PDE

Of course we have been doing PDE all along, since the Schrödinger equation is a PDE. But in the last part of the course the PDE analysis gets much more substantial. The main points are density functional theory, the Thomas–Fermi approximation for it, which we analyze using a semiclassical trace formula, and obtain as a byproduct some general Weyl asymptotics.

1. **Density functional theory and the Hohenberg–Kohn Theorem.** Density functional theory solves N-particle problems, i.e. problems over a subspace of

$$L^2(\mathbb{R}^d;\mathbb{C}^{2s+1}) \otimes \cdots \otimes L^2(\mathbb{R}^d;\mathbb{C}^{2s+1}),$$

where the tensor product has N factors, by reformulating them in terms of the density of particles, which is a function in $L^1(\mathbb{R}^d)$. The foundational theorem, the Hohenberg–Kohn theorem, gives general conditions under which no information is lost by this reformulation.

We present the theorem in the following setting.[1] Let

$$H = T + V_{ee} + V_{ext},$$

where

$$T = -\frac{1}{2}\sum_{j=1}^{N} \Delta_j, \qquad V_{ee} = \sum_{1\le i<j\le N} \frac{1}{|\vec{r}_i - \vec{r}_j|}, \qquad V_{ext} = \sum_{i=1}^{N} V(\vec{r}_i),$$

with $d = 3$ and $s = 1/2$, where V is an external potential. Typically,

$$V(\vec{r}) = \sum_{k=1}^{M} \frac{-Z_k}{|\vec{r} - \vec{R}_k|}, \tag{1.1}$$

where $\vec{R}_k$ is the position of the kth nucleus and Z_k is the number of protons it has, but V can also be more general. We will suppose that V is smooth and bounded except for a finite number of such Coulombic singularities.

A *ground state* of H is a minimizer of $\langle u, Hu\rangle$ over u in the domain[2] of H with $\|u\| = 1$. Because $|u(\vec{r}_1,\dots,\vec{r}_N)|$ is symmetric under any swap of $\vec{r}_j$ and $\vec{r}_k$, we have

$$\langle u, Hu\rangle = \langle u, Tu\rangle + \langle u, V_{ee}u\rangle + \int_{\mathbb{R}^3} Vn,$$

where

$$n(\vec{r}) = N\int_{\mathbb{R}^{N-1}} |u(\vec{r},\vec{r}_2,\dots\vec{r}_N)|^2\, dr_2\cdots dr_N.$$

This n is the *density* corresponding to u, because $\int_U n$ computes the expected number of electrons to be found in U.

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[1] This material comes from Appendix B of Tao and Zworski's `PDE Methods in Condensed Matter Physics`, which has more information, background, and references.

[2] The domain is vectors in $H^2(\mathbb{R}^3;\mathbb{C}^2) \otimes \cdots \otimes H^2(\mathbb{R}^3;\mathbb{C}^2)$ which are antisymmetric under any swap of factors in the tensor product. Recall $u \in H^2(\mathbb{R}^d)$ means the Fourier transform $\hat{u}$ obeys $(1+|\xi|^2)\hat{u}(\xi) \in L^2(\mathbb{R}^d)$, so u and its partial derivatives up to second order are in L^2. See Theorem 7.8 of Borthwick's *Spectral Theory* for more.

The Hohenberg–Kohn theorem states that the ground state density and energy determine V_{ext}, and hence determine everything about the system. The main result is the following:

THEOREM 1.2. *Suppose two external potentials V_A and V_B have Hamiltonians H_A and H_B with ground states u_A and u_B with the same density*

$$n(\vec{r}) = N \int_{\mathbb{R}^{N-1}} |u_A(\vec{r}, \vec{r}_2, \dots \vec{r}_N)|^2 \, dr_2 \cdots dr_N = N \int_{\mathbb{R}^{N-1}} |u_B(\vec{r}, \vec{r}_2, \dots \vec{r}_N)|^2 \, dr_2 \cdots dr_N.$$

Then $V_A - V_B$ is a constant.

The beautiful original proof of Hohenberg and Kohn makes the result almost obvious, up to some technical issues we discuss at the end.

Proof. Because each ground state is a minimizer of its corresponding Hamiltonian, we have

$$\langle u_A, H_A u_A \rangle \leq \langle u_B, H_A u_B \rangle,$$

and, canceling the V_A terms,

$$\langle u_A, (T + V_{ee}) u_A \rangle \leq \langle u_B, (T + V_{ee}) u_B \rangle.$$

Switching the role of A and B leads to

$$\langle u_B, (T + V_{ee}) u_B \rangle \leq \langle u_A, (T + V_{ee}) u_A \rangle,$$

and hence

$$\langle u_B, (T + V_{ee}) u_B \rangle = \langle u_A, (T + V_{ee}), u_A \rangle,$$

and hence u_A and u_B are both ground states of both Hamiltonians H_A and H_B. The result then follows from the Lemma below. □

LEMMA 1.3. *If there exists a state u which is an eigenstate of both Hamiltonians H_A and H_B, then $V_A - V_B$ is a constant.*

Proof. Subtracting $H_A u = E_A u$ from $H_B u = E_B u$ yields

$$Wu = 0, \qquad W(\vec{r}_1, \dots \vec{r}_N) = E_B - E_A + \sum_{j=1}^{N} (V_A - V_B)(\vec{r}_j).$$

We will prove that

$$W(\vec{r}_1, \dots \vec{r}_N) = 0, \qquad \text{for all } (\vec{r}_1, \dots \vec{r}_N) \in \mathbb{R}^{3N}. \tag{1.4}$$

This completes the proof because then

$$V_A(\vec{r}_1) - V_B(\vec{r}_1) = E_B - E_A + \sum_{j=2}^{N} (V_A - V_B)(\vec{r}_j),$$

and hence both sides are constant.

The technical step in deducing (1.4) from $Wu = 0$ is proving that the zero set of u must be small. We use the fact, from quantum tunneling / unique continuation, that

$$\int_{\Omega} |u|^2 > 0 \tag{1.5}$$

for any nonempty open $\Omega \subset \mathbb{R}^{3N}$ on which W is continuous. To use (1.5), multiply Wu by $\bar{u}$ and integrate over such an Ω to obtain

$$0 = \int_\Omega W|u|^2.$$

If r^* is a point of continuity of W, then for any $\varepsilon > 0$ there is Ω containing r^* such that $|W(r^*) - W| < \varepsilon$ on Ω, and hence

$$0 < (W(r^*) + \varepsilon) \int_\Omega |u|^2,$$

and similarly

$$(W(r^*) - \varepsilon) \int_\Omega |u|^2 < 0.$$

Chaining the inequalities, canceling $\int_\Omega |u|^2$, and rearranging, gives

$$-\varepsilon < W(r^*) < \varepsilon.$$

Since ε is arbitrary, $W(r^*) = 0$, and since r^* is an arbitrary point of continuity, we obtain (1.4). □

Exercise 1.6. Use a limiting argument to explain in more detail how to go from proving (1.4) for an arbitrary point of continuity, to proving it for all points. Do this either in the case where V_A and V_B have the nuclear form (1.1), or in the more general setting introduced in the following sentence.

This reduces the proof of Hohenberg–Kohn to the quantum tunneling / unique continuation property (1.5). The same property can also be used to prove uniqueness and nondegeneracy of ground states, as was done in the introduction in one dimension. The next exercise gives an example of this, and the corresponding result for particles in a box is Theorem 6.34 of Borthwick's *Spectral Theory*.

Exercise 1.7. Let $H = -\Delta + V$ have domain $H^2(\mathbb{R}^3)$ and form domain $H^1(\mathbb{R}^3)$. Prove that, if $\int_\Omega |u|^2 > 0$ whenever u is a ground state and $\Omega \subset \mathbb{R}^3$ is a nonempty open set, then the space of ground states is one-dimensional and no ground state ever changes sign. You may use without proof the fact that functions in $H^2(\mathbb{R}^3)$ are continuous, and also state and use without proof an appropriate fact about $\max(u, 0)$ when $u \in H^1(\mathbb{R}^3)$. [3]

[3] The first fact can be proved using Fourier transformation: see Theorem 4 `here`. The second uses mollification and the chain rule: see Section 4.2.2 of Evans and Gariepy's *Measure theory and fine properties of functions*.