Symmetric Potentials Beget Symmetric Ground States

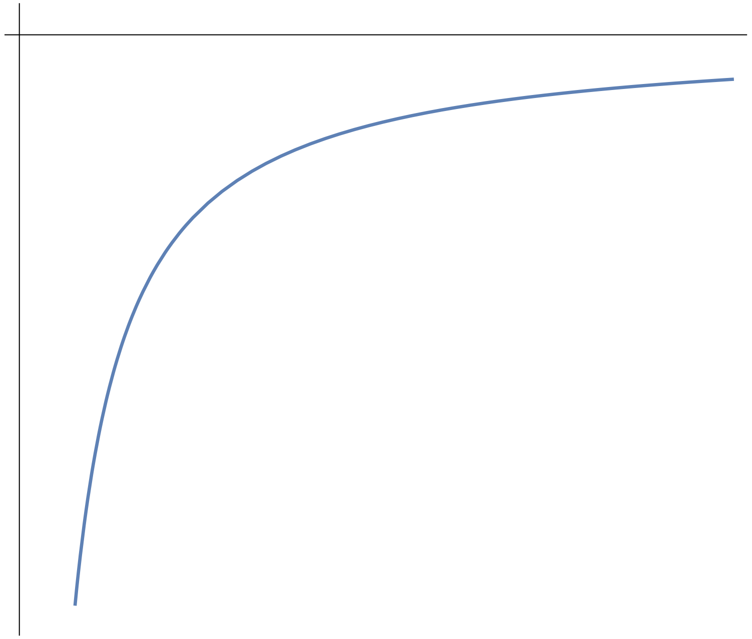
Richard Chapling

LMS Graduate Student Meeting, 11 November 2016

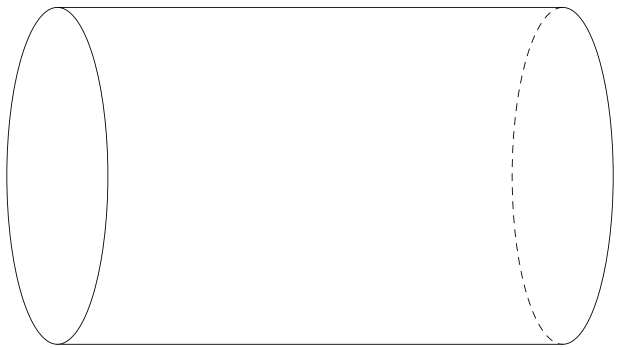
We are often told that systems described by symmetric equations, such as the hydrogen atom, will have a symmetric lowest-energy solution. The usual method of proving this only applies to certain radial systems. I shall describe an unusual symmetrisation technique, and use it to show for several systems with symmetric potentials, both linear and nonlinear, that if they have a ground state, it must be symmetric.

- In physics, one frequently discusses equations describing physical systems that possess certain symmetries.
- E.g. the potential of an atomic nucleus is spherically symmetric.
- Knowing a solution is symmetric is always useful: reduces the complexity of any problem, no matter how we study it subsequently.
- Often, the lowest-energy solution to these equations is simply assumed to be symmetric.
- Today, I will explain a simple technique to prove that such symmetric equations for scalar fields have symmetric ground states.
- The examples I discuss will be based on equations from quantum mechanics, and describe the distribution of spinless charged particles in electric fields.

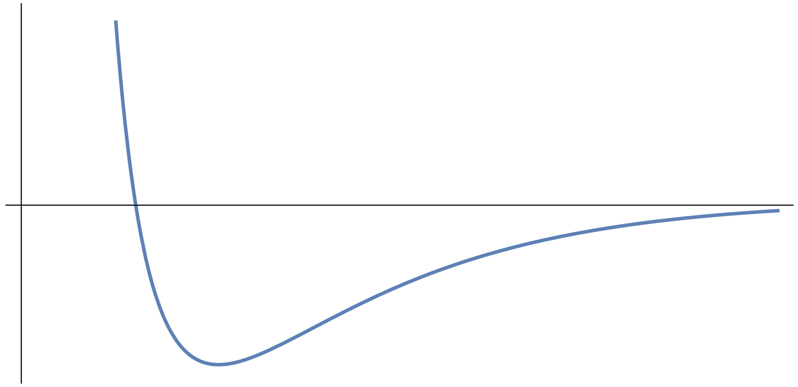
Previous techniques only work for radial, nondecreasing potentials, such as the hydrogen atom:



The technique I will describe today will work for other cases, e.g.



Charges on a cylinder



Charges in a more general radial potential

(And many more.)

Equations Euler–Lagrange differential equations of an energy functional.

Energy Functional A map $E : \mathcal{X} \to \mathbb{R}$. The examples we consider have domains contained in the Sobolev/Bessel space

$$H^1(X) = \left\{(u : X \to \mathbb{C}) : \int_X (|\nabla u|^2 + |u|^2) < \infty\right\}.$$

Ground State A function in $\mathcal{X}$ that minimises E.

Spaces and Groups X is a smooth manifold, G a compact group acting on X by symmetries, so the volume element dx is invariant.

Symmetric f is symmetric if $f(g.x) = f(x), \forall g \in G$.

A concrete example that is useful to think about is $X = \mathbb{R}^d$, $G = SO(d)$ acting by rotations—the spherically symmetric case. Then f is symmetric iff it is radial.

The *Schrödinger equation*,

$$-\Delta u + Vu = \omega u.$$

ω is a Lagrange multiplier, which enforces the condition

$$N[u] = \int_X |u|^2 = n.$$

The corresponding energy is

$$\begin{aligned} E_1[u] &= \frac{1}{2}\int_X |\nabla u|^2 + \frac{1}{2}\int_X V\,|u|^2 \\ &= \tfrac{1}{2}T[u] + \tfrac{1}{2}P[u] \end{aligned}$$

and we have

Problem 1. Minimise $E_1[u]$ subject to $N[u] = n$.

The *nonlinear Schrödinger equation*,

$$-\Delta u + Vu + \kappa |u|^2 u = \omega u,$$

The corresponding energy is

$$\begin{aligned} E_2[u] &= \frac{1}{2}\int_X |\nabla u|^2 + \frac{1}{2}\int_X V|u|^2 + \frac{1}{4}\kappa \int_X |u|^4 \\ &= \tfrac{1}{2}T[u] + \tfrac{1}{2}P[u] + \tfrac{1}{4}K[u] \end{aligned}$$

and we have

Problem 2. Minimise $E_2[u]$ subject to $N[u] = n$.

The *Hartree equation*,

$$-\Delta u + Vu + (G * |u|^2)u = \omega u,$$

G is the Green's function of the Laplacian.
The corresponding energy is

$$\begin{aligned} E_3[u] &= \frac{1}{2}\int_X (|\nabla u|^2 + V\,|u|^2) + \frac{1}{4}\int_X\int_X G(x;y)\,|u(x)|^2\,|u(y)|^2\;dx\,dy \\ &= \tfrac{1}{2}T[u] + \tfrac{1}{2}P[u] + \tfrac{1}{4}Q[|u|^2, |u|^2] \end{aligned}$$

and we have

Problem 3. Minimise $E_3[u]$ subject to $N[u] = n$.

In this talk I am considering the following implication:

$$\text{Equations symmetric} \quad + \quad \exists \text{ ground state}$$
$$\Downarrow$$
$$\text{Ground state symmetric}$$

In particular, I will *not* prove that the ground state exists.

We proceed by contradiction.

1. Start with a u that is *not* symmetric, has total charge n, and minimises E.
2. Apply some operation to make a new function, $\bar{u}$, which also has total charge n.
3. Show that the energy of this new function is *strictly smaller* than that of u.
4. Hence u does not minimise E.

Therefore if u does minimise E and have total charge n, it must be symmetric.

We work with the following *orbital mean*:

$$\bar{u}(x) = \left(\int_G |u(g.x)|^2 \; dg \right)^{1/2}$$

(. denotes the action, dg Haar probability measure on G.)

- This is a classical idea: used by Hardy and Littlewood when $G = S^1$ for analytic functions and their power series.
- But writing explicitly as an integral over a group makes life a lot clearer.
- This construction works for any compact group G. Nothing in the proof needs much structure on either X or G, so the results are quite general.

$$\bar{u}(x) = \left(\int_G |u(g.x)|^2 \, dg \right)^{1/2}$$

Problem. Minimise E subject to $N[u] = n$.

Suppose $N[u] = n$, u is not symmetric, and u minimises E. We show that

1. $N[\bar{u}] = N[u]$ ($\bar{u}$ is a possible solution to the Problem).
2. $E[\bar{u}] < E[u]$ ($\bar{u}$ has smaller energy than u), by looking at each term separately.

Therefore we have a witness to u not minimising E.

We want to show that:

1. $N[\bar{u}] = N[u]$ ($\bar{u}$ is a possible solution to the Problem).
2. $E[\bar{u}] < E[u]$ ($\bar{u}$ has smaller energy than u).

We do this by considering each term in E separately. So we need to understand what happens to

$$N[u] = \int_X |u|^2 \, dx \qquad \text{Total charge}$$

$$T[u] = \int_X |\nabla u|^2 \, dx \qquad \text{Kinetic energy}$$

$$P[u] = \int_X V \, |u|^2 \, dx \qquad \text{External PE}$$

$$Q[|u|^2, |u|^2] = \int_X \int_X G(x; y) \, |u(x)|^2 \, |u(y)|^2 \, dx \, dy \qquad \text{Internal PE}$$

when we replace u with $\bar{u}$.

$$N[u] = \int_X |u|^2 \, dx, \qquad T[u] = \int_X |\nabla u|^2 \, dx,$$
$$P[u] = \int_X V\, |u|^2 \, dx, \quad Q[u] = \int_X \int_X G(x;y)\, |u(x)|^2 \, |u(y)|^2 \, dx\, dy$$

Only T changes when $u \to |u|$.
Diamagnetic inequality,

$$|\nabla |u|| \leqslant |\nabla u|\,,$$

implies $T[|u|] \leqslant T[u]$. Hence $E[|u|] \leqslant E[u]$, and suffices to take $u \geqslant 0$.

For the total charge, we have

$$\begin{aligned} N[\bar{u}] &= \int_X \int_G |u(g.x)|^2 \; dg\, dx \\ &= \int_G \int_X |u(g.x)|^2 \; dx\, dg \\ &= \int_G \int_X |u(x')|^2 \; dx'\, dg \qquad\qquad (x' = g.x, \quad dx' = dx) \\ &= \int_G N[u]\, dg = N[u]. \end{aligned}$$

The external potential energy $P[u]$ works in exactly the same way, since $V(g.x) = V(x)$, so

$$P[\bar{u}] = P[u].$$

The other proofs are just more elaborate forms of this idea!

Kinetic Energy

For the kinetic energy $T[u]$, need a relative of Cauchy–Schwarz:

$$\int |\alpha|^2 \int |\beta|^2 \geqslant \left| \int \Re(\alpha^* \beta) \right|^2$$

Putting $\alpha = u(g.x)$, $\beta = (\nabla u)(g.x)$ and $\int = \int_G \, dg$,

$$\begin{aligned} \bar{u}(x)^2 \int_G |\nabla u(g.x)|^2 \, dg &\geqslant \left| \int_G \Re(u^* \nabla u)(g.x) \, dg \right|^2 \\ &= \cdots = \bar{u}(x)^2 \, |\nabla \bar{u}(x)|^2 \,. \end{aligned}$$

Cancelling $\bar{u}(x)^2$, integrating over X and changing the order of integration on the left, we obtain

$$T[u] \geqslant T[\bar{u}].$$

(Equality is strict if $u > 0$ and u not symmetric.)

Internal Potential Energy

For the internal potential energy $Q[|u|^2, |u|^2] = Q[u^2, u^2]$, we have that Q is *positive-definite*: if $f \neq 0$,

$$Q[f, f] > 0.$$

Write $u^2 = \bar{u}^2 + (u^2 - \bar{u}^2)$. Then

$$Q[u^2, u^2] = Q[\bar{u}^2, \bar{u}^2] + 2Q[\bar{u}^2, u^2 - \bar{u}^2] + Q[u^2 - \bar{u}^2, u^2 - \bar{u}^2]$$

Last term is *positive* unless $u = \bar{u}$.
For middle term, $G(g.x; g.y) = G(x; y)$, which implies the term is zero by an argument similar to that for the total charge. Hence

$$Q[u^2, u^2] > Q[\bar{u}^2, \bar{u}^2]$$

if u is not symmetric.

Conclusion

Suppose u minimises E and $u \neq \bar{u}$. We have found:

$$\begin{aligned} u &\geqslant 0, \\ N[u] &= N[\bar{u}], \\ T[u] &> T[\bar{u}], \\ P[u] &= P[\bar{u}], \\ Q[u^2, u^2] &> Q[\bar{u}^2, \bar{u}^2], \end{aligned}$$

Hence $\bar{u}$ has the correct total charge and $E[u] > E[\bar{u}]$, so u cannot minimise E.

Introduction
Examples
Proof Outline
Other
▹ Other Terms
Questions

Similar ideas can be used on

Relativistic KE In $\mathbb{R}^d$ this may be given by a Fourier transform

$$\langle u, \sqrt{p^2 + m^2 u}\rangle = \int_{\mathbb{R}^d} \sqrt{k^2 + m^2}\, |u(k)|^2 \; dk.$$

One can turn this back into a positive-definite convolution in position space and use the similar ideas as for Q (note we have u rather than u^2).

Other nonlinear terms For convex functions of $|u|^2$, one can use Jensen's inequality: e.g. since $x \mapsto |x|^2$ is strictly convex,

$$K[\bar{u}] = \int_X |\bar{u}|^4 < \int_X |u|^4 = K[u]$$

unless $|u| = \bar{u}$.

Open Questions

- Discrete symmetry groups are more mysterious: suppose we have an even potential on $\mathbb{R}$. Must the ground state be even?
- Can a singularity in an even potential affect whether the ground state is even or odd?
- These problems originate in the lack of connectivity in one-dimensional space and discrete groups: in one dimension, can't tell the difference between

$$(\nabla |x|)^2 \quad \text{and} \quad (\nabla x)^2$$