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6. Pseudorelativistic matter

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6. Stability of pseudorelativistic matter

Relativistic energy-momentum relation

$$E^2 = c^2p^2 + (mc^2)^2$$

$\rightsquigarrow$ pseudorelativistic Hamiltonian

$$\hat{H} = \sqrt{c^2p^2 + (mc^2)^2} + V$$

or, better, relativistic kinetic energy in quantum case:

$$(\psi, c\sqrt{p^2 + m^2c^2}\,\psi) = \int_{\mathbb{R}^3} c\left((2\pi\hbar k)^2 + m^2c^2\right)^{1/2} |\hat{\psi}(k)|^2 dk$$

$\rightsquigarrow$ $H^{1/2}(\mathbb{R}^d)$ space

Recall that, Sobolev inequality

$$\|f\|_{L^{\frac{2d}{d-2s}}(\mathbb{R}^d)} \leq C_{d,s} \|(-\Delta)^{s/2} f\|_{L^2(\mathbb{R}^d)}$$

for $d > 2s$ and $f \in H^s(\mathbb{R}^d)$. The relativistic kinetic energy corresponds to the space $H^{1/2}(\mathbb{R}^d)$

$\rightsquigarrow$ $d > 1 \Rightarrow d = 2, 3, \ldots$

Since $(c = 1, m = 1)$

$$|p| \geq \sqrt{p^2 + m^2} - m \geq |p| - m$$

it is enough to consider the ultra-relativistic kinetic energy

$$T_\varphi = (\varphi, |p|, \varphi)$$

which by Sobolev satisfies:

$$T_\varphi \geq C \, \|\varphi\|^2_{2d/(d-1)} \qquad d \geq 2.$$

Exercise

Assuming $V \in L^d(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$, show stability of relativistic matter in $d \geq 2$.

Solution:

We follow the previous proofs. To this end we need to establish the Hölder inequality for the potential part:

$$\int_{\mathbb{R}^2} |V(x)| \, |\varphi(x)|^2 \, dx \leq \left(\int |V_-|^\alpha\right)^{\frac{1}{\alpha}} \left(\int |\varphi|^{2\beta}\right)^{\frac{1}{\beta}}$$

with $\frac{1}{\alpha} + \frac{1}{\beta} = 1$ and $2\beta = \frac{2d}{d-1}$

$$\Rightarrow \frac{1}{\beta} = \frac{d-1}{d} \Rightarrow \frac{1}{\alpha} = \frac{1}{d} \Rightarrow \alpha = d$$

$\square$.

In order to deal with $d = 1$ we need another Sobolev inequality for $H^{1/2}(\mathbb{R})$.

Exercise

Let $f \in H^{1/2}(\mathbb{R})$. Show that

$$(f, |p| f) + \|f\|_2^2 \geq S_{1,q} \|f\|_q^2 \quad \forall q \in [2, \infty)$$

Hint: follow the proof of $\mathbb{R}^2$ Sobolev inequality

Solution

We have
$$\|f\|_2^2 + (f, |p| f) = \int_{\mathbb{R}} (1 + 2\pi |k|) |\hat{f}(k)|^2 \, dk$$

The rest of the proof is the same.

Corollary

Consider the pseudo-relativistic matter in $d = 1$. Then $E_0 > -\infty$ if $V \in L^{1+\varepsilon}(\mathbb{R}) + L^\infty(\mathbb{R})$. $\blacksquare$

7. Eigenvalues of one-body Schrödinger Hamiltonians

Point spectrum of an operator T:
$$\sigma_p(T) := \{ z \in \sigma(T) : \ker(T - z) \neq \{0\} \}$$

A number $z \in \sigma_p(T)$ is called an eigenvalue and any $0 \neq u \in \ker(T - z)$ is called a (corresponding) eigenvector.

Eigenvalue equation in QM $\quad H\varphi = E\varphi$.

Note that

$$\mathcal{E}(\varphi) = \langle \varphi | H \varphi \rangle = T_\varphi + V_\varphi = E$$

if φ is an eigenvector corresponding to eigenvalue E. Recall we defined $E_0 = \inf_{\|\varphi\|=1} \mathcal{E}(\varphi)$. One can ask whether this ground state energy is attained.

Thm Let $d=3$. Assume $V \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ and V vanishes at infinity, i.e. for all $a>0$

$$\left| \{ x \in \mathbb{R}^3 : |V(x)| > a \} \right| < \infty .$$

Then, if $E_0 < 0$, there is a unique function $\varphi_0 \in H^1(\mathbb{R}^3)$ with $\|\varphi_0\| = 1$ such that

$$\mathcal{E}(\varphi_0) = E_0 .$$

This φ_0 satisfies the equation

$H\varphi_0 = E_0 \varphi_0$ in the sense of distributions.

$\blacksquare$

We skip the proof as it is an exercise in calculus of variations which is beyond the scope of this course.

A similar statement allows to analyze excited states.

Define (under the assumption that $\varphi_0, \dots, \varphi_{k-1}$ exist)

$$E_k := \inf \{ \mathcal{E}(\varphi) : \varphi \in H^1(\mathbb{R}^n),\ \|\varphi\|_2 = 1 \text{ and } (\varphi, \varphi_i) = 0,\ i = 0, \dots, k-1 \}$$

We have an analogous statement

Thm Let $V \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ and V vanishes at ∞. If $E_k < 0$ then $\varphi_k \in H^1(\mathbb{R}^3)$ with $\|\varphi_k\| = 1$ exists and satisfies

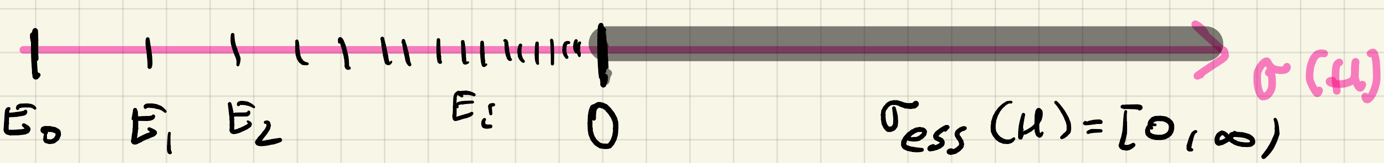
$$H \varphi_k = E_k \varphi_k .$$

Furthermore, each number $E_k < 0$ can only occur finitely many times in the list of eigenvalues. Conversely, any $\psi \in H^1(\mathbb{R}^3)$ that satisfies $H\psi = E\psi$ for some $E < 0$ is a linear combination of eigenfunctions to the eigenvalue E.

■

It turns out, that the eigenvalues E_k cannot accumulate at any point that is strictly smaller than zero.

Typical spectrum of a Schrödinger operator



Finding eigenvalues as described in the previous thm requires finding eigenfunctions. Might be difficult!

Below we present a way to compute the eigenvalues without the knowledge of eigenfunctions.

Theorem (Min-max principle)

Let $V \in L^{d/2}(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ and assume it vanishes at infinity as in the previous statements.

Then the eigenvalues are also given by

$$\boxed{E_k = \max_{\phi_0, \ldots, \phi_{k-1}} \min \{ \mathcal{E}(\phi_k) : \phi_k \perp \phi_0, \ldots, \phi_{k-1} \}}$$

and

$$\boxed{E_k = \min_{\phi_0, \ldots, \phi_k} \max \{ \mathcal{E}(\phi) : \phi_0 \in \operatorname{span}(\phi_0, \ldots, \phi_k) \}}$$

where the maximum (resp. minimum) extends over all collections of k (resp. $k+1$) orthonormal functions $\phi_j \in H^1(\mathbb{R}^d)$.

Remark: the assumptions on V guarantee that the eigenvalues exist, see previous statements.

Proof

•) Let $\gamma_k = \max_{\phi_0, \ldots, \phi_{k-1}} \min \{ \mathcal{E}(\phi_k) : \phi_k \perp \phi_0, \ldots, \phi_{k-1} \}$.

choosing $\phi_0, \dots, \phi_{k-1}$ to be the eigenfunctions $\varphi_0, \dots, \varphi_{k-1}$ we immediately see that $\gamma_k \geq E_k$.
Conversely, for any choice $\phi_0, \dots, \phi_{k-1}$ there is (as the sum below extends over $k+1$ linearly independent functions) always a linear combination

$$f = \sum_{j=0}^{k} c_j \varphi_j \qquad (\varphi_i \text{ - eigenfct.})$$

such that f is normalized and $\perp$ $\phi_0, \dots, \phi_{k-1}$.
then

$$\mathcal{E}(f) = \sum_{j=0}^{k} |c_j|^2 E_j \leq E_k \sum_{j=0}^{k} |c_j|^2 = E_k$$

and consequently $\min \{ \mathcal{E}(\phi_k) : \phi_k \perp \phi_0, \dots, \phi_{k-1} \} \leq E_k$
which implies $\gamma_k \leq E_k$.

•) To prove the second identity, let

$$\gamma_k := \min_{\phi_0, \dots, \phi_k} \max \{ \mathcal{E}(\phi) : \phi \in \operatorname{span} \{ \phi_0, \dots, \phi_k \} \}$$

choosing $\phi_0, \dots, \phi_k$ to be the eigenfctns $\varphi_0, \dots, \varphi_k$ we get that $\gamma_k \leq E_k$.
Conversely, for any orthogonal $\phi_0, \dots, \phi_k$ there is (as before) a linear combination $f = \sum_{j=0}^{k} c_j \phi_j$ such that f normalized and $\perp$ $\varphi_0, \dots, \varphi_{k-1}$.
Then by definition of eigenvalues $\mathcal{E}(f) \geq E_k$ and hence $\gamma_k \geq E_k$. $\blacksquare$

Corollary (monotonicity of eigenvalues)

Let V^A, V^B be two potentials satisfying the assumptions, $\mathcal{E}^A, \mathcal{E}^B$ the corresponding energy functionals and $E_0^A, E_1^A, \dots, E_0^B, \dots$ the eigenvalues. Then if

$V^A(x) \leq V^B(x)$ then $\mathcal{E}^A(\psi) \leq \mathcal{E}^B(\psi)$

and thus $E_k^A \leq E_k^B$ $\forall$ $k \geq 0$.

Riesz means

Let A be a self-adjoint operator. We define A_- by the functional calculus as $\varphi(A)$ where $\varphi(\lambda) = \max\{-\lambda, 0\} = \lambda_-$.

Clearly $A_- \geq 0$.

In our application to Schrödinger operators we know that $[-\Delta + V]_-$ will correspond to minus the projection onto the (negative) eigenvalues.

In that case we define the Riesz means

$$\operatorname{Tr} A_-^\gamma = \sum_j (\lambda_j(A))_-^\gamma$$

where $\lambda_1(A) \leq \lambda_2(A) \leq \dots$ is the enumeration of those negative eigenvalues.