Symmetric Potentials Beget Symmetric Ground States

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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.

Today I shall be talking about the connection between problems from physics that are defined by differential equations with certain symmetries, and their solutions.

There are a number of reasons for wanting to show that a solution to any problem is symmetric: probably the most important of these is that it normally reduces the complexity of the equations we have to solve (or more realistically, study with numerics or analytical techniques).

I shall focus on three examples, to demonstrate the techniques involved in the proofs. At the end I shall give a couple of other examples that have been of special interest to me.

Before we begin, I wish to emphasise one point:

I will be proving that if a the equations have a certain symmetry, and *if* a ground state exists, then the ground state also has the symmetry. *I shall not prove that there actually is a lowest-energy state.*

I should also define these terms that I am using:

Equations When I say this, I mean the Euler–Lagrange differential equations arising from an energy functional by the standard variational method. The parameter ω is a Lagrange multiplier, and generically ensures that $\int_X |u|^2 = 1$

Energy A map E from some Banach space of functions to the real numbers. The examples we consider generally use subsets of the Sobolev/Bessel space

$$H^1(X) = \left\{ (u : X \to \mathbb{C}) : \int_X |\nabla u|^2 + |u|^2 < \infty \right\} \tag{0.1}$$

as their domain.

Ground State The function that minimises E is called the ground state of the equation.

Spaces and Groups We take X to be a smooth manifold, G a compact group acting on X by symmetries, so that the infinitesimal volume element dx is invariant.[1] The action is denoted $g.x$.

Symmetric A function $f : X \to \mathbb{C}$ is called symmetric if $f(g.x) = f(x)$ for every $x \in X$ and $g \in G$.

(In all my examples, the equations are time-independent, obtained by assuming a solution of the form $e^{-i\omega t}u(x)$.)

1 The Main Idea

Now, this is the key idea. The following is not new in specifics, but its usefulness lies in the generality of its statement. Let dg be Haar probability measure for G. We define

$$M[u](x) = \left(\int_G |u(g.x)|^2 \, dg \right)^{1/2}, \tag{1.1}$$

which in the absence of a nicer name I have been calling the *orbital averaging of* u. (This idea goes back at least to Hardy and Littlewood for the circle.)

It turns out that writing this as an integral over a group (rather than, for example, over all the angles in the spherical case) makes certain manipulations far easier to carry out.

With those preliminaries out of the way, let us move to the examples.

2 Examples

2.1 Example 1: The Schrödinger Equation in n Dimensions

We start with a very simple example, although it is already important in applications.

$$-\Delta u + Vu = \omega u. \tag{2.1}$$

We've probably all seen this as undergraduates, at least for describing electrons in the hydrogen atom. It probably doesn't surprise you that this equation has a symmetric ground state, at least for the potentials where this is exactly solvable: separation of variables and local uniqueness give the ground state in three dimensions. The corresponding energy functional is

$$E_1[u] = \frac{1}{2} \int_X |\nabla u|^2 + \frac{1}{2} \int_X V \, |u|^2 =: \tfrac{1}{2} T[u] + \tfrac{1}{2} P[u], \tag{2.2}$$

comprising the kinetic energy $T[u]$ and potential energy $P[u]$. Writing also $N[u] = \int_X |u|^2$, we hence have

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

However, it is normally necessary to modify this equation to take into account other effects, which tends to make an exact solution unfeasible.

[1] For $\mathbb{R}^d$, if G acts by linear transformations, this translates to $\det g = 1$, for example.

2.2 Example 2: Nonlinear Schrödinger Equation

Another well-known example of this sort of equation is the *nonlinear* Schrödinger equation, which has applications in superconductivity, for example. As the name would suggest, one adds a nonlinear term:

$$-\Delta u + Vu + \kappa |u|^2 u = \omega u. \tag{2.3}$$

The energy is

$$E_2[u] = \frac{1}{2}T[u] + \frac{1}{2}P[u] + \frac{1}{4}K[u], \tag{2.4}$$

where $K[u] = \kappa \int_X |u|^4$. Thus we have

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

The proof here shall be based on what is essentially a convexity result.

2.3 Example 3: Nonlocal Equations

The *Hartree equation* is a self-consistent way to describe charged particles in an atom: in contrast to the Schrödinger equation, the field describing the electrons interacts with itself via a potential obtained from a Laplace-type equation. The equation itself is

$$-\Delta u + Vu + \left(G * |u|^2\right) u = \omega u, \tag{2.5}$$

where G is the inverse of the Laplacian, which we recall is

$$G(x;y) = G(x-y) = \begin{cases} \frac{1}{(d-2)S_{d-1}} |x-y|^{2-d} & d \neq 2 \\ \frac{1}{2\pi} \log |x-y| & d = 2 \end{cases}; \tag{2.6}$$

this describes the effect that the field at a point feels from the field's own charge at other points of the space.

Hence we can also write down the energy,

$$E_3[u] = \frac{1}{2}T[u] + \frac{1}{2}P[u] + \frac{1}{4}Q[u], \tag{2.7}$$

where $Q[u]$ is a self-energy term, $Q[u] = \kappa \int_X \int_X G(x;y) |u(x)|^2 |u(y)|^2 \, dx \, dy$. Thus we have

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

3 How The Proof Works

Suppose we have a u that is not symmetric, but minimises E. If we can show that $M[u]$ is a possible solution, and

$$E[M[u]] < E[u], \tag{3.1}$$

then $M[u]$ witnesses that u is not the ground state.

Hence it suffices to show that *one* of the terms in E is *decreased* when replacing u by $M[u]$, and the rest stay the same or at least are not increased.

4 Some Proofs

Now that we know what sort of terms we need to understand, I will give some of the proofs. To summarise, we want inequalities for

$$T[u] = \int_X |\nabla u|^2 \tag{4.1}$$

$$P[u] = \int_X V\,|u|^2 \tag{4.2}$$

$$K[u] = \kappa \int_X |u|^4 \tag{4.3}$$

$$Q[u] = \int_X \int_X G(x;y)\,|u(x)|^2\,|u(y)|^2\;dx\,dy. \tag{4.4}$$

We also need to show that $N[M[u]] = N[u]$.

This last is straightforward, and it is here we reap the first benefit of averaging over a group. Subsequently, we write $x' = g.x$. Since dx is G-invariant by assumption, the measure transforms, or rather doesn't transform, as $dx = dx'$.

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

That's encouraging. By exactly the same idea, we also find

$$\begin{aligned} P[M[u]] &= \int_X V(x) \int_G |u(g.x)|^2\;dg\,dx \\ &= \int_G \int_X V(x)\,|u(g.x)|^2\;dx\,dg \\ &= \int_G \int_X V(g^{-1}.x')\,|u(x')|^2\;dx'\,dg \\ &= \int_G \int_X V(x')\,|u(x')|^2\;dx'\,dg = \int_G P[u]\,dg = P[u]. \end{aligned}$$

Now we turn to the inequalities.

4.1 Kinetic

This looks much more difficult. To cut a long story short, the simplest proof is probably that based on the following: let α and β be square-integrable. Then we have the following identity:

$$\begin{aligned} &\frac{1}{4} \iint \left(|\bar\alpha(y)\beta(z) - \bar\alpha(z)\beta(y)|^2 + \left|\bar\alpha(y)\beta(z) - \alpha(z)\bar\beta(y)\right|^2 \right) dy\,dz \\ &= \|\alpha\|_2^2\,\|\beta\|_2^2 - \iint \Re(\bar\alpha\beta)(y)\cdot\Re(\bar\alpha\beta)(z)\,dy\,dz \\ &= \|\alpha\|_2^2\,\|\beta\|_2^2 - \left|\int \Re(\bar\alpha\beta)(y)\,dy\right|^2. \end{aligned}$$

The left-hand side is clearly nonnegative, so

$$\|\alpha\|_2^2 \|\beta\|_2^2 \geqslant \left| \int \Re(\bar{\alpha}\beta)(y)\, dy \right|^2$$

Replacing α by $u(g.x)$ and β by $(\nabla u)(g.x)$, and the integrals by integrals over G, we find

$$\begin{aligned} M[u](x)^2 \int_G |\nabla u(g.x)|^2 \, dg &\geqslant \left| \int_G \Re(\bar{u}\nabla u)(g.x)\, dg \right|^2 \\ &= \left| \tfrac{1}{2} \int_G \nabla |u(g.x)|^2 \, dg \right|^2 \\ &= \left| \tfrac{1}{2} \nabla (M[u](x)^2) \right|^2 \\ &= M[u](x)^2 \left| \nabla M[u](x) \right|^2 . \end{aligned}$$

Cancelling $M[u](x)$ and integrating over X,[2] we find

$$T[u] \geqslant T[M[u]], \tag{4.5}$$

as required.

4.2 Nonlocal

Fundamentally here we require *positive-definiteness*: a symmetric integral kernel h is said to be positive-definite if

$$\int_X \int_X h(x;y) f(x) f(y)\, dx\, dy > 0 \tag{4.6}$$

for any $f \not\equiv 0$. (Note that in our case, G satisfies this since it is the inverse of the positive Laplacian—one may check this using the Fourier transform, provided with sufficiently rapid decay.)

We show that:

Lemma 1. *Let $H[\alpha, \beta] = \int_X \int_X \alpha(x) h(x;y) \beta(y)\, dx\, dy$ be positive-definite, and k be G-invariant in the sense that $h(gx;gy) = h(x;y)$. Then*

$$H[M[u]^2, M[u]^2] \leqslant H[u^2, u^2], \tag{4.7}$$

with equality if and only if $M[u] \equiv u$.

Proof. Writing $U = M[u]$, we have

$$H[u^2, u^2] = H[U^2, U^2] + 2H[U^2, u^2 - U^2] + H[u^2 - U^2, u^2 - U^2].$$

The last term is positive unless $M[u] \equiv u$. It remains to understand the second term. Firstly, writing $W(y) = \int_X U(x)^2 h(x;y)\, dx$, we have

$$\begin{aligned} W(g.y) &= \int_X U(x)^2 h(x - g.y)\, dx \\ &= \int_X U(g.x')^2 h(g.x' - g.y)\, dx' \\ &= \int_X U(x')^2 h(x' - y)\, dx' \\ &= W(y). \end{aligned}$$

[2]Note that ∇ is the weak derivative, and $\nabla |f| = 0$ at points where $f = 0$, so we may cancel without fear.

But then the middle term is

$$\begin{aligned}
\int_X W(y)(u(y)^2 - U(y)^2)\,dy &= \int_X \left(\int_G W(g^{-1}.y)\,dg \right) (u(y)^2 - U(y)^2)\,dy \\
&= \int_G \left(\int_X W(g^{-1}.y)(u(y)^2 - U(y)^2)\,dy \right) dg \\
&= \int_G \left(\int_X W(y')(u(g.y')^2 - U(g.y')^2)\,dy' \right) dg \\
&= \int_X W(y') \left(\int_G (u(g.y')^2 - U(g.y')^2)\,dg \right) dy' \\
&= \int_X W(y') \left(\int_G u(g.y')^2\,dg - U(y')^2 \right) dy' \\
&= 0
\end{aligned}$$

by the definition of U, and we obtain the result. □

This gives us the strict inequality we desire.

For the linear case, we can obtain the result using a more subtle version of the kinetic inequality (where else?), provided that G is a Lie Group acting freely on X, so that X splits into a foliation of G-orbits. One may then use coordinates on each, computing the integrals separately. In particular, this is the case for spherical symmetry in $\mathbb{R}^d$, since it splits into the product $\mathbb{R}^d = \mathbb{R}^+ \times S^{d-1}$, and $SO(d)$ acts only the second factor.

4.3 Nonlinear

For the nonlinear equation, we prove a more general result:

Lemma 2. *Let $F(x,u) = f(x,|u|^p)$ be convex in $|u|^p$ for almost all x, and $F(g.x,u) = F(x,u)$ for almost every g. Then*

$$\int_X F(x,u(x))\,dx \geqslant \int_X F\left(x, M[u](x)\right)\,dx. \tag{4.8}$$

Moreover, if f is strictly convex in its second argument, equality holds precisely when $|u| = M[u]$.

Proof. We have

$$\int_X F(x,u(x))\,dx = \int_X \int_G F(g.x,u(g.x))\,dg\,dx = \int_X \int_G F(x,u(g.x))\,dg\,dx,$$

by the same process as the previous proofs. We now apply Jensen's inequality, which in this case says

$$\begin{aligned}
\int_G F(x,u(g.x))\,dg &= \int_G f\left(x, |u(g.x)|^p\right)\,dg \\
&\geqslant f\left(x, \int_G |u(g.x)|^p\,dg\right) \\
&= F\left(x, M[u](x)\right)
\end{aligned}$$

for almost every x, and integrating both sides gives the result. The second part follows from the equality case in Jensen's inequality. □

5 Other Equations, Other Questions

So far I have talked exclusively about equations containing the Laplacian. What about other operators?

One example that is useful to know about is a relativistic version of the Laplacian, often written $\sqrt{(-\Delta) + m^2}$. This may be succinctly given by a Fourier transform formula,

$$\langle u, \sqrt{(-\Delta) + m^2 u}\rangle_x = \langle \tilde{u}, \sqrt{k^2 + m^2 \tilde{u}}\rangle_k = \int_{\mathbb{R}^n} \sqrt{k^2 + m^2}\, |u(k)|^2 \, dk. \tag{5.1}$$

One may undo the Fourier transform to obtain a normal-space convolution with a positive-definite kernel involving Bessel functions. Hence the results above apply and we have

$$\langle u, \sqrt{(-\Delta) + m^2 u}\rangle \geqslant \langle M[u], \sqrt{(-\Delta) + m^2 M[u]}\rangle. \tag{5.2}$$

Finally, I would like to mention a couple of examples that are not yet completely understood.

Suppose we look again at the Schrödinger equation, taking $X = \mathbb{R}$, and $G \cong Z_2$ acts by reflection in 0. This relates to

$$-u'' + Vu = \omega u, \tag{5.3}$$

where V is even. Are the ground states of this equation even? Could there be cases where V has a singularity that forces the ground state to be odd? Because this equation is linear, and the group is discrete, the method I have given provides no information on the parity, and indeed, a weak solution cannot tell the difference if the derivative is discontinuous at a single point.