A variational approach for energy minimization of Schrödinger operators

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July 8, 2024

Overview

Consider the eigenvalue problem:

$$H\psi = (-\Delta + V)\psi = E\psi$$

Let us define the total energy of a quantum system as

$$\mathcal{E}\psi = \langle \psi | H\psi \rangle = \int_{\mathbb{R}^N} |\nabla \psi|^2 \, d\mathbf{x} + \int_{\mathbb{R}^N} V|\psi|^2 \, d\mathbf{x}$$

This functional is well-defined for $\psi \in H^1$ and $V \in L^1_{loc}$.

Steps for the Solution of the Problem

The steps for the solution of this problem follows:

1. Proving that the ground state energy is finite, i.e.

$$E_0 = \inf \sigma(H) = \inf_{\psi \in \mathcal{D}(H), \|\psi\|=1} \langle \psi | H\psi \rangle > -\infty$$

2. Proving the existence of a minimizer ψ_0 for the **variational** problem, namely that E_0 is a **minimum** for $\mathcal{E}$.
3. Re-conducting to the **weak** formulation of the eigenvalue problem.

Remark 1

$$\mathcal{D}(H) \subset \mathcal{D}(\mathcal{E}) \implies e_0 := \inf_{\psi \in \mathcal{D}(\mathcal{E})} \mathcal{E}\psi \leq E_0$$

The ground state energy is finite

Theorem 1

Let $\psi \in H^1(\mathbb{R}^N)$ and let $V \in L^{N/2}(\mathbb{R}^N) + L^\infty(\mathbb{R}^N)$, $N \geq 3$. Then:

1. E_0 is finite.
2. There exist some constants C, $D < \infty$ such that

$$T_\psi \leq C\mathcal{E}(\psi) + D\|\psi\|_2^2$$

where T_ψ is the kinetic energy functional.

Consequence of theorem 1

Assuming $V = -V_-$, we get $|V_\psi| \leq \frac{1}{2} T_\psi + D\|\psi\|_2^2$. *KLMN* theorem assures that such a perturbed (free) Hamiltonian is also **self-adjoint**.

Some technical tools

Lemma 1 (Sobolev's inequality in dimension $N \geq 3$)

Let $\psi \in D^1(\mathbb{R}^N)$. Then $\psi \in L^q(\mathbb{R}^N)$ with $q = 2N/(N-2)$ and

$$\|\nabla\psi\|_2^2 \geq S_n \|\psi\|_q^2$$

where

$$S_n = \frac{N(N-2)}{4}|\mathbb{S}^N|^{2/N}$$

Proposition 1

For every $\phi \in L^{N/2}(\mathbb{R}^N)$, there exists a constant λ such that the function $h(x) := min(\phi(x) - \lambda, 0)$ satisfies

$$\|h\|_{N/2} \leq \frac{1}{2} S_n$$

Existence of a Minimizer for E_0

Theorem 2

Let V be as in Theorem 1 and assume it vanishes at infinity. Also assume that

$$E_0 = \inf\{\mathcal{E}\psi : \psi \in H^1(\mathbb{R}^N), \|\psi\|_2 = 1\} < 0.$$

Then, $\exists \psi_0 \in H^1(\mathbb{R}^N)$, $\|\psi_0\|_2 = 1$ such that

$$\mathcal{E}\psi_0 = \min_{\phi \in H^1 : \|\phi\|_2 = 1} \{\mathcal{E}\phi\}$$

Furthermore, it satisfies weakly

$$H\psi_0 = E_0\,\psi_0.$$

Existence of a Minimizer for E_0 - cont'd

Our strategy for proving this result involves two main steps:

1. Proving the *weak lower semi-continuity* of the total energy.
2. Applying Fermat's theorem to a suitable (differentiable) ratio of quadratic forms.
3. Variational formulation $\longrightarrow$ weak formulation.

Remark 2:

$\mathcal{E}$ is (in general) neither a functional on $(L^2)^*$ nor $(H^1)^*$. Hence, it is not trivial to prove that it has a minimum on $\mathcal{D}(\mathcal{E})$ even after we know that it is coercive and w.l.s.c.

Derivation of the Weak Form

Define the **variation** of ψ_0 as $\psi_\epsilon = \psi_0 + \epsilon\phi$, for $\epsilon \in \mathbb{R}$, $\phi \in C_0^\infty(\mathbb{R}^N)$.
We can test the Schrödinger equation with ψ_ϵ and see what happens.

Consequence of Theorem 2 - Euler-Lagrange equation

From the previous theorem, we get

$$\left.\frac{d\mathcal{E}(\psi_\epsilon)}{d\epsilon}\right|_{\epsilon=0} = E_0 \left.\frac{d\langle\psi_\epsilon|\psi_\epsilon\rangle}{d\epsilon}\right|_{\epsilon=0} \iff \langle\phi|H\psi_0\rangle = E_0\langle\phi|\psi_0\rangle$$

Addendum: connection to Euler-Lagrange equation

Let us define

$$\Phi(\epsilon) := \frac{\mathcal{E}\psi_\epsilon}{\langle\psi_\epsilon|\psi_\epsilon\rangle} = \mathcal{L}(\psi_0 + \epsilon\phi)$$

Indeed, defining $\mathcal{L}u := \int_\Omega \mathcal{F}(\mathbf{x}, u(\mathbf{x}), \nabla u(\mathbf{x}))\, d\mathbf{x}\,,$

$$\Phi'(0) = 0 \iff \int_\Omega \frac{d\mathcal{F}}{d\epsilon}\, d\mathbf{x} = 0 \iff \frac{\partial\mathcal{F}}{\partial\psi_0} - \nabla\cdot\left(\frac{\partial\mathcal{F}}{\partial(\nabla\psi_0)}\right) = 0 \qquad (\textbf{E-L})$$

Moreover,

$$\Phi'(0) = 0 \iff \left.\frac{d\mathcal{E}(\psi_\epsilon)}{d\epsilon}\right|_{\epsilon=0} - \left. E_0\,\frac{d\langle\psi_\epsilon|\psi_\epsilon\rangle}{d\epsilon})\right|_{\epsilon=0} = 0$$

Namely, $(-\Delta + V)\psi = e_0\,\psi$, is the **Euler-Lagrange** equation for the functional $\mathcal{E}$ constrained to the unit sphere $\|\psi\|_2 = 1$.

Addendum: Lagrange multipliers

Define

$$Ju := \int_\Omega \left(\frac{1}{2} |\nabla u|^2 + \frac{1}{2}\, V |u|^2 \right) d\mathbf{x}$$

$$Gu := \int_\Omega \frac{1}{2} |u|^2 \, d\mathbf{x}$$

$$\mathcal{L}[u, E] := Ju - E(Gu - 1/2)$$

Remark 5

We seek for stationary points of a Lagrangian subjected to the **constraint** $Gu = 1$. This is equivalent to setting

$$\frac{\partial \mathcal{L}}{\partial E} = 0 \qquad \Longleftrightarrow \qquad \|u\|_2 = 1$$

Addendum: Lagrange multipliers - cont'd

Let us also define

$$\mathcal{F}(u, \nabla u) := \frac{1}{2}\left(|\nabla u|^2 + V|u|^2 - E_0|u|^2\right)$$

Then,

$$\frac{\partial \mathcal{F}}{\partial u} = Vu - E_0 u \qquad \frac{\partial \mathcal{F}}{\partial(\nabla u)} = \nabla u \qquad \mathcal{L}u = \int_\Omega \mathcal{F}(u, \nabla u)\, d\mathbf{x}$$

Now, we plug the **Euler-Lagrange** equation $(u = \psi_\epsilon = \psi_0 + \epsilon f)$:

$$\left.\frac{d\mathcal{L}[\psi_0 + \epsilon f]}{d\epsilon}\right|_{\epsilon=0} = 0 \iff \frac{\partial \mathcal{F}}{\partial \psi_0} - \nabla \cdot \left(\frac{\partial \mathcal{F}}{\partial(\nabla \psi_0)}\right) = 0$$

$$\iff V\psi_0 - E\psi_0 - \Delta\psi_0 = 0 \iff (-\Delta + V)\psi_0 = E_0\psi_0$$

Addendum: FT of Calculus of Variations

Let $\epsilon \in \mathbb{R}$ and $f \in C_0^\infty(\mathbb{R}^N)$. Then,

$$\frac{d\mathcal{L}[\psi_0 + \epsilon f]}{d\epsilon}\bigg|_{\epsilon=0} = 0 \iff \int_\Omega \frac{d\mathcal{F}}{d\epsilon}\bigg|_{\epsilon=0} d\mathbf{x} = 0$$

$$\iff \int_\Omega \left(\frac{\partial \mathcal{F}}{\partial \psi_\epsilon} \frac{d\psi_\epsilon}{d\epsilon} + \frac{\partial \mathcal{F}}{\partial (\nabla \psi_\epsilon)} \frac{d\nabla \psi_\epsilon}{d\epsilon} \right)\bigg|_{\epsilon=0} d\mathbf{x} = 0$$

$$\overset{by\ parts}{\iff} \int_\Omega \frac{\partial \mathcal{F}}{\partial \psi_0} f \, d\mathbf{x} + \frac{\partial \mathcal{F}}{\partial (\nabla \psi_0)} f \,\bigg|_{\partial\Omega} - \int_\Omega \nabla \cdot \left(\frac{\partial \mathcal{F}}{\partial (\nabla \psi_0)} \right) f \, d\mathbf{x} = 0$$

$$\overset{FTCV}{\iff} \quad \frac{\partial \mathcal{F}}{\partial \psi_0} - \nabla \cdot \left(\frac{\partial \mathcal{F}}{\partial (\nabla \psi_0)} \right) = 0$$

References

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