LOSS OF THE CONSTRAINT IN CONVEX VARIATIONAL PROBLEMS

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Dedicated to J.-L. Lions, with great admiration

1. Introduction

In this paper we collect together a number of examples from mechanics and physics which can be formulated as the minimization of a strictly convex functional subject to a convex constraint, and show how they fit into a common abstract framework. The principal feature of the examples is the occurrence of a critical value of the constraint above which the minimum is not attained, and of a corresponding critical minimizer that acts as a fake minimizer for larger values of the constraint.

Perhaps the easiest of the examples to visualize is the problem of equilibrium of a given volume ρ of a homogeneous incompressible fluid above a given surface $\mathcal{S}$. We suppose that the equation of $\mathcal{S}$ is

$$x_3 = f(x_1, x_2) \tag{1.1}$$

where $f : \mathbb{R}^2 \to \mathbb{R}$ is continuous, and where (x_1, x_2, x_3) denote coordinates with respect to fixed Cartesian axes, the x_3-direction being vertical. We suppose, solely for simplicity, that at infinity the surface has the form of a horizontal plane, so that

$$f(z) \to 0 \text{ as } |z| \to \infty, \tag{1.2}$$

where $z = (x_1, x_2)$. If the height of the liquid surface above $\mathcal{S}$ is denoted by $h(z)$ then the total potential energy of the liquid (taking $x_3 = 0$ to be the zero energy level) is given by

$$V(h) = \int_{\mathbb{R}^2} \left(\int_{f(z)}^{f(z)+h(z)} g x_3 dx_3 \right) dz = g \int_{\mathbb{R}^2} [f(z)h(z) + \frac{1}{2}(h(z))^2] dz, \tag{1.3}$$

where g is the acceleration due to gravity, assumed constant, and where the fluid is taken to have unit density. We seek to minimize $V(h)$ among functions $h \geq 0$

satisfying the volume constraint $H(h) = \rho$, where

$$H(h) := \int_{\mathbb{R}^2} h(z) dz. \tag{1.4}$$

The volume of the region $f(z) \leq x_3 \leq 0$ is given by

$$\rho_s = \int_{\mathbb{R}^2} [f(z)]^- dz, \tag{1.5}$$

where $[t]^- = \max\{-t, 0\}$. If $0 \leq \rho \leq \rho_s$, $\rho < \infty$, then it is intuitively clear that the minimum of V is attained by a unique function h^ρ such that

$$h^\rho(z) = 0 \quad \text{or} \quad f(z) + h^\rho(z) = -d(\rho) \tag{1.6}$$

for all z, where $d(\rho) \geq 0$, i.e. the fluid surface is part of the plane $x_3 = -d(\rho)$. If, however, $\rho_s < \rho < \infty$ then the minimum is *not* attained, but minimizing sequences for V tend in an appropriate sense to the function

$$h^{\rho_s}(z) = [f(z)]^- \tag{1.7}$$

that does not satisfy the constraint. The excess volume $\rho - \rho_s$ of fluid disperses to infinity. This simple example is discussed in detail in Section 3.

The abstract analysis in Section 2 is based on the idea of replacing the equality constraint by an inequality. This is the method used by Lieb & Simon [8] in their treatment of the Thomas-Fermi problem, the relevant results from their work being recovered from the theory in Section 5. The treatment of the behaviour of minimizing sequences was motivated by the analysis in Ball, Carr & Penrose [3] of coagulation-fragmentation equations, their results for the equilibrium problem being deduced in Section 6. The theory is also applied in Section 4 to a well known model predicting a finite height for the atmosphere ; a related example from one-dimensional nonlinear elasticity is treated in [1]. In the example discussed in Section 4 the loss of the constraint occurs because minimizing sequences concentrate at a spatial point, while in the other examples there is a loss of the constraint 'at infinity' ; these two possibilities are analyzed by P.-L. Lions [9][10], whose theory of concentration-compactness has applications to a large class of problems of the type considered here.

Although there are some minor new remarks in the analysis of the examples, the main aim of the paper is to draw attention to their common variational structure and make this structure more accessible for other applications. One such application to Bose-Einstein condensation appears in van den Berg & Lewis [12].

2. Minimization of convex functionals subject to a convex constraint.

Let X be a Hausdorff topological vector space, and let $K \subset X$ be sequentially closed and convex. Let $V : K \to \mathbb{R} \cup \{+\infty\}$ be convex, with V strictly convex on dom $V := \{u \in K : V(u) < \infty\}$. Let $H : K \to [0,\infty]$ be convex, sequentially lower semicontinuous (slsc) and take every value in $[0,\infty)$. Given $\rho \in [0,\infty)$ and $M \in \mathbb{R}$ we set

$$K_\rho = \{u \in K : H(u) \leq \rho\},$$
$$K_\infty = \{u \in K : H(u) < \infty\},$$
$$K_{\rho,M} = \{u \in K : H(u) \leq \rho, V(u) \leq M\},$$
$$S_\rho = \{u \in K : H(u) = \rho\}.$$

We suppose that there exists M_o such that, for any $\rho \geq 0$ and $M \geq M_o$, $K_{\rho,M}$ is nonempty and sequentially precompact with V restricted to $K_{\rho,M}$ slsc.

Given $\rho \in [0,\infty)$ let

$$\theta(\rho) = \inf_{S_\rho} V. \tag{2.1}$$

We are interested in whether or not the minimum in (2.1) is attained, in the behaviour of minimizing sequences, and in how $\theta(\rho)$ depends on ρ. Since the level sets S_ρ are not in general closed, it turns out to be easier to consider first the problem of determining

$$\varphi(\rho) = \inf_{K_\rho} V \tag{2.2}$$

and the corresponding minimizers.

Proposition 2.1

The function $\varphi : [0,\infty) \to \mathbb{R}$ is continuous and convex. For each $\rho \in [0,\infty)$ the minimum in (2.2) is attained by a unique u^ρ that varies continuously with ρ, and every minimizing sequence converges to u^ρ. There exists $\rho_s \in [0,\infty]$ such that $\varphi(\rho)$ is strictly decreasing and strictly convex for $0 \leq \rho < \rho_s$ and constant for $\rho_s \leq \rho < \infty$. The case $\rho_s < \infty$ occurs if and only if $\inf_{K_\infty} V$ is attained, and then the corresponding unique minimizer is u^{ρ_s} and $u^\rho = u^{\rho_s}$ for all $\rho \geq \rho_s$.

Proof

Our hypotheses imply that the sets $K_{\rho,M}$ are sequentially closed, so that any minimizing sequence for V in K_ρ has a subsequence converging to some minimizer u^ρ. Since V is strictly convex u^ρ is unique, and since X is Hausdorff every minimizing sequence converges to u^ρ.

It is obvious that φ is nonincreasing, and our convexity hypotheses imply that φ is convex ; in particular φ is continuous on $(0,\infty)$. If $\rho_j \to \rho$ then $u^{\rho_\mu} \to v$, $v \in K$ for some subsequence $\{\rho_\mu\}$ of $\{\rho_j\}$, and $V(v) \leq \liminf_{\mu\to\infty} V(u^{\rho_\mu})$,

$H(v) \leq \liminf_{\mu\to\infty} \rho_\mu = \rho$. Thus $\varphi(\rho) \leq V(v) \leq \liminf_{\mu\to\infty} \varphi(\rho^\mu)$. Applying this with $\rho = 0$ we deduce that φ is continuous on $[0,\infty)$. The continuity implies that in the above argument $v = u^\rho$, and since X is Hausdorff it follows that u^ρ is continuous in ρ.

From the above properties it follows that there exists $\rho_s \in [0,\infty]$ such that φ is strictly decreasing for $0 \leq \rho < \rho_s$ and constant for $\rho_s \leq \rho < \infty$. If $\rho_s < \infty$ then, since $\varphi(\rho) \geq \varphi(\rho_s)$ for all $\rho \geq 0$ and V is strictly convex, u^{ρ_s} is the unique minimizer of V on K_∞. If $\rho_s = \infty$ then V cannot attain a minimum on K_∞, since the infimum is less than $\varphi(\rho)$ for every $\rho < \infty$. Finally, since $\varphi(\rho)$ is strictly decreasing for $0 \leq \rho < \rho_s$, each u^ρ is different for $0 \leq \rho < \rho_s$. Therefore, by the strict convexity of V, $\varphi(\rho)$ is strictly convex for $0 \leq \rho < \rho_s$. □

Clearly $\theta(\rho) \geq \varphi(\rho)$ for all ρ. Equality does not hold in general (take, for example, $K = [0,\infty)$, $V(u) = (u-1)^2$, $H(u) = u$), but we always have the following result.

Proposition 2.2

If $0 \leq \rho \leq \rho_s$, $\rho < \infty$, then $H(u^\rho) = \rho$ and thus $\theta(\rho) = \varphi(\rho)$.

Proof

Clearly $H(u^o) = 0$. Suppose for contradiction that $H(u^\rho) < \rho$ for some $\rho \in (0,\rho_s]$, $\rho < \infty$. Then $H(u^\rho) \leq \rho - \varepsilon$ for some $\varepsilon \in (0,\rho)$. Hence

$$\varphi(\rho) = V(u^\rho) \geq \varphi(\rho - \varepsilon),$$

which is impossible since φ is strictly decreasing on $[0,\rho_s)$. □

The next result gives a useful method of calculating u^ρ and ρ_s via Lagrange multipliers. For $\lambda \geq 0$ define $V_\lambda : K \to \mathbb{R} \cup \{+\infty\}$ by

$$V_\lambda(u) = V(u) + \lambda H(u). \tag{2.3}$$

If $\rho \geq 0$ we define the subdifferential $\partial\varphi(\rho)$ by

$$\partial\varphi(\rho) = \{\mu \in \mathbb{R} : \varphi(\bar\rho) \geq \varphi(\rho) + \mu(\bar\rho - \rho) \text{ for all } \bar\rho \geq 0\}.$$

(This is the usual definition of the subdifferential provided φ is set equal to $+\infty$ on $(-\infty,0)$; note that if the right derivative $D^+\varphi(0)$ exists then $\partial\varphi(0) = (-\infty, D^+\varphi(0)]$.)

Proposition 2.3

If $\lambda \geq 0$ then V_λ attains an absolute minimum on K_∞ if and only if $-\lambda \in \partial\varphi(\rho)$ for some $\rho \geq 0$, and then the unique minimizer is u^ρ.

Proof

Suppose $-\lambda \in \partial\varphi(\rho)$ for some $\rho \geq 0$. Let $u \in K_\infty$ and $H(u) = \rho_1$. If $\rho > \rho_s$ then $\lambda = 0$. Hence by Proposition 2.2

$$\begin{aligned} V_\lambda(u) - V_\lambda(u^\rho) &= V(u) - \varphi(\rho_1) + \varphi(\rho_1) - \varphi(\rho) + \lambda(\rho_1 - \rho) \\ &\geq \varphi(\rho_1) - \varphi(\rho) + \lambda(\rho_1 - \rho) \\ &\geq 0, \end{aligned}$$

and hence u^ρ minimizes V_λ. Conversely, if $\bar{u}$ minimizes V_λ on K_∞ and $H(\bar{u}) = \rho$ then for any $\rho_1 \geq 0$

$$\begin{aligned} 0 &\leq V_\lambda(u^{\rho_1}) - V_\lambda(\bar{u}) \\ &\leq \varphi(\rho_1) - V(\bar{u}) + \lambda(\rho_1 - \rho). \end{aligned} \tag{2.4}$$

Taking $\rho_1 = \rho$ we deduce that $\bar{u} = u^\rho$, and from this and (2.4) it follows that $-\lambda \in \partial\varphi(\rho)$. The uniqueness of the minimizer is a consequence of the strict convexity of V_λ. □

It follows from Proposition 2.3 that V_λ attains an absolute minimum on K_∞, with corresponding minimizer $\bar{u}(\lambda)$, if and only if λ belongs to a semi-infinite interval $J \subset [0,\infty)$. If $\psi(\lambda) = H(\bar{u}(\lambda))$ then $\psi(\lambda) = (\partial\varphi)^{-1}(-\lambda)$, ψ is nonincreasing, $\lim_{\lambda\to\infty}\psi(\lambda) = 0$ and $\sup_J \psi = \rho_s$. Furthermore $\rho_s < \infty$ if and only if $J = [0,\infty)$, and then $\rho_s = \psi(0)$.

We now give a criterion for $\theta(\rho)$ to equal $\varphi(\rho)$ for all $\rho \geq 0$.

Theorem 2.4

A necessary and sufficient condition that $\theta(\rho) = \varphi(\rho)$ for all $\rho \geq 0$ is that there exists a number $\delta > 0$ such that, given any $\bar{u} \in K_\infty$ and any $\varepsilon > 0$, there exists $u \in K_\infty$ with $H(u) \geq H(\bar{u}) + \delta$ and $V(u) \leq V(\bar{u}) + \varepsilon$.

Proof

Necessity. Let $\bar{u} \in K_\infty$ and suppose $H(\bar{u}) = \rho_o$. Let $\delta > 0$ and choose $\rho \geq \rho_o + \delta$. By assumption, given $\varepsilon > 0$, there exists $u \in S_\rho$ with $V(u) \leq \varphi(\rho) + \varepsilon$. Thus $H(u) \geq H(\bar{u}) + \delta$ and $V(u) \leq \varphi(\rho_o) + \varepsilon \leq V(\bar{u}) + \varepsilon$, as required.

Sufficiency. By Proposition 2.2 it suffices to show that θ is nonincreasing. Let $0 \leq \rho < \rho_1 < \infty$ and let $\bar{u} \in S_\rho$. By applying the condition in the theorem a finite number of times we deduce that given $\varepsilon > 0$ there exists $u \in K_\infty$ with $H(u) \geq \rho_1$ and $V(u) \leq V(\bar{u}) + \varepsilon$. Define, for $0 \leq s \leq 1$, $u_s = s\bar{u} + (1-s)u$. Then $H(u_1) = \rho$, $H(u_o) \geq \rho_1$ and the function $s \mapsto H(u_s)$ is finite, convex and lsc, and thus continuous. Hence there exists $s \in [0,1]$ such that $u_s \in S_{\rho_1}$. But

$$V(u_s) \leq s\,V(\bar{u}) + (1-s)V(u) \leq V(\bar{u}) + \varepsilon,$$

and since ε is arbitrary, $\theta(\rho_1) \leq \theta(\rho)$. □

Various other necessary and sufficient conditions that $\theta(\rho) = \varphi(\rho)$ for all $\rho \geq 0$ can be established in a similar way ; one such condition is that there exists a sequence $u_j \in K$ with $H(u_j) \to \infty$ and $V(u_j) \to \inf_{\rho\geq 0}\varphi(\rho)$.

If $X = \mathbb{R}^n$ and H has an extension to a convex function $\tilde{H} : \mathbb{R}^n \to \mathbb{R}$ then H is necessarily continuous, and thus the level sets S_ρ are closed for every $\rho \in [0,\infty)$. Consequently the minimum in (2.1) is always attained and hence $\theta(\rho) > \varphi(\rho)$ for $\rho_s < \rho < \infty$. The following example shows, however, that when $\rho_s < \infty$ the case $\theta(\rho) = \varphi(\rho)$ for all $\rho \geq 0$ can occur even in finite dimensions.

Example

Let $X = \mathbb{R}^2$, $K = \{(x,y) : x \geq 0\}$, $V(x,y) = x^2 + y^2$, and $H(x,y) = y^4/x^2$ if $x > 0$, $H(0,0) = 0$, $H(x,y) = +\infty$ otherwise. Then H is convex and lsc. For any $\rho > 0$, $\varepsilon > 0$, $H(\varepsilon, \rho^{1/4}\varepsilon^{1/2}) = \rho$ and $V(\varepsilon, \rho^{1/4}\varepsilon^{1/2}) = \varepsilon^2 + \rho^{1/2}\varepsilon$. It follows that $\rho_s = 0$ and that $\theta(\rho) = \varphi(\rho) = 0$ for all $\rho \geq 0$.

Finally we note that extra equality constraints can sometimes be handled using the above results by redefining K. Suppose, for example, that the problem to be studied is to minimize V on S_ρ subject to the extra constraint $G(u) = \gamma$, where $G : K \to \mathbb{R} \cup \{+\infty\}$ is convex and slsc. Assume further that $\gamma \in \mathbb{R}$ is such that, given any $\rho \in [0,\infty)$ and $u \in S_\rho$ with $G(u) \leq \gamma$ there exists $\bar{u} \in S_\rho$ such that $G(\bar{u}) = \gamma$ and $V(\bar{u}) \leq V(u)$. Then the problem is equivalent to that of minimizing V on $S_\rho \cap \tilde{K}$, where $\tilde{K} = \{u \in K : G(u) \leq \gamma\}$.

3. Equilibrium of an incompressible fluid above a surface.

So as to fit this example into the framework of Section 2, we set $X = L^1(\mathbb{R}^2) \cap L^2(\mathbb{R}^2)$ endowed with the weak topology of $L^2(\mathbb{R}^2)$, $K = \{h \in X : h \geq 0\}$, and we define V, H by (1.3), (1.4) respectively. Since f is bounded and

$$V(h) \geq g[\tfrac{1}{2}\|h\|^2_{L^2} + \left(\min_{z\in\mathbb{R}^2} f(z)\right)H(h)], \tag{3.1}$$

it follows that $V : K \to \mathbb{R}$. Furthermore, for each $\rho \geq 0$, $M \geq 0$ the set $K_{\rho,M}$ is nonempty and sequentially precompact. If $h_j \in K_{\rho,M}$ with $h_j \rightharpoonup h$ in $L^2(\mathbb{R}^2)$ then for any $R \geq 0$

$$\int_{\mathbb{R}^2} fh_j dz = \int_{|z|<R} fh_j\, dz + \int_{|z|\geq R} fh_j\, dz,$$

and the first integral on the right-hand side tends to $\int_{|z|<R} fh\, dz$ as $j \to \infty$, while the second is bounded above by $\rho \max_{|z|\geq R}|f(z)|$. By (1.2) we thus have $\lim_{j\to\infty}\int_{\mathbb{R}^2} fh_j\, dz = \int_{\mathbb{R}^2} fh\, dz$, and hence that V restricted to $S_{\rho,M}$ is slsc. It is easily shown that K is sequentially closed and convex, that H is convex and slsc, and that V is strictly convex. Thus Propositions 2.1-2.3 hold. The minimizers $\bar{h}(\lambda)$ of the functional (cf. (2.3))

$$V_\lambda(h) = g\int_{\mathbb{R}^2}(\tfrac{1}{2}h^2 + fh)dz + \lambda\int_{\mathbb{R}^2} hdz \tag{3.2}$$

on K are easily calculated by minimizing the integrand for each z. Thus we find that

(3.3) $$\bar{h}(\lambda)(z) = [f(z) + g^{-1}\lambda]^-,$$

and that

(3.4) $$\psi(\lambda) := H(\bar{h}(\lambda)) = \int_{\mathbb{R}^2} [f(z) + g^{-1}\lambda]^- dz,$$

and hence

(3.5) $$\rho_s = \int_{\mathbb{R}^2} [f(z)]^- dz.$$

If $\rho_s = \infty$ (resp. $\rho_s < \infty$) then V_λ attains a minimum on K for all $\lambda > 0$ (resp. $\lambda \geq 0$). Since $\psi : [0, -g\min_{\mathbb{R}^2} f] \to [0, \rho_s]$ is strictly decreasing and continuous, it has an inverse ψ^{-1}. The minimizer h^ρ of V on K_ρ is therefore given by

(3.6) $$h^\rho(z) = [f(z) + d(\rho)]^-,$$

where

(3.7) $$d(\rho) = \begin{cases} g^{-1}\psi^{-1}(\rho) & \text{if} \quad 0 \leq \rho \leq \rho_s, \rho < \infty \\ 0 & \text{if} \quad \rho_s \leq \rho < \infty. \end{cases}$$

Thus where $h^\rho(z) > 0$ the fluid surface is given by $x_3 = -d(\rho) =$ constant. To check that h^ρ is also the minimizer of V on S_ρ we need to verify the condition in Theorem 2.4. To do this define for $j = 1, 2, \ldots$,

$$\sigma_j(z) = \begin{cases} j^{-1} & \text{if } j \leq |z| \leq j+1 \\ 0 & \text{otherwise.} \end{cases}$$

Then it is easily shown that for any $\bar{h} \in K_\infty$

$$\lim_{j\to\infty} H(\bar{h} + \sigma_j) = H(\bar{h}) + 2\pi, \quad \lim_{j\to\infty} V(\bar{h} + \sigma_j) = V(\bar{h}),$$

as required. From (3.6) we thus have that for all $\rho \geq 0$

(3.8) $$\theta(\rho) = \varphi(\rho) = \frac{1}{2} g \int_{f(z) \leq -d(\rho)} (d(\rho)^2 - f^2) dz.$$

Other formulations of the problem treated in this section are possible. For example, one can minimize the potential energy of a given volume of fluid given that it occupies a subset of the region above the surface $\mathcal{S}$, without assuming initially that this subset has the form $f(z) \leq x_3 \leq f(z) + h(z)$, as done here ; a material (Lagrangian) description is also possible. Although these formulations

may in some ways be preferable they do not have the same convex structure as (1.3), (1.4).

It is interesting that in the problem considered here, and despite its convex structure, there are configurations that can be regarded as metastable, such as that represented by a lake in the mountains. In the latter case the total potential energy can be reduced by transferring a drop of liquid to a lower level, so that the configuration is not a local minimizer with respect even to small $C_o^\infty(\mathbb{R}^2)$ perturbations. This raises questions pertaining to the appropriate choice of metric and role of dynamics in metastability similar to those arising in problems concerning solid and fluid phase transitions.

4. A simplified model of the atmosphere.

Consider a vertical column of height $\rho > 0$ and unit cross-sectional area of an ideal gas with constant specific heats. We use a one-dimensional Lagrangian description with respect to a reference configuration $[0, 1]$ in which the gas has constant density $r_o > 0$ and constant pressure $p_o > 0$, the material point at $x \in [0, 1]$ in the reference configuration being displaced to the point with vertical coordinate $z(x)$, where z is increasing and

(4.1) $$z(0) = 0, \quad z(1) = \rho.$$

The gas is assumed to deform adiabatically, so that the pressure p and density r satisfy

(4.2) $$p\, r^{-\gamma} = p_o\, r_o^{-\gamma},$$

where $\gamma > 1$ is a constant. (The adiabatic assumption, while capturing some features of the lower atmosphere, is a considerable oversimplification : see, for example, Houghton [6].) The potential energy of the column is given by

(4.3) $$I(z) = \int_0^1 \left[\frac{p_o}{(\gamma - 1)(z'(x))^{\gamma-1}} + r_o g z(x) \right] dx,$$

which we write in the form

(4.4) $$I(z) = r_o g \int_0^1 \left[\frac{k}{(z'(x))^{\gamma-1}} + (1 - x) z'(x) \right] dx,$$

where $k = \dfrac{p_o}{r_o g(\gamma - 1)}$. We seek to minimize $I(z)$ subject to the boundary conditions (4.1). To fit this problem into the framework of Section 2 we set $z' = u^2$, so that the problem becomes to minimize

(4.5) $$V(u) = r_o g \int_0^1 \left[\frac{k}{u^{2(\gamma-1)}} + (1 - x) u^2(x) \right] dx$$

subject to the constraint

$$H(u) := \int_0^1 u(x)^2 dx = \rho. \tag{4.6}$$

We set $X = L^2(0,1)$ with the weak topology, and $K = \{u \in L^2 : u \geq 0\}$. Standard methods show that the hypotheses of Proposition 2.1-2.3 hold. The minimizers $\bar{u}(\lambda)$ of $V_\lambda(u) = V(u) + \lambda H(u)$ are easily calculated by minimizing the integrand for each x. Thus

$$\bar{u}(\lambda)(x) = \left[\frac{p_o}{\lambda + r_o g(1-x)}\right]^{1/2\gamma}, \tag{4.7}$$

and

$$\psi(\lambda) := H(\bar{u}(\lambda)) = \frac{\gamma}{\gamma - 1}\cdot\frac{p_o^{1/\gamma}}{r_o g}((\lambda + r_o g)^{\frac{\gamma-1}{\gamma}} - \lambda^{\frac{\gamma-1}{\gamma}}). \tag{4.8}$$

Hence

$$\rho_s = \frac{\gamma}{\gamma-1}\left[\frac{p_o}{r_o g}\right]^{1/\gamma} < \infty, \tag{4.9}$$

and the minimizer u^ρ of V on K_ρ is given by

$$u^\rho(x) = \left[\frac{p_o}{\mu(\rho) + r_o g(1-x)}\right]^{1/2\gamma}, \tag{4.10}$$

where

$$\mu(\rho) = \begin{cases} \psi^{-1}(\rho) & \text{if } 0 \leq \rho \leq \rho_s \\ 0 & \text{if } \rho_s \leq \rho < \infty. \end{cases} \tag{4.11}$$

To check the condition in Theorem 2.4 define for $j = 1, 2, \ldots$,

$$\sigma_j(x) = \begin{cases} 0 & \text{if } 0 \leq x \leq 1 - j^{-1}, \\ j & \text{if } 1 - j^{-1} < x \leq 1. \end{cases} \tag{4.12}$$

Then if $\bar{u} \in K_\infty$,

$$\lim_{j\to\infty} H((\bar{u}^2 + \sigma_j)^{1/2}) = H(\bar{u}) + 1, \quad \lim_{j\to\infty} V((\bar{u}^2 + \sigma_j)^{1/2}) = V(\bar{u}),$$

as required. Hence, for all $\rho \geq 0$, $\theta(\rho) = \varphi(\rho)$ and u^ρ minimizes V on S_ρ.

From (4.9) we see that the adiabatic model predicts a finite height $h = \rho_s$ for the atmosphere. The corresponding pressure, density and temperature profiles are easily obtained from (4.10) with $\rho = \rho_s$ using the formulae $rz' = r_o$, $p = c_p(\frac{\gamma-1}{\gamma})\theta r$, where θ denotes the absolute temperature and c_p the specific heat at constant

pressure. If $\bar{p}, \bar{r}$ denote the values of the pressure and density respectively at the earth's surface $z = 0$ we find that

$$h = \frac{\gamma}{\gamma - 1}\frac{\bar{p}}{\bar{r}g}, \tag{4.13}$$

$$p(z) = \bar{p}(1 - \frac{z}{h})^{\frac{\gamma}{\gamma-1}}, \tag{4.14}$$

$$r(z) = \bar{r}(1 - \frac{z}{h})^{\frac{1}{\gamma-1}}, \tag{4.15}$$

$$\theta(z) = \frac{gh}{c_p}(1 - \frac{z}{h}). \tag{4.16}$$

These well known formulae can be found, for example, in Sommerfeld [11, pp 49-55].

5. The Thomas-Fermi model

In the Thomas-Fermi theory of atoms and molecules one is led to the problem of minimizing the energy functional

$$V(r) = \frac{3}{5}\nu\int_{\mathbb{R}^3} r(x)^{5/3}dx - \int_{\mathbb{R}^3}\gamma(x)r(x)dx + \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{r(x)r(y)}{|x-y|}dx\,dy \tag{5.1}$$

subject to the constraint

$$H(r) := \int_{\mathbb{R}^3} r(x)dx = \rho. \tag{5.2}$$

Here $r(x) \geq 0$ is the electron density,

$$\gamma(x) = \sum_{j=1}^{k}\frac{z_j}{|x - a_j|} \tag{5.3}$$

is the Coulomb potential corresponding to $k \geq 1$ nuclei of charges $z_j > 0$ located at the distinct points $a_j \in \mathbb{R}^3$ and ν is a positive constant.

To apply the results of Section 2 we let $X = L^1 \cap L^{5/3}$ endowed with the weak topology of $L^{5/3}$, and we let

$$K = \{r \in X : r \geq 0\}. \tag{5.4}$$

(Here L^p denotes $L^p(\mathbb{R}^3)$.) The convexity, semicontinuity and other hypotheses of Propositions 2.1-2.3 are easily verified (see Lieb & Simon [8], Lieb [7]). To prove the condition in Theorem 2.4 we let $\eta \in C_o^\infty(\mathbb{R}^3)$, $\eta \geq 0$, and for $\bar{r} \in K_\infty$, $\varepsilon > 0$, define (cf. Benguria, Brezis & Lieb [4])

$$\bar{r}_\varepsilon(x) = \bar{r}(x) + \varepsilon^3\eta(\varepsilon x). \tag{5.5}$$

Then it is not hard to prove that

$$\lim_{\varepsilon\to 0+}\frac{V(\bar r_\varepsilon)-V(\bar r)}{\varepsilon} = \Big(\int_{\mathbb{R}^3}\bar r(x)dx - Z\Big)\int_{\mathbb{R}^3}\frac{\eta(x)}{|x|}dx + \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{\eta(x)\eta(y)}{|x-y|}dx\,dy, \tag{5.6}$$

where $Z=\sum_{j=1}^k z_j$. In particular,

$$\lim_{\varepsilon\to 0} H(\bar r_\varepsilon) = H(r)+H(\eta), \quad \lim_{\varepsilon\to 0} V(\bar r_\varepsilon) = V(\bar r),$$

as required.

From (5.6) we see also that if $\bar r\in K_\infty$ with $H(\bar r)<Z$ then for a suitable η and $\varepsilon>0$ we have that $H(\bar r_\varepsilon)>H(\bar r)$ and $V(\bar r_\varepsilon)<V(\bar r)$. Hence $\rho_s\geq Z$. In fact, by showing that the Lagrange multiplier for the minimizer r^Z of V subject to $H(r)=Z$ is zero we find (see the above references and the work of Benilan & Brezis reported in Brezis [5]) that $\rho_s=Z$. Since the second term in (5.1) is sequentially continuous on X, while the first and third terms are slsc, it follows that any minimizing sequence r_j for V in K_ρ satisfies $\lim_{j\to 0}\|r_j\|_{L^{5/3}}=\|r^\rho\|_{L^{5/3}}$, so that $r_j\to r^\rho$ strongly in $L^{5/3}$, and hence strongly in L^p for $1<p\leq 5/3$. If $0\leq\rho\leq Z$, and if r_j is a minimizing sequence for V in S_ρ, then we also have that $\int_{\mathbb{R}^3} r_j dx=\int_{\mathbb{R}^3} r^\rho dx$, from which it is easily proved that $r_j\to r^\rho$ strongly in L^1. Combining these remarks with the results of Section 2 gives the following version of the basic result of Lieb & Simon [8].

Theorem 5.1

(i) If $0\leq\rho\leq Z$ then V attains an absolute minimum on K subject to $H(r)=\rho$ at a unique r^ρ, and every minimizing sequence converges strongly to r^ρ in L^p for $1\leq p\leq 5/3$.

(ii) If $Z<\rho<\infty$ then the infimum of V on K subject to $H(r)=\rho$ equals $V(r^Z)$ and is not attained. Every minimizing sequence converges to r^Z strongly in L^p for $1<p\leq 5/3$, but not strongly in L^1.

For more information concerning the minimizers r^ρ, and for other results, the reader is referred to the papers by Lieb & Simon and Lieb. The results of Section 2 also apply to the Thomas-Fermi-von Weisäcker theory treated in Benguria, Brezis & Lieb [4].

6. Coagulation-fragmentation equations

The discrete coagulation-fragmentation equations

$$\dot c_r = \frac{1}{2}\sum_{s=1}^{r-1}[a_{r-s,s}c_{r-s}c_s - b_{r-s,s}c_r] - \sum_{s=1}^{\infty}[a_{r,s}c_rc_s - b_{r,s}c_{r+s}], \quad r=1,2,\dots, \tag{6.1}$$

(where the first sum is absent if $r=1$) are a model for the time evolution of the expected numbers $c_r(t)\geq 0$ of r-particle clusters in a system of a large number of clusters of particles that can coagulate to form larger clusters or fragment to form smaller ones. We suppose that the coagulation rates $a_{r,s}$ and fragmentation rates $b_{r,s}$ are nonnegative constants satisfying for each $r,s\geq 1$

$$a_{r,s}=a_{s,r},\quad b_{r,s}=b_{s,r},\quad a_{r,s}Q_rQ_s=b_{r,s}Q_{r,s}, \tag{6.2}$$

where the Q_r are strictly positive constants with $Q_1=1$, and we confine attention to the physically interesting case when

$$0<z_s<\infty, \tag{6.3}$$

where

$$z_s^{-1}=\limsup_{r\to\infty} Q_r^{1/r}. \tag{6.4}$$

Formal calculations show that for solutions $c=(c_r)$ of (6.1) the density

$$H(c)=\sum_{r=1}^{\infty} rc_r \tag{6.5}$$

is a conserved quantity, and that the function

$$E(c)=\sum_{r=1}^{\infty} c_r\Big(\ell n\Big(\frac{c_r}{Q_r}\Big)-1\Big) \tag{6.6}$$

is nonincreasing with time. For these and other reasons it is natural to consider the problem of minimizing E subject to $H(c)=\rho$. Following Ball, Carr & Penrose [3] we study the equivalent problem of minimizing, in the notation of (2.3), the functional

$$V(c)=E(c)-\ell n z_s H(c), \tag{6.7}$$

which has advantageous continuity properties. We introduce the Banach sequence space

$$Y=\{c=(c_r):\|c\|<\infty\},\quad \|c\|=\sum_{r=1}^{\infty} r|c_r|, \tag{6.8}$$

and denote by X the space Y endowed with the weak star topology (see [3, p 672]); a sequence $c^{(j)}$ converges to c in this topology if and only if the norms $\|c^{(j)}\|$ are uniformly bounded and $c_r^{(j)}\to c_r$ for each r.

We let $K = \{c \in X : c_r \geq 0 \text{ for all } r\}$. Since

$$V(c) = \sum_{r=1}^{\infty} c_r(\ell n(c_r) - 1) + \sum_{r=1}^{\infty} \gamma_r r c_r,$$

where $\gamma_r = -\ell n(Q_r^{1/r} z_s)$, and since $\liminf_{r\to\infty} \gamma_r = 0$, it follows using the methods in [3, pp 680-682] that V is slsc on K. The other hypotheses of Propositions 2.1-2.3 also hold. To check the condition in Theorem 2.4 we let $\{r_j\}$ be a sequence such that $\lim_{j\to\infty} \gamma_{r_j} = 0$ and define $\sigma^{(j)}$ by

$$\sigma_r^{(j)} = \begin{cases} r_j^{-1} & \text{if } r = r_j \\ 0 & \text{otherwise.} \end{cases}$$

Then for any $\bar{c} \in K_\infty$, it is easily checked that

$$\lim_{j\to\infty} H(\bar{c} + \sigma^{(j)}) = H(\bar{c}) + 1, \quad \lim_{j\to\infty} V(\bar{c} + \sigma^{(j)}) = V(\bar{c}),$$

as required.

Defining V_λ as in (2.3) (a different notation is used in [3]) we find by minimizing the summand for each r that the minimizers $\bar{c}(\lambda)$ of V_λ on K_∞ have the form

$$\bar{c}(\lambda)_r = Q_r(e^{-\lambda} z_s)^r. \tag{6.9}$$

Therefore

$$\psi(\lambda) = H(\bar{c}(\lambda)) = \sum_{r=1}^{\infty} r Q_r (e^{-\lambda} z_s)^r. \tag{6.10}$$

Let

$$F(z) = \sum_{r=1}^{\infty} r Q_r z^r. \tag{6.11}$$

By (6.4) this series has radius of convergence z_s. Thus

$$\rho_s = \sum_{r=1}^{\infty} r Q_r z_s^r, \tag{6.12}$$

and if $0 \leq \rho \leq \rho_s$, $\rho < \infty$, the unique minimizer of V (and hence of E) on S_ρ is given by

$$c_r^\rho = Q_r z(\rho)^r \tag{6.13}$$

where $F(z(\rho)) = \rho$.

In terms of the original free energy functional E the conclusion of Theorem 2.4 implies that if $\rho_s < \rho < \infty$ then

$$\inf_{S_\rho} E = E(c^{\rho_s}) + \ell n z_s (\rho - \rho_s), \tag{6.14}$$

and by Proposition 2.1 every minimizing sequence of E on S_ρ converges weak star to c^{ρ_s}. If $0 \leq \rho \leq \rho_s$, $\rho < \infty$ then every minimizing sequence of E on S_ρ converges strongly in Y to c^ρ ; this follows from Proposition 2.1 and from [3 Lemma 3.3]. These and the remaining conclusions of Section 2 were established in [3 Proposition 2.3, Theorem 2.4] in the context of the Becker-Döring equation, a special case of (6.1). Results for (6.1) are reported in Ball & Carr [2]. The reader is referred to these papers for the relevant physical background, a discussion of the validity of density conservation, and a dynamical analysis of the approach to equilibrium.

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