Homework 3, Mathematics of Quantum Mechanics

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1 Perturbed Magnetic Laplcian

1.1 Preliminaries

Before starting, we recall that $C_0^\infty(\mathbb{R}^3)$ is dense in $H^2(\mathbb{R}^3)$. Hence, $-\Delta$ (Kinetic energy) is essentially self-adjoint on the set of smooth functions with compact support. Recall also that for any vector field A, the following identity holds:

$$\nabla \cdot (\psi A) = \psi \nabla \cdot A + A \cdot \nabla \psi$$

Moreover, the expanded (perturbed) Hamiltonian reads

$$H_A = \frac{\hbar}{2m}(-i\nabla + \gamma A)^2 - \frac{e^2}{r} = \frac{\hbar}{2m}(-\Delta + \gamma^2 A^2 + 2\gamma A \cdot (-i\nabla)) - \frac{e^2}{r}$$

We recall also that Kato-Rellich theorem on small perturbations let us find (essentially) self-adjoint operators which derive from a sum of a starting self-adjoint operator and one or more of its small perturbations. Note also that self-adjointness of those perturbations must not be checked in general: it is enough to check for symmetry on the domain of (essentially) self-adjointness of the first operator.

1.2 Self-adjointness

Let us consider the following decomposition:

$$H_A = -\frac{\hbar}{2m}\Delta + V_A$$

where

$$V_A = \frac{\hbar}{2m}(\gamma^2 A^2 + 2\gamma A \cdot (-i\nabla)) - \frac{e^2}{r}$$

and $A \in C_0^\infty(\mathbb{R}^3)$ a Coulomb-Gauge vector potential. Indeed, V_A can be further decomposed into three sub-components. The third one (e^2/r) is familiar: it is a well-known small perturbation of the kinetic energy. For the first two, we need a little more effort.

We have that for any $\psi \in H^2(\mathbb{R}^3)$, $a > 0$ arbitrary small and $b < \infty$ it holds that

$$\|\gamma^2 A^2 \psi\|_\infty \leq \gamma^2 \|A\|_\infty \|A\|_\infty \|\psi\|_\infty \leq a\| - \Delta\psi\|_2 + b\|\psi\|_2$$

where the last inequality is a Sobolev inequality characterizing vectors of $H^2(\mathbb{R}^3)$. This is enough to say that this potential is a small perturbation of the kinetic energy on $C_0^\infty(\mathbb{R}^3)$: symmetry is granted by the fact that this potential is real.

Take now ϕ and ψ in $C_0^\infty(\mathbb{R}^3)$. Then,

$$\langle \phi \mid 2\gamma A(-i\nabla)\psi\rangle = \int_{\mathbb{R}^3} \phi^* 2\gamma A \cdot (-i\nabla)\psi \, d\mu = -2\gamma i \int_{\mathbb{R}^3} \phi^* A \cdot \nabla\psi \, d\mu$$

$$= -2\gamma i \left(\int_{\mathbb{R}^3} \phi^* \nabla \cdot (\psi A) \, d\mu - \int_{\mathbb{R}^3} \phi^* \psi \nabla \cdot A \, d\mu \right)$$

$$= -2\gamma i \left(\int_{\partial K} \phi^* \psi A \, ds - \int_{\mathbb{R}^3} \psi A \cdot \nabla \phi^* \, d\mu \right) = (*)$$

for some compact subset $K \subset \mathbb{R}^3$. The first integral vanishes and

$$(*) = \int_{\mathbb{R}^3} \psi 2\gamma A \cdot (i\nabla)\phi^* \, d\mu = \int_{\mathbb{R}^3} 2\gamma A \cdot (-i\nabla\phi)^* \psi \, d\mu$$

$$= \langle 2\gamma A \cdot (-i\nabla)\phi \mid \psi\rangle$$

Hence, the operator proves symmetric on this domain.

Let's now prove that this operator can indeed be considered a small perturbation of the free kinetic energy. For any two positive integers a and b, we have:

$$0 \leq (a-b)^2 = a^2 - 2ab + b^2$$

This implies:

$$ab \leq \frac{a^2}{2} + \frac{b^2}{2}$$

Next, by substituting $b' = b/\sqrt{\epsilon}$ and $a' = a\sqrt{\epsilon}$, we get, for all positive ϵ,

$$ab \leq \frac{a^2}{2\epsilon} + \frac{\epsilon b^2}{2}$$

Therefore,

$$\|A \cdot \nabla\psi\|_2 \leq \|A\|_\infty \|\nabla\psi\|_2$$

Using the inner product notation, we get:

$$\|A \cdot \nabla\psi\|_2 \leq \|A\|_\infty \langle -\Delta\psi, \psi\rangle^{1/2}$$

By applying the Cauchy-Schwarz inequality, we obtain:

$$\|A \cdot \nabla\psi\|_2 \leq \|A\|_\infty \| - \Delta\psi\|_2^{1/2} \|\psi\|_2^{1/2}$$

Using the previous bound, we find:

$$\|A \cdot \nabla\psi\|_2 \leq \|A\|_\infty \frac{\epsilon}{2} \| - \Delta\psi\|_2 + \|A\|_\infty \frac{1}{2\epsilon} \|\psi\|_2$$

where $\epsilon > 0$. Thus, also $2\gamma A(-i\nabla)$ is Kato small w.r.t. the kinetic energy on $C_0^\infty(\mathbb{R}^3)$.

We conclude that V_A is a small perturbation of $-\Delta$. Self-adjointness and boundedness from below of H_A follows by Kato-Rellich theorem.

1.3 Spectral Analysis of H_A

1.3.1 Essential spectrum

For the sake of clarity, we propose a decomposition of H_A where differential operators are separated from the multiplication operators (i.e., the potential). Omitting constants for clarity, as they do not affect the thesis of the following arguments, consider:

$$H_A = \widetilde{H} + \widetilde{V}$$

where $\widetilde{H} = -\Delta + A \cdot P$, with P being the momentum operator, and $\widetilde{V} = A^2 + V_e$, incorporating the Coulomb potential V_e.

As discussed earlier, $\widetilde{H}$ represents a small perturbation of $-\Delta$ and is bounded from below. Meanwhile, $\widetilde{V}$ behaves similarly to V_e because A is smooth with compact support (thus belonging to $L^2(\mathbb{R}^3)$). Consequently, we can apply Weyl's lemma on compact differences to $\widetilde{H}$ and $-\Delta$, as in the Hamiltonian of the Hydrogen atom with only Coulomb potential. Specifically,

$$\sigma_{ess}(H_A) = \sigma_{ess}(-\Delta) = \mathbb{R}_+$$

1.3.2 Discrete spectrum

Unfortunately, H_A cannot be decomposed as a sum of free kinetic energy and a multiplication potential due to the presence of the term $A \cdot P$ in the expansion of the square of the magnetic Laplacian. Therefore, results concerning the existence of a ground state for Schrödinger-like operators in the context of eigenvalued PDEs cannot be applied. A simpler approach involves inspection, specifically by considering a suitable candidate eigenstate such as

$$\psi_\lambda(\mathbf{x}) = c_\lambda e^{-\frac{1}{2}\lambda|\mathbf{x}|}$$

and then directly computing

$$\langle\psi_\lambda|H_A|\psi_\lambda\rangle.$$

Another (far less precise, but at least theoretically grounded) way to show non-emptiness of $\sigma_{disc}(H_A)$ and further to get some estimates on the position of the candidate ground state is to use some useful results from [1]. In particular, we state the following:

Theorem 1 *Let A be a self adjoint operator and B a small perturbation of A in the sense of Kato, i.e.,*

$$\|B\psi\| \leq a\|A\psi\| + b\|\psi\|$$

for some $a < 1$ and $b < \infty$. Let also E_0 be an isolated non degenerate eigenvalue of A, namely

$$dist(E_0, \sigma(A) \setminus \{E_0\}) = 2\epsilon > 0$$

Then, for all

$$\beta \in B_0 = (0, (a + (a(|E_0| + \epsilon) + b)\epsilon^{-1})^{-1})$$

there is exactly one spectral point $E(\beta)$ of $A + \beta B$ in the interval (E_0, ϵ), where $E(\beta)$ is a non degenerate eigenvalue.

Remark: Indeed, being ϵ arbitrary small and $a < 1$, we can choose $\beta = 1$. Furthermore, we are implicitly considering a one parameter family B_γ of small perturbation of A given by the postive coupling constant.

A direct consequence of this theorem is that H_A has a non empty discrete spectrum. In fact,

$$H_A = H_e + 2\gamma A \cdot (-i\nabla) + \gamma^2 A^2$$

and we have already shown that it is a small perturbation of H_e in Kato's sense. Since H_e admits a ground state energy E_0 which is non degenerate and isoleted, we can find another eigenvalue of H_A with non degeneracy in the negative interval $(E_0, 0) \subset (E_0, \epsilon)$.

1.3.3 Upper and Lower Bounds for the Total Energy

We define the total energy functional as

$$\mathcal{E}_A\psi = \langle\psi|H_A|\psi\rangle$$

If $\lambda \in \mathbb{R}$ is an eigenvalue of H_A, then $\exists\psi_\lambda$ such that $H_A\psi_\lambda = \lambda\psi_\lambda$. This implies that

$$\langle\psi_\lambda|H_A|\psi_\lambda\rangle = \lambda\|\psi_\lambda\|^2$$

In particular,

$$\inf_{\|\psi\|=1} \sigma(H_A) = \inf_{\|\psi\|=1} \mathcal{E}_A\psi$$

Now,

$$\inf_{\|\psi\|=1} \mathcal{E}_A\psi = \inf_{\|\psi\|=1} \langle\psi|H_A|\psi\rangle$$

$$\geq \inf_{\|\psi\|=1} \langle\psi|H_e|\psi\rangle + \inf_{\|\psi\|=1} \{\gamma^2\langle\psi|A^2\psi\rangle + 2\gamma\langle\psi|A \cdot (-i\nabla)\psi\rangle\} = (*)$$

Letting E_0 be the ground state energy for the Hydrogen atom,

$$(*) \geq E_0 + \inf_{\|\psi\|=1} \{\gamma^2 \int_{\mathbb{R}^3} A^2 |\psi|^2 \, dx + 2\gamma \langle \psi | A \cdot (-i\nabla)\psi \rangle \}$$

$$\geq E_0 + \inf_{\|\psi\|=1} \{\gamma^2 \min_{supp(A)} \{A^2\} \|\psi\|_2^2 + 2\gamma \min_{supp(A)} \{A\} \int_{\mathbb{R}^3} |\psi^* \, (-i\nabla)\psi| \, dx \}$$

$$\geq E_0 + \inf_{\|\psi\|=1} \{2\gamma \min_{supp(A)} \{A\} \|\psi\|_2 \|\nabla\psi\|_2 \} \geq E_0$$

Remark: $\min_{supp(A)}\{A\} \leq 0$ since $A \in C_0^\infty(\mathbb{R}^3)$.

This is coherent to what we already know from Theorem 1, namely that $E(\beta)$ belongs to $(E_0, 0)$. It remains to find an upper bound. We proceed as follows:

$$\inf_{\|\psi\|=1} \mathcal{E}_A \psi \leq E_0 + \inf_{\|\psi\|=1} \{\gamma^2 \|A^2\|_\infty \|\psi\|_2^2 + \gamma \langle \psi | (-i\nabla)\psi \rangle \}$$

$$\leq E_0 + \gamma^2 \|A^2\|_\infty + \gamma \inf_{\|\psi\|=1} \{ \|A\|_\infty \|\psi\|_2 \|\nabla\psi\|_2 \} \leq E_0 + \gamma^2 \|A^2\|_\infty$$

Remark: We implicitly set the Plank constant and the mass to 1 and 1/2 respectively.

References

[1] Tosio Kato. *Perturbation theory for linear operators; 2nd ed.* Grundlehren der mathematischen Wissenschaften : a series of comprehensive studies in mathematics. Berlin: Springer, 1976. URL: `https://cds.cern.ch/record/101545`.