$k_i^n = k_i^{n-1} + dt \frac{\tau_e}{\eta} F_i^{n-1},$$

$$x_i^n = x_i^{n-1} + dt \frac{\Delta l}{2\hbar v_M} \sin(k_i^n).$$

For stability reasons, we use k_i^n to update x_i^n . We have also used multi-step methods but they yield worse results.

The boundary conditions are taken into account as follows:

- If $k_i^n > \pi$, we set $k_i^n = k_i^n - 2\pi$. If $k_i^n < -\pi$, we set $k_i^n = k_i^n + 2\pi$.
- If $x_i^n > L$, we set $x_i^n = x_i^n - L$ and $f_i^{n-1} = f_i^+$. If $x_i^n < 0$, we set $x_i^n = x_i^n + L$ and $f_i^{n-1} = f_i^-$. Here f_i^+ and f_i^- are calculated by discretization of the integrals using Simpson's rule on an equally spaced mesh $K_{m'}$ with step Δk .

To calculate x_i , k_i and f_i at the next time step t^{n+1} , we need to update the electric field and the Fermi-Dirac distribution in the equations for the particles. This updating requires an interpolation procedure to generate an approximation of the distribution function on a regular mesh X_m , $K_{m'}$ which is then used to approximate the electric field and the chemical potential. To approximate the values of the distribution function over the mesh, $f_{m,m'}^n$, we use its values for the particles, f_i^n . The idea is obtain a weighted mean by:

$$f_{m,m'}^n = \frac{\sum_{i=1}^N f_i^n W_{m,m'}^i}{\sum_{i=1}^N W_{m,m'}^i}$$

where

$$W_{m,m'}^i = \max \left\{ 0, 1 - \frac{|X_m - x_i^n|}{\Delta x} \right\} \cdot \max \left\{ 0, 1 - \frac{|K_{m'} - k_i^n|}{\Delta k} \right\}$$

and Δx and Δk are the spatial and wave vector steps.

An approximation for the density and average energy at the mesh points, $n(X_m, t^n) \approx n_m^n$ and $(k_B T)^{-1} E(X_m, t^n) \approx (k_B T)^{-1} E_m^n$, are obtained using Simpson's rule and the interpolated values of the distribution function on the mesh.

We calculate the nondimensional chemical potential μ by using a Newton-Raphson iterative scheme to solve the equations. The extended Simpson's rule is employed to approximate the integrals for $n(\mu)$ and $dn(\mu)/d\mu$. Once we know the chemical potential μ , we find the Fermi-Dirac distribution function at mesh points, $f^{FD}(K_{m'}; n_m^n)$, which is then interpolated to get the Fermi-Dirac distribution function for the particles.

To compute the electric field at time t^n , we use finite differences to discretize the Poisson equation on the grid X_m :

$$\begin{aligned} V_{m+1}^n - 2V_m^n + V_{m-1}^n &= n_m^n - 1, \\ F_m^n &= \frac{V_{m+1}^n - V_{m-1}^n}{2\Delta x}. \end{aligned}$$

Here $V(0, t^n) = 0$ and $V(L, t^n) = \phi L$. Let V_m^n and F_m^n denote our approximations of $V(X_m, t^n)$ and $F(X_m, t^n)$ on the equally spaced mesh X_m . Finally, the electric field is interpolated at the location of the particle i

$$F_i^n = \left(\frac{X_{m+1} - x_i^n}{\Delta x} \right) F_m^n + \left(\frac{x_i^n - X_m}{\Delta x} \right) F_{m+1}^n.$$

The total current density J is given by

$$J(t) = \frac{\varsigma}{L} \int_0^L \left[\int_{-\pi}^{\pi} \sin(k) f(x, k, t) dk \right] dx,$$

in which

$$\varsigma = \frac{l\Delta}{4\pi\hbar v_M}.$$

We use the Simpson rule to approximate $J(t^n)$.

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